125th Anniversary
NYACS
NEW YORK SECTION of the
AMERICAN CHEMICAL SOCIETY

COLLEGE OF
MOUNT SAINT VINCENT

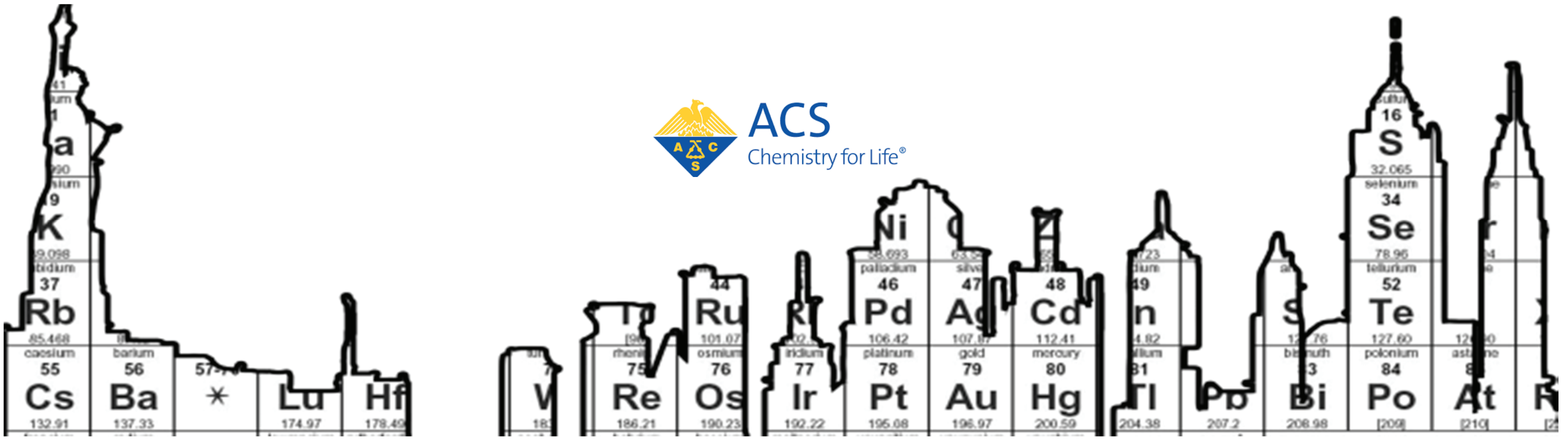
44th Middle Atlantic Regional Meeting

June 9 – June 12, 2016

Chemistry: Past, Present, and Future

New York – A Chemistry State of Mind

College of Mount Saint Vincent
Riverdale, New York



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COLLEGE OF MOUNT SAINT VINCENT

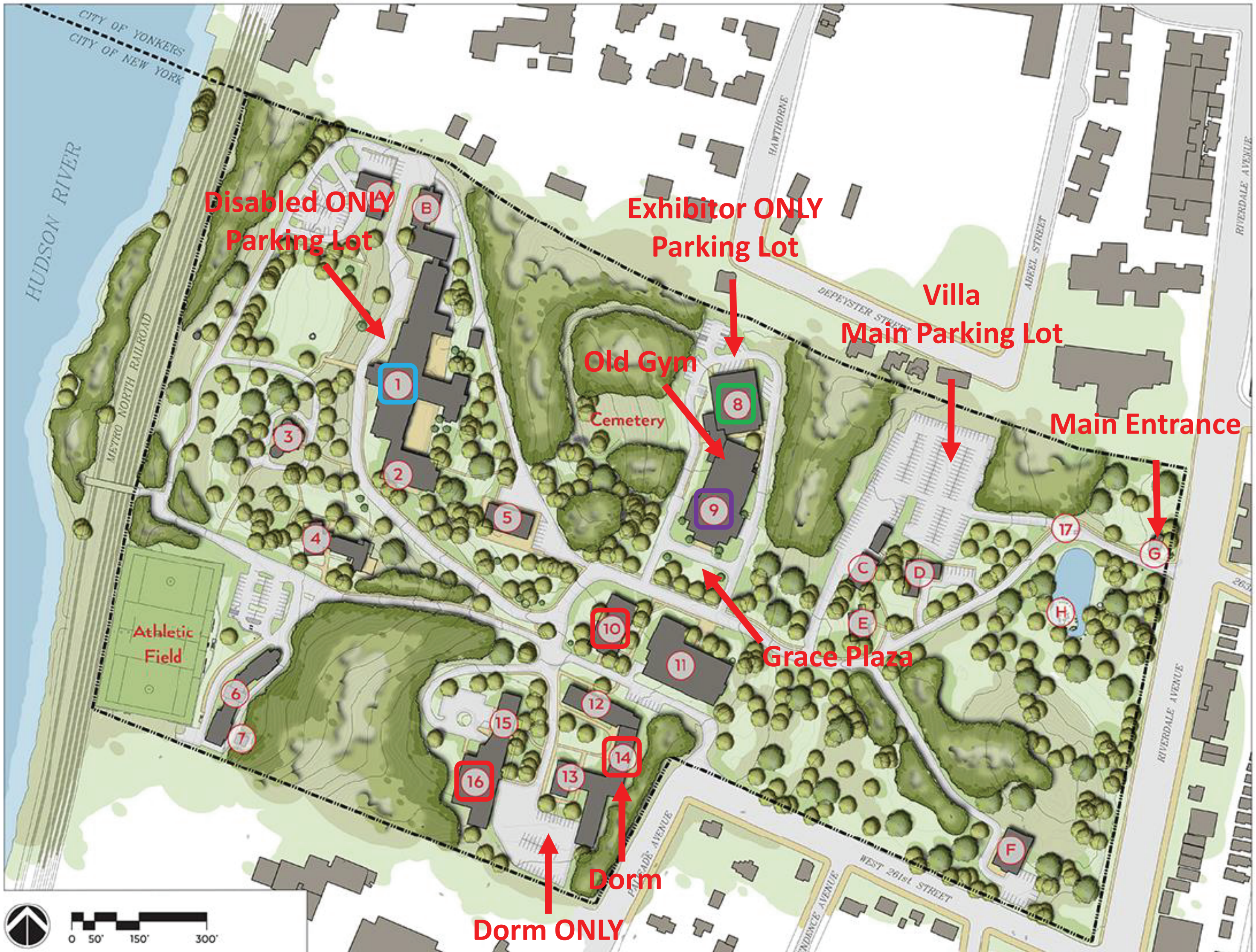
#	Building Name	Events
1	Founders Hall	All Technical Sessions and Workshops (3rd and 4th Floor), Awards Dinner & 125th Anniversary Dinners (2nd Floor)
8	Peter Jay Sharp Athletic and Recreation Center (Gym)	On-site Registration, Posters & Exhibitions
9	Grace Center (Hayes Auditorium)	Keynote Address, Chemagination

CMSV Buildings

1. Founders Hall
2. The Academy
3. Fonthill Castle
4. Maryvale Hall
5. Seton Hall
6. Marillac
7. The Lodge
8. Peter Jay Sharp Athletic and Recreation Center
9. Grace Center (Hayes Auditorium)
10. Science Hall
11. Seton Library
12. Mastronardi Hall
13. Alumnae Pavilion
14. Alumnae Hall
15. Spellman Hall
16. Hudson Heights (Dining Hall)
17. Guard Booth

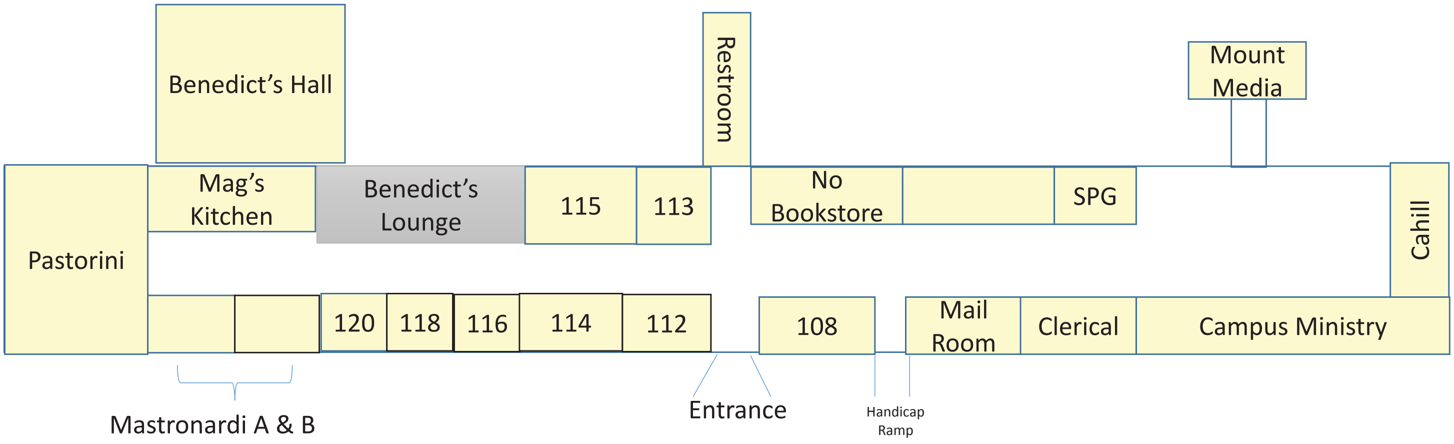
Sisters of Charity Buildings

A. Rosary Hall
B. The Convent
C. Boyle Hall
D. Ely Hall
E. The Villa
F. LeGras Hall
G. The Gate House
H. The Grotto

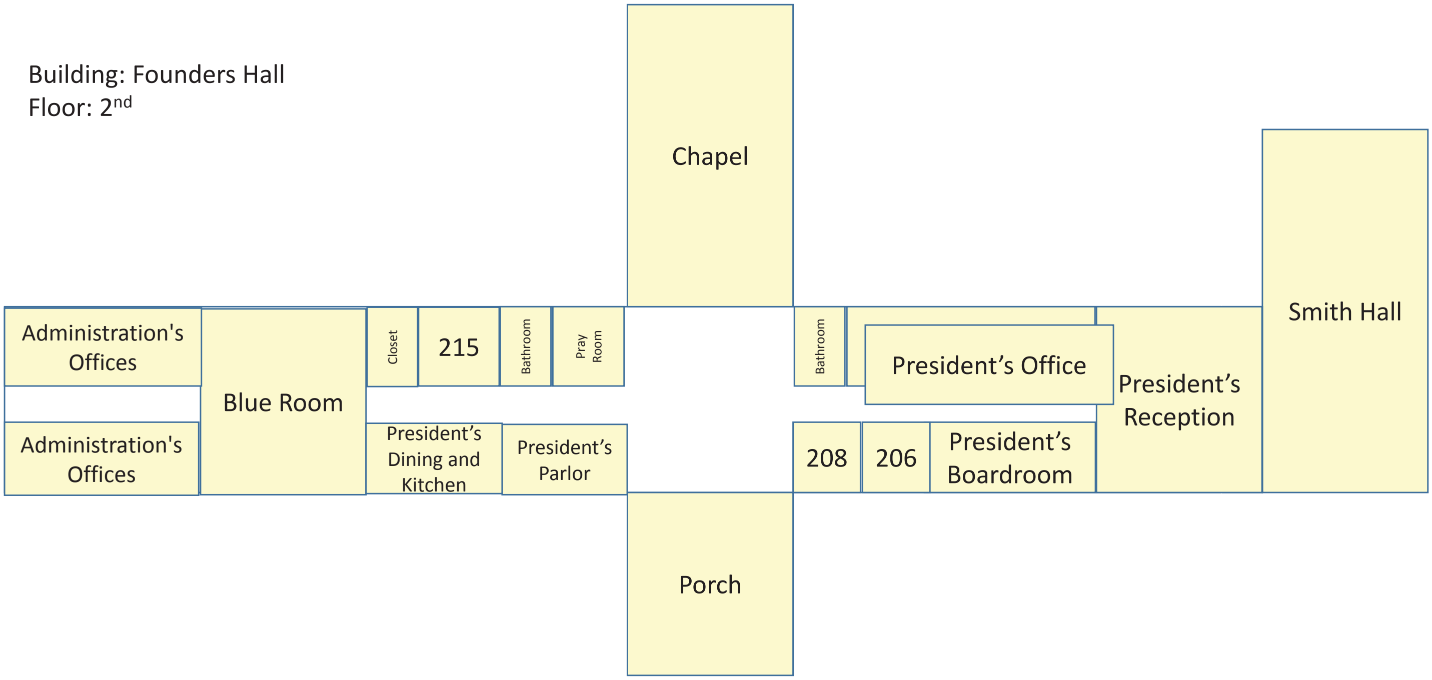


CAMPUS MAP

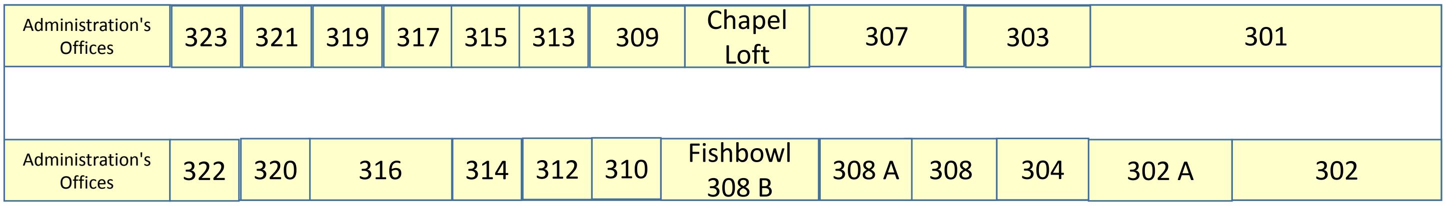
Building: Founders Hall
Floor: 1st



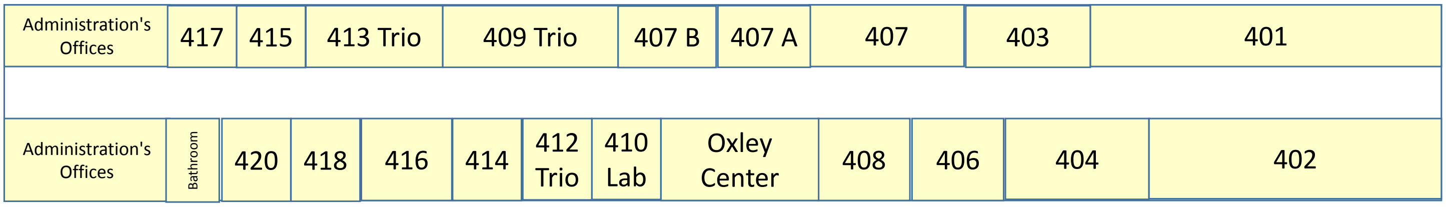
Building: Founders Hall
Floor: 2nd



Building: Founders Hall
Floor: 3rd



Building: Founders Hall
Floor: 4th



MEETING SCHEDULE AT A GLANCE

EVENT	THURS. PM June 9	FRI. AM June 10	FRI. PM June 10	SAT. AM June 11	SAT. PM June 11	LOCATION
TECHNICAL SESSIONS						
Clinical Diagnostics	1:00 – 4:45					Founder’s Hall/306
Crystal Engineering & Mechanisms of Crystallization	1:00 – 3:50					Founder’s Hall/304
Lithium Ion Batteries	1:00 – 3:55					Founder’s Hall/303
Analytical Chemistry & Toxicology		9:00 – 12:55	2:30 – 3:50			Founder’s Hall/309
Chemical Education Traditional & Online		9:00 – 11:15	1:00 – 3:35			Founder’s Hall/304
Computational/Physical Chemistry Excited-State Materials: Perspectives from Theory & Experiment		9:00 – 11:50				Founder’s Hall/409
Drug Analysis		9:00 – 12:38				Founder’s Hall/404
Energy for a Sustainable Future		9:00 – 12:45				Founder’s Hall/302
Entrepreneur’s Toolkit: Resources & True Stories		9:00 – 12:00				Founder’s Hall/310
Functional Supramolecular Architectures		9:00 – 11:20	1:00 – 3:55			Founder’s Hall/312
History of Chemistry in the New York Local Section		9:00 – 12:15				Founder’s Hall/303
Microwave Chemistry: Bridging Synthetic Research & Instructional Innovation		9:00 – 12:15				Founder’s Hall/307
NSF Chemistry: Funding Opportunities Symposium		9:15 – 11:30				Founder’s Hall/308
Association for Women in Science (AWIS)		9:30 – 11:50				Founder’s Hall/306
Molecular Electronics		10:00 – 12:40				Founder’s Hall/314
Nucleic Acid Chemistry		10:00 – 11:30				Founder’s Hall/406
Biospectroscopy			1:00 – 3:45			Founder’s Hall/307
Chemistry & Neutrino Physics			1:00 – 4:55			Founder’s Hall/406
Chemistry & the Arts			1:00 – 4:50			Founder’s Hall/314
Computational/Physical Chemistry Quantum Chemical Methods for Excited-State Systems			1:00 – 3:05			Founder’s Hall/409
Environmental Remediation: Methods & Applications			1:00 – 3:45			Founder’s Hall/310
Green Chemistry			1:00 – 4:30			Founder’s Hall/306
Polymer Chemistry Undergraduate Research & Teaching			1:00 – 3:50	9:00 – 11:50		Founder’s Hall/303
Protein Structure & Design			1:00 – 2:55			Founder’s Hall/402
Research & Education in Nuclear Magnetic Resonance & Mass Spectrometry			1:00 – 4:50			Founder’s Hall/415
Energy for a Sustainable Future			1:30 – 4:45			Founder’s Hall/302
Medicinal Chemistry			1:30 – 4:15			Founder’s Hall/404
Biotechnology				9:00 – 12:30		Founder’s Hall/302
Environmental Chemistry: Fate of Contaminants Measurements, Predictions & Reactions in Water				9:00 – 11:25		Founder’s Hall/309
Frontiers in Gel Chemistry				9:00 – 11:50	1:00 – 3:50	Founder’s Hall/308
Inorganic Chemistry				9:00 – 12:15		Founder’s Hall/307
Ionic Liquids Properties & Interactions with Biopolymers				9:00 – 12:00		Founder’s Hall/310
Material Chemistry				9:00 – 12:40		Founder’s Hall/402
Nano-Chemistry & Technology				9:00 – 11:20	1:00 – 3:10	Founder’s Hall/301
Organic Electronics				9:00 – 12:20		Founder’s Hall/314
Photocatalysis & Solar Fuel				9:00 – 12:30		Founder’s Hall/306
Teaching Chemistry to Students with Disabilities				9:00 – 12:55		Founder’s Hall/304
Teaching Nanoscience				9:00 – 11:50		Founder’s Hall/404
Organic Synthesis & Catalysis				9:30 – 11:45	1:00 – 3:30	Founder’s Hall/317
Computational/Physical Chemistry Structure & Thermodynamics in Biological Systems				10:00 – 1:20		Founder’s Hall/409
Radiation Photochemistry & Photophysics				10:00 – 11:35	1:00 – 2:15	Founder’s Hall/312
Chemical Biology				10:30 – 12:00	2:30 – 5:15	Founder’s Hall/315

MEETING SCHEDULE AT A GLANCE

EVENT	THURS. PM June 9	FRI. AM June 10	FRI. PM June 10	SAT. AM June 11	SAT. PM June 11	LOCATION
TECHNICAL SESSIONS						
Activation & Transformations of Small Molecules by Metal Centers					1:00 – 3:40	Founder’s Hall/307
Ambient Mass Spectrometry for Forensic Science					1:00 – 3:45	Founder’s Hall/314
Bioinformatics					1:00 – 3:05	Founder’s Hall/302
Environment & Forensics					1:00- -3:35	Founder’s Hall/306
Environmental Chemistry: Fate of Contaminants Measurements & Reactions in Soil					1:00 – 3:55	Founder’s Hall/309
Enzyme Catalysis & Inhibition					1:00 – 3:45	Founder’s Hall/304
Organic Synthesis & Catalysis					1:00 – 3:30	Founder’s Hall/317
Organizing Research Programs at the Undergraduate Level					1:00 – 4:20	Founder’s Hall/303
Ionic Liquids Radiation Chemistry & Interactions with Transition Metals					1:30 – 4:20	Founder’s Hall/310
POSTER SESSIONS						
Graduate & Post-Docs		10:00 – 12:00				Peter Jay Sharp Athletic & Recreation Center (Gym)
Undergraduate				9:00 – 11:00	2:00 – 4:00	Peter Jay Sharp Athletic & Recreation Center (Gym)
Faculty				11:30 – 1:30		Peter Jay Sharp Athletic & Recreation Center (Gym)
SOCIAL EVENTS						
MARM 2016 Welcome Barbeque	5:00 – 6:00					Grace Plaza
Women Chemists Committee Luncheon Dr. Elise Megehee			12:00 – 2:00			Benedict’s (1st Floor FH)
Chips and Chat with ACS Governance			2:00 – 3:00			President’s Reception room - Founders Hall second Floor
Election Town Hall			3:00 – 4:00			President’s Reception room - Founders Hall second Floor
Awards Cocktail Hour			6:30 – 7:30			Blue Room (2nd Floor FH)
Awards Dinner			7:30 – 10:00			Smith Hall (2nd Floor FH)
Undergraduate Continental Breakfast				8:00 – 9:00		Grace Plaza
Undergraduate Picnic					12:00 – 1:00	Grace Plaza
Undergraduate Chemistry Demo Exchange					1:00 – 2:00	Grace Plaza
Undergraduate Ice Cream Social					4:00 – 5:00	Grace Plaza
Keynote Address with Dr. Ronald Breslow					5:00 – 6:00	Hayes Auditorium
125th Anniversary Cocktail Hour					6:30 – 7:30	Blue Room (2nd floor FH)
125th Anniversary Dinner					7:30 – 10:00	Smith Hall (2nd Floor FH)
WORKSHOPS						
ACS Leadership Course: Fostering Innovation		8:30 – 12:30				Founder’s Hall/317
ACS Career Workshop: Finding Your Pathway		8:30 – 12:30				Founder’s Hall/408
Chemical Hygiene Officer (CHO) Workshop		8:30 – 12:30				Founder’s Hall/315
ACS Career Workshop: Resume Reviews			1:30 – 5:00			Founder’s Hall/408
Laboratory Waste Management Workshop			1:30 – 5:30			Founder’s Hall/315
Green Chemistry Workshop for Science Teachers				8:00 – 4:30		Science Hall, room #117 classroom and 301/313 Lab
MARM Chemagination!					12:00 – 5:00	Old Gym
ACS ChemIDP: Planning for Your Career Workshop					2:00 – 4:00	Founder’s Hall/408

TABLE OF CONTENTS MARM 2016

Participating MARM ACS Sections
(Representing Over 30,000 Members)

Chemical Society of Washington DC
Central Pennsylvania
Delaware
Lehigh Valley
Maryland
Monmouth County
New York
North Jersey
Ocean County
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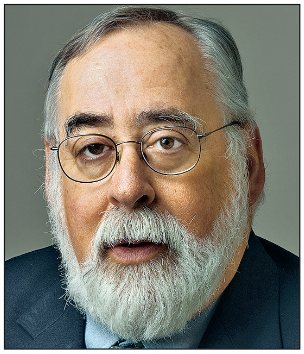
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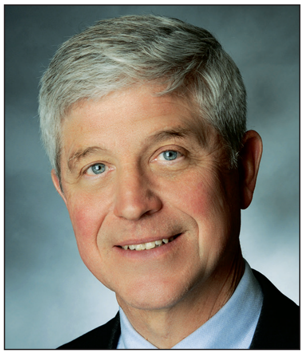
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Immediate Past President


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12/14/15

MARM 2016 Organizing Committee

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	Sujun Wei Queensborough Community	SWei@qcc.cuny.edu
Treasurer	Frank Romano Agilent	Frank.Romano@agilent.com
Secretary	Marlon Moreno Queensborough Community	MMoreno@qcc.cuny.edu
Exhibits & Sponsorship Co-Chairs	Ping Furlan United States Merchant Marine	furlanp@usmma.edu
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	Farai Tsokodayi American Chemical Society	F_Tsokodayi@acs.org
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	Ronald D'Amelia Hofstra University	Ronald.P.Damelia@hofstra.edu
2016- ACS New York Section Chair	Alison Hyslop St. John's University	hyslopa@stjohns.edu

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AMERICAN CHEMICAL SOCIETY
1155 Sixteenth Street, NW
Washington, DC 20036
T [202] 872 4534

Thomas M. Connelly, Jr., Ph.D.
Executive Director & Chief Executive Officer

May 11, 2016

Dr. Alison G. Hyslop
Chair & Program Chair
New York Local Section
c/o St. John's University
8000 Utopia Parkway
Jamaica, NY 11439

Dear Colleagues in the New York Local Section:

On behalf of the American Chemical Society with nearly 157,000 members, I wish to commend the New York Local Section as it observes the 125th anniversary of its founding in 1891. The New York Local Section is to be congratulated for its long standing commitment to serving its members and its efforts to create a positive awareness in the community about the importance of chemistry in day-to-day life. Your section has a rich history and should be proud of its many stellar achievements. The history of the section is in many ways the history of the ACS itself!

I firmly believe that the success of the American Chemical Society is due in large part to the strength and contributions of our local sections. I salute your members, volunteers, section officers past and present, and all those who have contributed in some fashion to the New York Local Section. Your collective efforts reach far beyond the borders of the section and have continued to make it one of the leading sections in the ACS. You have truly helped ACS to achieve its vision of improving people's lives through the transforming power of chemistry.

Again, heartfelt thanks and congratulations for 125 years of excellence! I wish the New York Local Section continued success and look forward with you to a bright future.

Sincerely yours,

T M Connelly Jr.

Dr. Thomas M. Connelly, Jr.
ACS Executive Director & CEO

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Donna J. Nelson, Ph.D.
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1155 SIXTEENTH STREET, N.W.
WASHINGTON, D.C. 20036
Phone 405-325-2288
Fax 202-872-6338
djnelson@ou.edu
twitter: @drdjnelson

June 9, 2016

Dear Middle Atlantic Regional Meeting participants,

On behalf of the more than 156,000 members of the American Chemical Society, I am happy to welcome all of you to the College of Mount Saint Vincent in Riverdale, New York for the 2016 Middle Atlantic Regional Meeting.

The meeting, hosted by the ACS New York Section, will highlight the theme “Chemistry: Past, Present & Future.” In addition to 50 technical symposia and a poster session, the meeting will also feature keynote speaker Ronald Breslow of Columbia University, a 125th anniversary banquet of the ACS New York Section, a Chemagination competition by high school students, and green chemistry training for high school teachers on pollution prevention in New York City schools.

Career Workshops, Leadership Courses, and the Women Chemists Committee luncheon are all designed to help you network and learn from your peers. Join your colleagues on Thursday evening for the Welcome Barbeque, and at a ‘Chips and Chat’ with ACS Governance and the Awards Dinner on Friday.

With all these events and great symposia, I want to express my special thanks to the MARM co-chairs Pamela Kerrigan and Daniel Amarante and to our hosts at the New York Section for their hard work and dedication to create a great experience here in Riverdale.

All the best for a wonderful MARM 2016!

Sincerely,

Donna J Nelson

Donna J. Nelson
2016 President
American Chemical Society

COLLEGE OF
MOUNT SAINT VINCENT
OFFICE OF THE PRESIDENT

June 2016

Welcome to the College of Mount Saint Vincent. We are delighted to host this 125th anniversary celebration and meeting of the New York Section of the American Chemical Society.

Scholarship defines the academic life and our professional lives. This organization has been especially distinguished in recognizing and furthering the fundamental role of scholarly research to excellent undergraduate education.

Thank you for featuring the excellent research of students from Mount Saint Vincent and other strong programs. We should celebrate the proficient skills, self-discipline, independent judgment, and creativity reflected in this work.

With best wishes for you all,

Sincerely,

Charles Flynn

6301 RIVERDALE AVENUE, RIVERDALE, NEW YORK 10471-1093 • P: (718) 405-3233 • F: 718.549.2603 • PRESIDENT@MOUNTSAINTVINCENT.EDU

COLLEGE OF
MOUNT SAINT VINCENT
DIVISION OF NATURAL SCIENCES

American Chemical Society
New York Section, Inc.

Dear Meeting Participants,

Welcome to the College of Mount Saint Vincent. We are delighted and proud to be hosting the 44th Middle Atlantic Regional Meeting (MARM) of the American Chemical Society. We, also, would like to congratulate the New York Section on its 125th Anniversary.

This organization has been especially distinguished in recognizing and furthering the fundamental role of not only the scientific community but the community at large. The theme of this MARM meeting is "Chemistry: Past, Present and Future". This event will afford to your fellow scientists the opportunity to learn from the past and utilize the research of the present in order to influence the future of chemistry and its related disciplines.

This is the first MARM meeting in four years and it has been eight years since it was held in New York. This year's meeting has 50 technical symposia, 4 poster sessions, an undergraduate program, a Green Chemistry workshop for high school teachers and the Chemamgination. There were over 500 abstracts submitted.

In addition, there will be several specials events. The regional awards for advancing diversity in the chemical sciences, teaching at a small college, volunteering and high school teacher will be presented at the Award dinner on Friday June 10. The keynote address will be presented on Saturday, June 11, by Dr. Ronald Breslow from Columbia University. His talk entitled "The Invention of SAHA, An Effective Anticancer Compound with an Important New Mechanism, and And of New Analogs with Exciting Properties" will be an example of research that is presently being pursued. During the 125th Anniversary dinner there will be a brief presentation on the history of the New York section followed by an example of future of chemistry research presented by Dr. Tianning Diao from New York University entitled "Bimolecular Strategies for Sustainable Chemical Syntheses."

We would like to thank all our sponsors for their contributions. A special thanks for our exhibitors, all of whom are listed in this program book. This meeting would not be possible without the tremendous effort and dedication of the MARM 2016 organizing committee and to all the volunteers who have taken time from their busy schedules to help in all the scheduled events.

We hope your stay here in Riverdale puts you in a "Chemistry State of Mind".

With best wishes for you all,

Daniel Amarante
General Co-Chair

Pamela Kerrigan
General Co-Chair

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The Bronx County Building
851 Grand Concourse, 161st St.
Bronx, New York 10451

Ruben Diaz Jr.
BOROUGH PRESIDENT

TEL: 718-590-3500
FAX: 718-590-3537

June 11, 2016

American Chemical Society - New York Section, Inc.
St. John's University
8000 Utopia Parkway
Jamaica, NY 11439

Dear Friends,

Congratulations on the occasion of your 44th Middle Atlantic Regional Meeting, a time to reflect and be proud of all that your organization has accomplished and continues to do for the people of The Bronx, New York City and the entire State of New York.

Through the years, the American Chemical Society - New York Section has shown an outstanding commitment to improving and addressing the concerns and needs of the scientific and academic community throughout our great borough.

On behalf of the 1.4 million residents of The Bronx, I salute the American Chemical Society - New York Section and I wish you all continued success in your future endeavors.

Sincerely,

Ruben Diaz Jr.

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New York Section
125 Years of Excellence
http://www.NewYorkACS.org

May 25, 16

Dear Middle Atlantic Regional Meeting Participants,

On behalf of the New York Section of the American Chemical Society, I am pleased to extend greeting to all of the attendees of the 44th Middle Atlantic Regional Meeting (MARM 2016) at the College of Mount Saint Vincent in Riverdale, New York.

In celebration of the 125th anniversary of the founding of the New York Section, Professors Pamela Kerrigan and Daniel Amarante, the General Chairs, and the MARM organizers have designated this MARM as Chemistry: Past, Present, and Future, New York – A Chemistry State of Mind as the theme for this event. Take advantage of this meeting to learn about how chemistry is now transforming our world and how it will impact our future.

While you are here, take advantage of the symposia, workshops, and special session, attend the social events, visit the exhibits, and take advantage of New York City. You can even attend a Yankees vs. Angels baseball game.

Thank you to all of the organizers and volunteers, the MARM Steering Committee, the other fifteen participating sections of the Middle Atlantic Region, and the the especially our host, the College of Mount Saint Vincent, for their hard work and dedication to making this meeting a success.

Regards,

Alison Hyslop

Alison Hyslop

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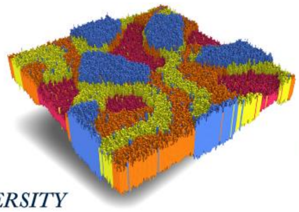

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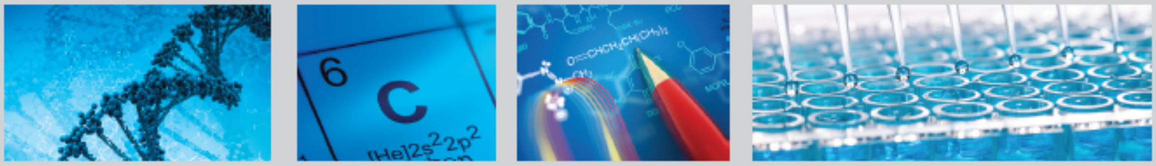
American Chemical Society

Division of Organic Chemistry



OUR MISSION is to foster and promote the advancement of the field of organic chemistry.

NURTURING YOUNG CHEMISTS

- Student Travel Awards
- Graduate Research Symposium and Workshops
- Graduate Research Fellowships
- Organic Division Undergraduate Awards
- Summer Undergraduate Research Fellowships

FOSTERING PROFESSIONAL DEVELOPMENT

- Workshops at ACS Meetings
- Faculty Travel Awards
- Young Investigator Symposium (non-academic)
- Assistant Professor Symposium

RECOGNIZING EXCELLENCE

- Technical Achievement Awards in Organic Chemistry
- Paul G. Gassman Distinguished Service Award
- Edward Leete Award
- ACS Awards Symposia at National Meetings

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- ACS National Meeting ORGN Programs
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Journal of Medicinal Chemistry

Organic Syntheses

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MARM 2016 EXPOSITION

When: June 10 & June 11, 2016, 9:00 AM—5:30 PM

Where: Peter Jay Sharp Athletic & Recreation Center, College of Mount Saint Vincent, Riverdale, NY

Why: Meet face-to-face with leaders & representatives of prominent Corporations and Universities as they demonstrate new products, discuss exciting programs, and answer your questions

Who:

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NSF SYMPOSIUM: FUNDING OPPORTUNITIES IN CHEMISTRY
FRIDAY, JUNE 10, 9:15 AM—NOON

College of Mount Saint Vincent, Founder's Hall Room: 308

9:15 AM—9:45 AM	**NATIONAL SCIENCE FOUNDATION AND BROADER IMPACTS** Eric Pfeiffer | Program Specialist | Division of Chemistry
9:45 AM—10:15 AM	**FUTURE FACULTY, EARLY CAREER FACILITY, AND NEW PRINCIPLE INVESTIGATORS: INTERACTIONS WITH NSF CHEMISTRY** Sarah Stoll | Program Officer | Division of Chemistry
10:15 AM—10:30 AM	**BREAK**
10:30 AM—11:00 AM	**SUPPORT FOR UNDERGRADUATES, GRADUATE STUDENTS, AND POSTDOCTORAL FELLOWS** C. Michelle Jenkins | Program Analyst | Division of Chemistry
11:00 AM—11:30 AM	**FACULTY INTERACTIONS WITH NSF CHEMISTRY** Lin he | Program Officer | Division of Chemistry
11:30 AM	**QUESTIONS AND ANSWERS**
NOON	**SESSION END**

National Science Foundation
WHERE DISCOVERIES BEGIN

NSF DIVISION OF CHEMISTRY BOOTH EXHIBIT
FRIDAY, JUNE 10 AND SATURDAY, JUNE 11

College of Mount Saint Vincent, Peter Jay Sharp Athletic and Recreation Center (Gym)

9:30 AM - 5:30 PM	Learn about current NSF and Chemistry funding opportunities, initiatives, programs and how to participate!

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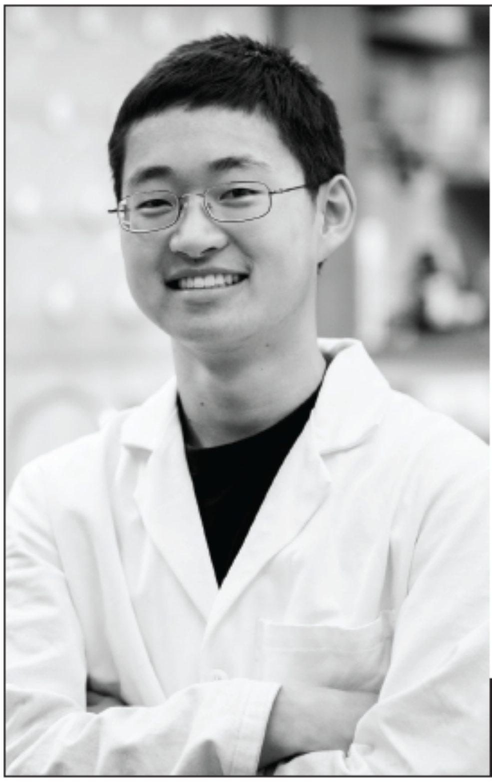

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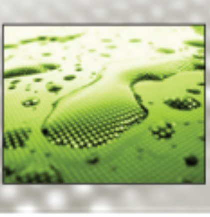

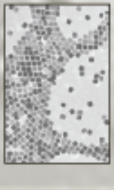

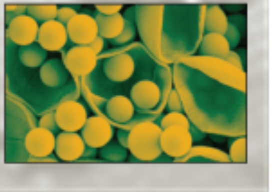

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The Institute for Soft Matter Synthesis and Metrology was established in 2012, and now comprises 12 regular faculty members across Physics, Chemistry, and Oncology, together with research faculty and staff devoted to facilities development and industrial liaison.

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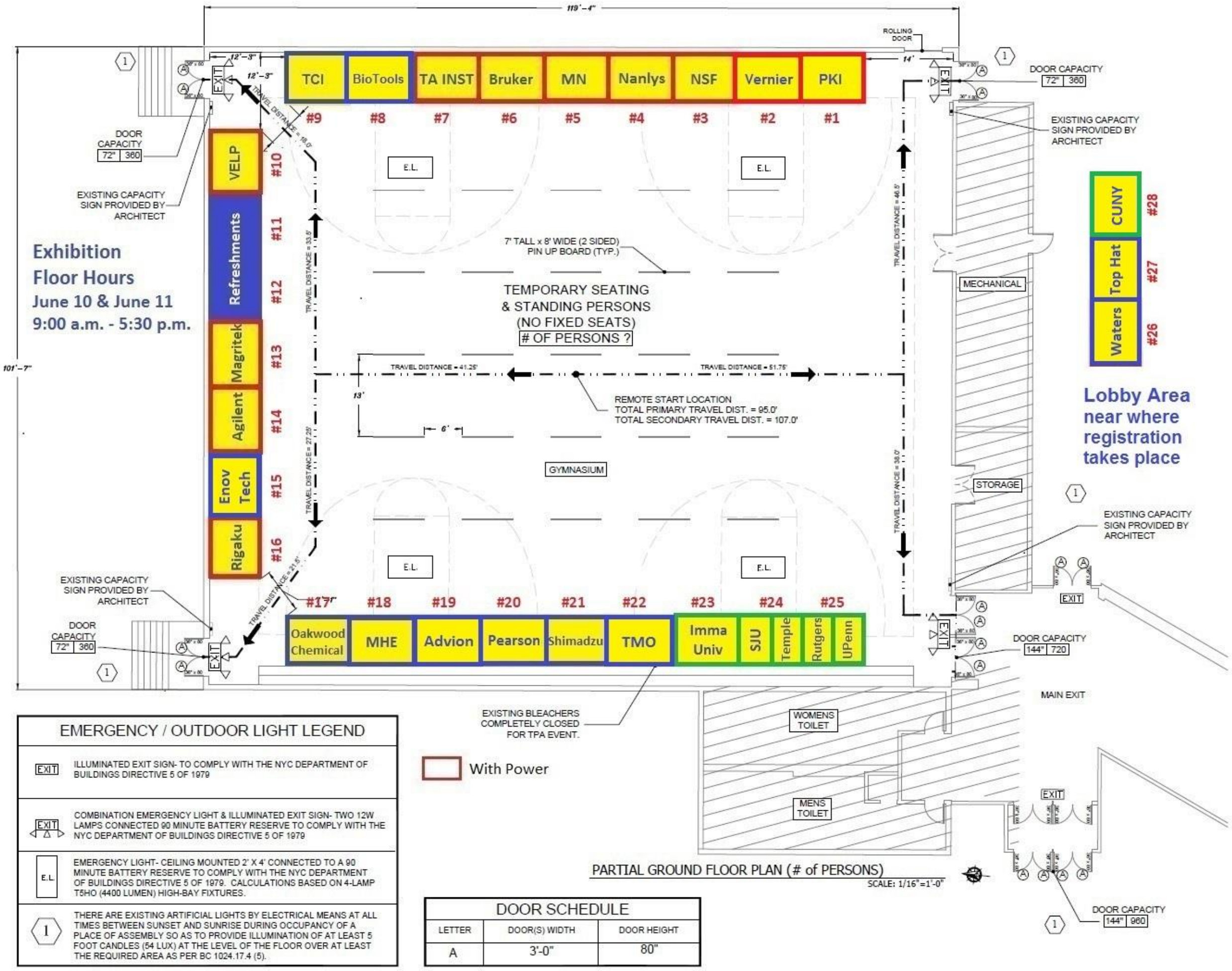
44th Middle Atlantic Regional Meeting Exhibitor Booth Assignments



Exhibition Floor Hours
June 10 & June 11
9:00 a.m. - 5:30 p.m.

Lobby Area near where registration takes place

🟥 With Power

EMERGENCY / OUTDOOR LIGHT LEGEND	
EXIT	ILLUMINATED EXIT SIGN- TO COMPLY WITH THE NYC DEPARTMENT OF BUILDINGS DIRECTIVE 5 OF 1979
EXIT	COMBINATION EMERGENCY LIGHT & ILLUMINATED EXIT SIGN- TWO 12W LAMPS CONNECTED 90 MINUTE BATTERY RESERVE TO COMPLY WITH THE NYC DEPARTMENT OF BUILDINGS DIRECTIVE 5 OF 1979
E.L.	EMERGENCY LIGHT- CEILING MOUNTED 2' X 4' CONNECTED TO A 90 MINUTE BATTERY RESERVE TO COMPLY WITH THE NYC DEPARTMENT OF BUILDINGS DIRECTIVE 5 OF 1979. CALCULATIONS BASED ON 4-LAMP T5HO (4400 LUMEN) HIGH-BAY FIXTURES.
1	THERE ARE EXISTING ARTIFICIAL LIGHTS BY ELECTRICAL MEANS AT ALL TIMES BETWEEN SUNSET AND SUNRISE DURING OCCUPANCY OF A PLACE OF ASSEMBLY SO AS TO PROVIDE ILLUMINATION OF AT LEAST 5 FOOT CANDLES (54 LUX) AT THE LEVEL OF THE FLOOR OVER AT LEAST THE REQUIRED AREA AS PER BC 1024.17.4 (5).

DOOR SCHEDULE		
LETTER	DOOR(S) WIDTH	DOOR HEIGHT
A	3'-0"	80"

Advion (Booth #19)	Pearson (Booth #20)
Agilent Technologies (Booth #14)	PerkinElmer (Booth #1)
Biotools (Booth #8)	Rigaku Oxford Diffraction (Booth #16)
Bruker (Booth #6)	Rutgers University (Booth #25)
City University of New York (Booth #28)	Saint John's University (Booth #24)
Enovative Technologies (Booth #15)	Shimadzu (Booth #21)
Immaculata University (Booth #23)	TA Instruments (Booth #7)
Machery-Nagel, Inc. (Booth #5)	TCI America (Booth #9)
Magritek (Booth #13)	Temple University (Booth #24)
Magritek (Booth #13)	Thermo Fisher Scientific (Booth #22)
McGraw-Hill Education (Booth #18)	Top Hat (Booth #27)
Nanalysis (Booth #4)	University of Pennsylvania (Booth #25)
National Science Foundation (Booth #3)	VELP Scientific, Inc. (Booth #10)
Oakwood Chemical (Booth #17)	Waters (Booth #26)

MARM 2016 EXHIBITORS

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www.nsf.gov	**Exhibit Time: 9:30 AM – 5:30 PM** Come stop past to learn about current NSF and Chemistry funding opportunities, initiatives, programs and how to participate!

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KEYNOTE SPEAKER

The Invention Of SAHA, An Effective Anticancer Compound With An Important New Mechanism, And Of New Analogs With Exciting Properties

Ronald Breslow, Columbia University

S.L. Mitchill Professor of Chemistry and University Professor

Saturday, June 11, 2016, 5:00 PM-6:00 PM
Hayes Auditorium

The 2016 ACS Middle Atlantic Regional Meeting (MARM) is honored to have Dr. Ronald Breslow, the 2003 Welch and the 2004 Willard Gibbs Medalist, the 1995 President-Elect of the American Chemical Society and 1996 ACS President, presenting a keynote lecture. Dr. Breslow is a distinguished chemist, with research interests in several different physical-/bio-organic chemistry areas: his specialties are the design, synthesis, and study of new molecules with interesting properties. Breslow is noted for his pioneering research in nonbenzenoid aromatic chemistry; enzyme-catalyzed reactions; biomimetic approaches to synthesis of enzymes and complex carbohydrates; and synthesis of simple anticancer compounds.

Breslow has written more than 400 published articles and three books. His numerous honors include the prestigious National Medal of Science, awarded to him in 1991, the American Chemical Society Bader Award in Bioorganic or Bioinorganic Chemistry, the New York City Mayor's Award in Science, the American Chemical Society Priestley Medal, the U.S. National Academy of Sciences Award in Chemical Sciences, the Columbia Alumni Association Great Teacher Award, the British Chemical Society Centenary Medal, and the American Chemical Society Award in Pure Chemistry. He is also a member of the National Academy of Sciences.

His achievements and service to chemistry have been additionally recognized with many honors and awards; the 2016 Pupin Medal, the 2014 American Institute of Chemists Gold Medal, the 2003 National Academy of Sciences Award for Chemistry in Service to Society, the 2002 Perkin Medal, and the 1995 E.B. Hershberg Award to name a few.

MARM 2016 Awards Dinner
Friday June 10, 2016
Founder's Hall – 2nd Floor

Reception

6:30 – 7:30 PM Blue Room

Beer, Wine, Cheese, Crackers, Fruit, Vegetables

Dinner

7:30 PM – 8:45 PM Smith Hall

Salad 7:30 PM (placed at table)

Buffet Dinner 8:00 – 8:45 PM

Chicken Marsala, Grilled Salmon, Vegetarian Lasagna, Scalloped Potatoes, Green Beans Almandine, Roasted Vegetable, Assorted Dessert Bars

Awards Ceremony

8:45 – 9:15 PM Smith Hall

MARM 2016 Awards

The Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences

Sponsored by the Committee on Minority Affairs of the American Chemical Society

Winner for MARM 2016

Department of Chemistry

St. John's University, Queens, New York

St. John's University's Chemistry Department advances diversity in the chemical sciences and fosters activities that promote inclusiveness. Guided by SJU's focus of educating to the students of New York, and a policy that a minimum of 40% of the student-body be Pell-eligible, our Department has embraced this mission through our academic, co-curricular, community outreach programming, and student support services. Our Chemistry students actively participate in research with faculty mentors and internships with industrial partners. They actively participate in Student ACS events, and have received numerous outstanding or honorable mention recognition awards from the National ACS. We provide *Chemistry is Fun* shows to local elementary schools and participate in National Chemistry Week at the New York Hall of Science. Through our departmental commitment to diversity, inclusive excellence, and service, we seek to level the playing field so that all of our students can be successful and thrive.

ST. JOHN'S
UNIVERSITY

DEPARTMENT OF
CHEMISTRY

The E. Emmet Reid Award in Chemistry Teaching at Small Colleges in the ACS Mid-Atlantic Region

Winner for MARM 2016

Dr. Ronald P. D’Amelia

Dr. Ronald P. D’Amelia graduated with a B.S. degree in Chemistry from the City College of New York (CCNY). As a recipient of a NASA research grant and an Adelphi teaching fellowship, he earned his master’s and doctoral degrees in Chemistry at Adelphi University, Garden City, N.Y. After graduate school, Dr. D’Amelia served in the Army Chemical Corps as an instructor at the Ft. McClellan Army Chemical School in Alabama. In 1971 he joined the Life Savers Company as a physical polymer chemist. After several company mergers, he was promoted to the rank of Director of Polymer Chemistry. He received 25 patents in the areas of reduced calorie fats, chewing gum technology and breath freshening ingredients. In 2000, he received the L.I. Innovator of the Year Award for developing the breath freshening technology used in the Life Saver’s Breath Savers product. He retired after 32 years of continuous service from the Kraft/Nabisco Food Group as a Senior Principal Scientist, the second highest technical position in the Company. He is now an adjunct full Professor of Chemistry at Hofstra University, where he teaches general and organic Chemistry. He was inducted as a Fellow of the American Chemical Society in 2011.

The ACS Division of Chemical Education Middle Atlantic Region Award for Excellence in High School Teaching

Winner for MARM 2016

Ms. Maria Calvert

Mary Calvert attended The University of Illinois in Champaign-Urbana earning a B.S. in Chemistry. After working in industry for a couple of years she went back to school and earned a master's in Chemistry from Princeton University. Calvert taught at the College of New Jersey before teaching at The Lawrenceville School where she has taught for the last 18 years. Calvert holds Lawrenceville's Oscar H. McPherson '01 Distinguished Teaching Chair. In addition to her duties in the science department, Calvert is the Housemaster of Kirby House and coaches the Kirby House Frisbee, volleyball, and basketball teams. She also co-coaches the Science and Robotics club, which enters about a dozen competitions a year. Calvert has served as a member of the following Lawrenceville committees: Selection of a New Headmaster, Health and Wellness Initiatives, Crescent Initiative: New Crescent House and Student Center, Coeducation, Review and Propose New Athletic Requirements, Student Leadership, and the Quarter Century Society. In 2012, she received Lawrenceville's Henry C. Woods Faculty Award for Service to the School and in 2000 she was honored with the School's Ritter Award for Fostering a Nurturing Academic Environment. Calvert has also chaperoned Lawrenceville International Programs trips to Austria, Cuba, and Germany.

The E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society

Winner for MARM 2016

Dr. Paris Svoronos

Dr. Paris Svoronos earned his PhD in organic synthesis under Professor Vaclav Horak at Georgetown University in 1979 and joined Queensborough Community College (CUNY) in 1981 where he is currently a full professor and former chair (2001-10). Dr. Svoronos was elected as the chair of the ACS-Long Island subsection (2002) as well as director-at-large (2013) and chair of the ACS-New York section (2015). In 2008 he was the General co-Chair of the MARM 2008, the first time this conference was ever held in New York City and was hosted by his home institution. He is currently the program co-chair of MARM 2016 and was the advocate for the ACS-New York Section Undergraduate Research Symposium (URS) that was held at Queensborough both in 2004 and 2008. As chair of the ACS-Long Island subsection he was the force behind the instituting of the Annual Chemistry Challenge which has been held with as many as 27 three-student teams for twelve straight years. He was bestowed the Stanley Israel award in 2008 but decided to share it with his Queensborough colleagues. He is a firm believer in undergraduate research, even at the community college level. He was declared the Community College Professor of the Year in 2003 by CASE and the Carnegie Foundation for the Advancement of Teaching- the first ever chemist to that point.

Partners for Progress and Prosperity (P3) Award

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Winner for MARM 2016

New York Local Section and William Nichols Foundation

Throughout its 125 year history, the New York Local Section of the American Chemical Society has collaborated with the William H. Nichols Foundation in its efforts to improve the public's perception of chemistry. This partnership is expressed in three programs that continue to have a sustained impact on the broader chemical enterprise and its practitioners. First and foremost, the New York Local Section with the support of the Nichols Foundation annually awards the William H. Nichols Medal, the first award authorized by the American Chemical Society. The Nichols Medal is given in recognition of an outstanding contribution in the field of chemistry and its list of recipients is a Who's Who of Chemistry that includes 18 Nobel Laureates and 22 recipients of the National Medal of Science. Second, the Nichols Foundation and the New York Local Section established the annual Nichols Foundation Chemistry Teacher Award in 1958. This award fosters the innovative and effective chemistry education needed to inspire high school students to pursue their interests in STEM fields. Lastly, the latest expression of the intimate partnership between the New York Local Section and the Nichols Foundation, Inc. is the establishment of the William H. Nichols Fellows program in 2015. This program fosters the early careers of chemical researchers by providing Fellowships to support their immersion into authentic research experiences over the summer of their junior year. The New York Local Section and the Nichols Foundation, Inc. have successfully partnered for more than a century to improve people's lives through the transforming power of chemistry.

MARM 2016 Awards criteria

The Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences

(Sponsored by the Committee on Minority Affairs of the American Chemical Society)

Nomination Guidelines:

Purpose: To recognize individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the region.

Nature: The award consists of a medal and a $1,000 grant to support and further the activities for which the award was made. The award also will include funding to cover the recipient's travel expenses to the ACS regional meeting at which the award will be presented.

Rules of Eligibility: Individuals nominated for the award may come from any professional setting: academia, industry, government, or other independent facility. Nominees may also be organizations, including ACS local sections and divisions. The awardees will have increased the participation and leadership of persons from diverse or underrepresented minority group(s), persons with disabilities, or women.

To Nominate: For nomination of individuals, a letter of nomination of no more than three pages and a CV or resume is required. The CV or resume should contain relevant diversity promotion activities and factual data on outcomes. At least one, but no more than three supportive letters, one of which must come from the nominee's ACS Local Section. Mailing address, phone number(s), and e-mail address of nominee/supporter must be provided

The E. Emmet Award in Chemistry Teaching at Small Colleges in the ACS Mid-Atlantic Region

This award is administered by the Organizing Committee of the Middle Atlantic Regional Meeting (MARM) of the American Chemical Society for outstanding achievements in teaching chemical sciences at small colleges within the Middle Atlantic Region.

Nomination Guidelines

Purpose: To recognize, encourage and stimulate high quality teaching and research at small colleges.

Nature: The Award will consist of $1,000 and a major award plaque.

To nominate: Nominations for the Award are made by the Local Sections of the Middle Atlantic Region. The Chairman or Secretary of the Section must sign and transmit the nomination to the MARM Award Committee Chairman. A committee may be appointed to solicit names of candidates for final selection. No special form is required but the MARM Award Chair must receive the nominee's short curriculum vitae, list of publications, and evaluation of the nominee's achievements as a teacher in a small college. This document should clearly demonstrate the candidate's attributes: the quality of the candidate's teaching; organization and efficiency of lab work; research and/or development work; ability to challenge and inspire students; extra-curricular work in chemistry; courses, meetings, presentations, awards, etc. Seconding letters are not essential but as many as three may be included with each nomination. Letters may include careful evaluations of the teacher's abilities by his superiors, associates, or by local section members. The candidate need not be a member of the American Chemical Society.

The Award committee of MARM will review the candidates and select the nominee. The nominee will be presented the Award during the forthcoming MARM. The nominee is expected to deliver a short acceptance speech. Unsuccessful candidate's files will be kept active for a period of three years upon receipt of a letter from the nominating section chairman or secretary. Any further updating of the candidates file will be welcomed at that time but are not mandatory.

The E. Ann Nalley Regional Award for Volunteer Service to the American Chemical Society

Nomination Guidelines

Purpose: To recognize the volunteer efforts of individuals who have served the American Chemical Society, contributing significantly to the goals and objectives of the Society through their Regional Activities.

Nature: This award was instituted in 2006 by ACS President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism. It is Dr. Nalley's wish that the award continue in perpetuity at each regional meeting. The award consists of a plaque honoring the recipient with an imbedded medallion commemorating Dr. Nalley.

Rules of Eligibility: A nominee must be a member of the American Chemical Society residing in a local section within the region, and will have made significant contributions to their Region of the American Chemical Society. The volunteerism to be recognized may include a variety of activities, including but not limited to the initiation or sponsorship of a singular endeavor or exemplary leadership in the region. Past and present members of the ACS Board of Directors and staff are ineligible for this award.

Submittal process: For each nominee, a Nomination (which includes a bio or curriculum vitae) and one or two Support Forms must be completed. As indicated in the form, these materials should be completed and forwarded to the MARM Awards Chair.

The ACS Division of Chemical Education Middle Atlantic Region Award for Excellence in High School Teaching

Nomination Guidelines

Purpose: To recognize, encourage, and stimulate outstanding teachers of high school chemistry in the Middle Atlantic Region.

Nature: The Award consists of a cash award and a plaque. Reasonable travel expenses to the Regional Meeting at which the award will be presented will be reimbursed. A certificate/plaque may also be provided to the recipient's institution for display. The awardee may be asked to give an address and/or participate in a symposium with other teachers.

Rules of Eligibility: Any individual, except a member of the award selection committee or currently enrolled student of the nominee, may submit one nomination or support form in any given year. Local Sections are especially encouraged to submit nominations for the award. The nominee must be actively engaged in the teaching of chemistry or a chemical science in a high school (grades 9-12) on at least a half-time basis. The nomination should clearly demonstrate as many of the following attributes as possible: The quality of the nominee's teaching; unusually effective methods of presentation should be emphasized; the nominee's ability to challenge and inspire students; extracurricular work in chemistry or a chemical science by the nominee, including science fairs, science clubs, and activities that stimulate the interest of young people in chemistry and related sciences; a willingness to keep up-to-date in the field, as evidenced by the pursuit of a higher degree in chemistry or a chemical science, enrollment in refresher courses and summer institutes, regular attendance at scientific meetings, membership in professional organizations, and other means of self-improvement; evidence of leadership and/or active involvement within the profession.

Required Nomination Components: A completed Nomination Form that consists of a Nominator; Information form; A Nominee; Information form; A Nominator Recommendation letter of not more than 750 words submitted by the nominator; A curriculum vitae or resume that includes a list of the nominee's honors, professional activities, and additional evidence of service to the profession. This must be limited to no more than two pages and the activities listed must have occurred within the past five years. At least one, but not more than three letters of support. One must be from the teacher's current principal or supervisor. Additional letters of support may be sent by colleagues, members of the American Chemical Society who are familiar with the nominee's achievements, or former students and parents of former students. Unsuccessful candidates' files will be kept active for a period of one year.

Partners for Progress and Prosperity (P3) Award

Nomination Guidelines:

Purpose: To encourage and recognize successful and exemplary partnerships, a Partners for Progress and Prosperity (P3) Award is to be established as a new award to be given by Local ACS Sections, ACS International Chapters, and ACS Regional Meetings. These partnerships can be between industry, academia, government, small business and/or other organizations, including ACS local sections, ACS divisions, ACS international chapters, other societies or various entities domestic or overseas resulting in impactful outcomes in one or more of the following categories such as improving the public perception and appreciation for chemistry; promoting career advancement opportunities and/or supporting entrepreneurship in the chemistry enterprise; advancing advocacy efforts with government and other thought leaders; supporting STEM (Science, Technology, Engineering & Mathematics) education and/or research

Nature and Establishment: This award was instituted in 2014 by a contribution from Marinda Li Wu out of her Immediate Past ACS President's budget as part of her presidential initiatives to promote partnering for progress and prosperity. The funds will be evenly distributed at the end of 2014 to all Regional Meeting Boards who wish to participate. It will be up to each Regional Meeting Board how much to fund each P3 Award and whether any of the funds should be used to help support travel if needed. It is Dr. Wu's hope that this will be an ongoing award to recognize the importance of partnering and working together towards common goals to advance the global chemistry enterprise. At the Regional Meeting level, the award will consist of a special Partners for Progress and Prosperity silver/gold medallion plus a framed certificate of recognition (one for each Partner representing an entity or organization) plus up to $1,000 grant split equally between the partners to further the activities for which the award is made.

Eligibility: A nominee may represent academia, industry, government, small business or other organizations such as a Local Section. Partnerships can include international ACS chapters, ACS divisions, or other entities domestic or overseas. The awards committee of the ACS Regional Meeting Board will select the P3 Award winners. Any individual, except a member of the award selection committee, may nominate or support only one nominee package for this award in any given year.

Required Nomination Components: It is requires a letter of nomination describing the partnership, its activities, outcomes and impact and at least one, but no more than three supporting letters plus the mailing addresses, phone numbers, and e-mail addresses for nominee and supporters.

125th Anniversary Dinner
Saturday June 11, 2016
Founder's Hall – 2nd Floor

Reception

6:30 – 7:30 PM Blue room

Beer, Wine, Cheese, Crackers, Fruit, Vegetables

Dinner

7:30 – 10:00 PM Smith Hall

Salad 7:30 PM

Welcome from Special Guests and History of the section between salad and entrée

"New York, the American Chemical Society at 125 years of Shared History"

(Dr. Brian Gibney) 7:40 – 8:00 PM

Entrée 8:00 – 8:30 PM

Choice of: NY Strip Au Jus and Fried Onions, Chicken Francaise, Lemon Butter Sauce, Eggplant Parmesan, served with Roasted Yukon Potatoes and Seasonal Grilled Vegetables

""Bimolecular Strategies for Sustainable Chemical Syntheses"

(Dr. Tianning Diao) 8:30 – 8:50 PM

Dessert (Chocolate Molten Lava Cake) 8:30 PM

125th Anniversary
NYACS
NEW YORK SECTION of the
AMERICAN CHEMICAL SOCIETY

A BRIEF HISTORY OF THE NEW YORK SECTION OF THE AMERICAN CHEMICAL SOCIETY

By
John B. Sharkey

The New York Section was chartered on September 30, 1891, as the second local section of the American Chemical Society. From 1876, when the society itself was founded, until 1891, the society was very much a New York organization. The society was founded on April 6, 1876 in the lecture room of the College of Pharmacy of the City of New York, now New York University. The society was incorporated in the State of New York in 1877, and its Charter required that its Board of Directors, the legal representatives of the society, be residents of New York State. The society would remain so until 1938 when it received its Federal Charter, and moved its official headquarters to Washington D.C. It is not surprising that most of the early members of the society, and all of the scientific meetings were held in New York City.

It was the localization of the society in New York that eventually led to the need to form local sections. During the years 1876 to 1890, the society failed to develop an active membership outside of New York City. Out of State members, plagued by the inconvenience of travel and lack of regular mail delivery soon became disillusioned, and began to resign. The membership, which had reached a high of 243 in 1881, declined to 167 in 1889. Dissident members, such as Harvey Wiley and Frank W. Clarke, formed the Washington Chemical Society in 1884, thus bringing pressure on the ACS for needed reform. In addition, Charles F. Chandler, Professor of Chemistry at Columbia in New York City, and Charles F. Monroe of Rhode Island, worked within the society to make it into a truly national chemical society. The result of these efforts led to a new constitution, which was adopted on June 6, 1890, providing for meetings outside of the New York City area, and also for the formation of local section of the society. The first general meeting under the new constitution took place in Newport, Rhode Island in August 1890. In January 1891, the society approved the formation of the Rhode Island Section as its first local section. New York received its charter in September 1891 as the second local section of the society.

Early History of the New York Section

The twenty chemists who made application for the formation of the New York Section constitute the charter members of the section. Among this group were two past presidents of the ACS, Charles F. Chandler and T. Sterry Hunt, and three future section chairs, A. A. Breneman, C. A. Doremus, and A. H. Sabin. Charter members also included Albert K. Leeds, Herman Endemann, and Albert C. Hale, men who distinguished themselves through long and dedicated service to the society.

The first elected officer of the New York Section was Alvah H. Sabin as Chairperson, Morris Loeb as Secretary/Treasurer, and an executive Committee consisting of Henry Carrington Bolton, Abram A, Breneman, and William McMurtrie. Space only permits brief mention of the accomplishments of several of these distinguished chemists.

Alvah Sabin spent most of his career with the American Lead Company, and was an expert in drying oils and the technology of paints, varnishes, and lacquers, and for 30 years, was an abstracter for Chemical Abstracts in these fields.

Morris Loeb served as Secretary/Treasurer from 1892 to 1895, and also was the section Chairperson in 1909-1910. Loeb studied under the great physical chemist Wilhelm Ostwald, and was one of the pioneers in America in this new field of science. A philanthropist, Loeb donated the land for the original Chemists' Club building on East 41st Street, and made possible, in 1912, the Wolcott Gibbs Laboratory for Physical Chemistry at Harvard.

William McMurtrie served on the first Executive Committee and also as section Chairperson from 1896 to 1899. McMurtrie was the first of six New York Section Chairpersons who would serve as President of the American Chemical Society. He worked as chief chemist for the Department of Agriculture, and, in 1883, was succeeded by Harvey W. Wiley, whose great work led to the Pure Food and Drugs Act of 1906.

Henry Carrington Bolton, also a member of the first Executive Committee, was regarded as one of the leading scientists in America at that time. Author, lecturer and bibliophile, it was Bolton who suggested that chemists meet in Northumberland PA in 1874 to celebrate the 100th anniversary of Joseph Priestley's discovery of oxygen. Bolton's legacy lives on today through the Bolton Society of the Chemical Heritage

Foundation, a group of bibliophiles devoted to the discussion and preservation of books and related material in the chemical sciences.

Many other prominent chemists would serve as officers of the New York Section over its hundred and twelve-year history. Chemists who served as chairpersons of the section would distinguish themselves in many ways; six would serve as president of the society; five would be awarded the Nichols Medal; two would receive the Priestley Medal; and one the Nobel Prize in Chemistry.

The first regular meeting of the New York Section was held on May 6, 1892, and the first paper to be presented was "On the Application of Graphic methods in Certain Chemical Studies" by A. Bourgougnon. Over the next hundred and twelve years, many distinguished chemists would present the results of their research at meetings of the section.

The William H. Nichols Medal Award

In 1902, William H. Nichols, a charter member of the ACS and President in 1918 and 1919, established an award for the purpose of encouraging original research in chemistry. Dr. Nichols, himself a pioneer in the development of the chemical industry in the United States, was among the first to realize the importance of encouraging chemical research in America. The William H. Nichols Medal Award, the oldest award presented by a local section of the ACS, recognizes outstanding achievement in chemical research. To date, 17 recipients of the Nichols Medal have also received the Nobel Prize, the most recent being K. Barry Sharpless, who received the Nobel Prize in 2001 and the Nichols Medal in 2006.

The evolution of the Nichols Medal award has been varied and interesting throughout the 20th century. Unaltered, however, are two things: First is the loyal interest and continued generous support of the Nichols family and second is the high quality of the recipients of the award.

Memorable Meetings of the New York Section

Many memorable meetings have taken place in New York City during the section's hundred and twelve-year history. Among the most memorable perhaps were the ACS National Meetings hosted by the New York Section, commemorating the 25th, 75th, and 100th anniversaries of the society. (The 50th anniversary meeting was held in Philadelphia, and also in Northumberland PA, site of the 1874 Priestley Centennial meeting which commemorated Joseph Priestley's discovery of oxygen in August 1, 1774.

A number of section meetings were also of historical significance. Among these was a 1914 Conference on Chemicals and Dyestuffs, which called attention to the U.S.

dependence on imported chemicals and to the need for American chemical companies to expand into dyestuffs, pharmaceuticals, and other organic chemicals. Action was taken by ACS President Charles H. Herty, a former section chairperson, in mobilizing American manufacturing resources in the interest of industrial preparedness. In general, the usefulness of the Society to the government in the war effort was greatly enlarged.

Among the innovations associated with the New York Section, perhaps the most noteworthy were the formation of the Chemists' Club, the ACS News Service, and the concept of meetings-in-miniature; innovations with us to the present day. The Section is particularly proud of its meetings-in-miniature, now called the Undergraduate Research Symposium, which this year held its 64th anniversary meeting.

National Historic Chemical Landmarks

In 1993, the ACS Division of Public Outreach and the Division of the History of Chemistry sponsored a new program to increase awareness among professionals and the general public of historic chemical and chemical engineering sites, artifacts, and collections and to encourage their preservation. Of the 47 designations that have taken place so far, four have been associated with the New York Section and the fifth will take place in conjunction with this National Meeting on Wednesday, September 3rd at the Polytechnic University in Brooklyn.
The New York Section designates the location of historical achievements in chemistry as New York Section Historical Landmarks. To date, these include:

- The Chemistry Building at Brookhaven National Laboratories (Upton, NY) for the synthesis of the positron emission tomography tracer 2-deoxy-2-[^{18}F]fluoro-D-glucose (^{18}FDG)
- The Chemist's Club at 41st Street in New York, NY
- The IBM Watson Research Center in Westchester, NY
- The New York Hall of Science in Queens, NY

The New York Section also works with the American Chemical Society on selecting recipients for the National Chemical Historical Landmark Designation. It has successfully nominated seven National Historical Landmarks, the greatest number of any ACS Local Section. These include:

- The Bakelizer, National Museum of American History, Smithsonian Institution, Washington DC (Jointly with the ACS North Jersey Section
- Foundations of Polymer Science: Herman Mark and the Polymer Research Institute, New York, NY
- Havemeyer Hall at Columbia University, New York, NY
- John W. Draper and the Founding of the American Chemical Society, New York,
- Penicillin Production through Deep-tank Fermentation, New York, NY

- NMR and MRI: Applications in Chemistry and Medicine, Stony Brook, NY
- Nucleic Acid and Protein Chemistry Research at Rockefeller University, New York, NY

The New York Section - Recent History

The territory of the Section has greatly changed compared to more than a century ago, when membership included those members within a 50-mile radius of New York City Hall. The most dramatic change occurred in 1925, when the North jersey Section was chartered. In 1926, the North Jersey and New York local sections joined forces with the publication of The Indicator, a special issue of which has been published for this meeting.

The Nichols Foundation Chemistry teacher Award, established in 1958, was made possible through the generosity of Charles W. Nichols Jr., grandson of William H. Nichols. The purpose of the award is to encourage and stimulate good teaching of chemistry and to recognize dedicated teachers who inspire students to fully utilize their intellectual resources. The section continues to support education at all levels through its participation in activities such as the Chemistry Olympiad and Project SEED.

Today the New York Section, through its six subsections, ten topical discussion groups, and thirty-seven committees, provides its more than 4000 members over 100 technical events each year. The Section continues its proud tradition of service in the advancement of the chemical sciences initiated by its charter members more than a century ago, by hosting the 125th Middle Atlantic Regional Meeting (MARM) of the American Chemical Society tonight. And all of us gathered tonight to celebrate this milestone.

125th Anniversary
NYACS
NEW YORK SECTION of the
AMERICAN CHEMICAL SOCIETY

SPECIAL EVENTS MARM 2016

Thursday, June 9th:

5:00-6.30 PM - MARM 2016 Welcome Barbeque, ($25), Grace Plaza

Friday, June 10th:

8:30 AM - 12:30 PM - ACS Leadership Course: Fostering Innovation, ($10), Founder's Hall, Room 317

8:30 AM - 12:30 PM - ACS Career Workshop: Finding Your Pathway, ($5), Founder's Hall, Room 408

8:30 AM - 12:30 PM - Chemical Hygiene Officer (CHO) Workshop, ($150), Founder's Hall, Room 315

9:00 AM – 5:30 PM - MARM Exhibition, Peter Jay Sharp Athletic and Recreation Center

12:00 PM - 2:00 p.m. - Women Chemists Committee Luncheon, ($20**),** Founder's Hall, Benedict's (1st Floor)

1:30 PM - 5:00 PM - ACS Career Workshop: Resume Reviews, ($5, Sign up for a time slot at registration), Founder's Hall, Room 408

1:30 PM - 5:30 PM - Laboratory Waste Management Workshop, ($150), Founder's Hall, Room 315

2:00 PM - 3:00 PM - Chips and Chat with ACS Governance, (Complimentary), Founder's Hall, President's Reception Room (2nd Floor)

3:00 PM - 4:00 PM - ACS N&E Vote 20/20 Taskforce Regional Meeting Town Hall, (Complimentary), Founder's Hall, President's Reception Room (2nd Floor)

6:00 PM - 7:00 PM - Awards Cocktail Hour, ($25**),** Founder's Hall, Blue Room (2nd Floor)

7:00 PM - 10:00 PM - Awards Dinner, ($60), Founder's Hall, Smith Hall (2nd Floor)

Saturday, June 11th:

8:00 AM – 9:00 AM - Undergraduate Continental Breakfast, Grace Plaza

8:00 AM - 4:30 PM - Green Chemistry Workshop for Science Teachers, Science Hall, Classroom 117 and Lab 313

9:00 AM – 5:30 PM - MARM Exhibition, Peter Jay Sharp Athletic and Recreation Center

9:00 AM – 10:00 AM - Undergraduate Career Workshop: How to write a resume (presented by Cheretta Robinson from CMSV), Science Hall, Room 004

10:00 AM – 11:00 AM - Undergraduate Career Workshop: Interview skills (presented by Cheretta Robinson from CMSV), Science Hall, Room 004

12:00 PM - 5:00 PM - MARM Chemagination!, Peter Jay Sharp Athletic and Recreation Center

12:00 PM - 1:00 PM - Undergraduate Picnic, ($5), Grace Plaza

1:00 PM - 2:00 PM Undergraduate Chemistry Demo Exchange, ($5), Grace Plaza

2:00 PM – 4:00 PM - ACS ChemIDP: Planning for Your Career Workshop (presented by Nancy Bakowski from ACS), Founder's Hall, Room 408

2:30 PM - 3:30 PM - Undergraduate Talk titled "Differentiation and Identification of Cachaça Wood Extracts using Peptide-based Receptors and Multivariate Data Analysis" by Dr. Eman Ghanem from Sigma Xi, Science Hall, Room 004

4:00 PM - 5:00 PM - Undergraduate Ice Cream Social, ($5), Grace Plaza

5:00 PM - 6:00 PM - Keynote Lecture by Dr. Ronald Breslow from Columbia University, Hayes Auditorium

6:00 PM - 7:00 PM - 125th Anniversary Cocktail Hour, ($25), Founder's Hall, Blue Room (2nd Floor)

7:00 PM - 10:00 PM - 125th Anniversary Dinner, ($75), Founder's Hall, Smith Hall (2nd Floor)

Sunday, June 12th:

11:00 AM- 1:00 PM - Meeting with Board of MARM 2017, Hudson Heights

Green Chemistry Training for High School Teachers: Pollution Prevention in New York City Schools

American Chemical Society of New York's Green Chemistry Training for High School Teachers: Pollution Prevention in New York City Schools initiative was awarded one of the 2015-2016 New York State Pollution Prevention Institute's (NYSP2I) Community Grants.

NYACS teamed up with Beyond Benign, a national non-profit organization dedicated to green chemistry education. Co-founded by Dr. John Warner, a founder of the field of green chemistry. Beyond Benign has led the charge, nationally, on green chemistry in education through their many green chemistry training workshops to high school teachers. The initiative will reduce hazardous chemical use in classrooms by training and providing high school teachers with resources that focus on green chemistry alternatives and concepts.

Funding provided by the NYS Pollution Prevention Institute through a grant from the NYS Department of Environmental Conservation. Any opinions, findings, conclusions or recommendations expressed are those of the author(s) and do not necessarily reflect the views of the NYS Pollution Prevention Institute or Department of Environmental Conservation.

Chemagination

For this event, high school students are asked to imagine that they are living 25 years in the future and have been invited to write an article and design the cover art for ChemMatters, an ACS magazine for high school students. The subject of the article is: “Describe a recent breakthrough or innovation in chemistry that has improved the quality of people’s lives today." The article must cover a topic related to the categories of Alternative Energy, Environment, Medicine/Health, or New Materials.

The 2016 Mid-Atlantic Regional Chemagination Competition will be held Saturday, June 11 from 12:00 pm to 5:00 pm. The student teams representing ACS Local Sections from the region must display the science behind their article on a poster and demonstrate their knowledge of the topic in interviews with judges.

2016 MARM Chemagination Competition

Saturday, June 11

Peter Jay Sharp Athletic and Recreation Center, Old Gym

Set-Up & Lunch:	12:00 pm 1:00 pm
Competition & Judging:	1:00 pm - 2:55 pm
Chemistry Presentation	3:00 pm - 4:00 pm
Awards Presentation	4:00 pm - 5:00 pm

Sponsored by the Mid-Atlantic Regional Meeting
Executive Board of the American Chemical Society

Co-Chairs, Barbara Hillery and Louise Lawter
Louise Lawter, louise.lawter@gmail.com.
Barbara Hillery, hilleryb@oldwestbury.edu.

MARM 2016 PROGRAM

P. Svoronos and S. Wei*, Program Chairs*

THURSDAY AFTERNOON

College of Mount Saint Vincent
306, Founder's Hall

Clinical Diagnostics

P. W. Dillon, *Organizer, Presiding*

1:00 1. Clinical diagnostics: An overview. **P.W. Dillon**

1:30 2. Immunoassays in clinical diagnostics: The good, the bad, and the ugly. **J. Hayden**

2:00 3. Harmonization of vitamin D results. **N. Parker**

2:30 4. Effects of overhanging analyte oligo tails in model DNA and morpholino arrays. **U. Koniges**, R. Levicky

3:00 Intermission.

3:15 5. Methods for characterization of hyaluronan from biological samples. **H. Yuan**, R. Amin, X. Ye, C. de la Motte, M.K. Cowman

3:45 6. Label-free bio-sensing based on whispering gallery modes that beat the surface plasmon resonance (SPR) approach in sensitivity, analyticity, and multiplexing. **S. Arnold**

4:15 7. Biochemical characterization of platelet-rich plasma (PRP). **D.M. Ferreira**, J.A. Rocha Filho, E.R. Figueira

4:45 Concluding Remarks.

College of Mount Saint Vincent
304, Founder's Hall

Crystal Engineering & Mechanisms of Crystallization

Cosponsored by PHYS‡
D. Musumeci, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 8. Exploring new regions of polymorphic space through polymer-induced heteronucleation. **V. López-Mejías**

1:35 9. Stopping crystal growth in its tracks: Pathways to therapies for pathological crystallization. **M.D. Ward**, L. Poloni, A. Shtukenberg, B.E. Kahr

2:05 10. Helicoidal dichroism. **B.E. Kahr**, A. Shtukenberg, X. Cui, S. Nichols

2:35 Intermission.

2:50 11. Solid phase transformation during pharmaceutical processing. **L. Zhu**

3:20 12. Precipitation-based microparticle synthesis in continuous-flow microfluidic platforms: design and application. **G. Kumi**, A. Obaid, J. Anstice, S. Belh

3:50 Concluding Remarks.

College of Mount Saint Vincent
303, Founder's Hall

Lithium Ion Batteries

P. Sideris, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 13. Imidazolium-based ionic liquids for the ionothermal synthesis of $LiFePO_4$. **P. Sideris**

1:25 14. ^{7}Li and ^{31}P nuclear magnetic resonance studies of single crystal LiMPO4 and $LiM_1M'_{1-x}PO_4$ (M = Mn, M'=Fe, x=0.5). **L. Cirrincione**, P. Stallworth, S. Greenbaum

1:45 15. Natural abundance ^{17}O, ^{23}Na and diffusion NMR studies in carbonate-based electrolytes. **J. Peng**, **S. Munoz**, **M. Gobet**, **S. Greenbaum**, **K. Xu**, **A. Cresce**, **S. Russell**

2:05 16. Synthesis of copper birnessite, Cu_xMnO_y nH_2O with crystallite size control: Impact of crystallite size on electrochemistry. **Y. Li**, A.C. Marschilok, E.S. Takeuchi, K.J. Takeuchi

2:25 Intermission.

2:35 17. The electrochemistry of the Li/$CuFe_2O_4$ system: An x-ray absorption spectroscopy study. **C. Cama**, C. Pelliccione, A.C. Marschilok, E.S. Takeuchi, K.J. Takeuchi

2:55 18. NMR studies of ion transport in ultra-concentrated aqueous lithium electrolytes. J. Peng, K. Xu, C. Wang, L. Suo, M. Gobet, **S.A. Munoz**, S. Greenbaum

3:15 19. Characterizing dendrite growth in lithium batteries using *in situ* MRI. **A. Ilott**, H. Chang, M. Mohammadi, N.M. Trease, C. Grey, A. Jerschow

3:35 20. Silicon-based anodes for lithium-ion batteries. **T. Jiang**, M. Whittingham

3:55 Concluding Remarks.

FRIDAY MORNING

College of Mount Saint Vincent
309, Founder's Hall

Analytical Chemistry & Toxicology

Financially supported by SCIEX, Waters
M. Concheiro-Guisan, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 21. Oral fluid drug testing: A new look at applications, advantages, and methods. **R. Stripp**

9:40 Discussion.

9:45 22. Quantitative analysis of licit & illicit drugs in river & wastewater samples. **M. Concheiro-Guisan**, A. Jacox, J. Wetzel, S. Cheng

10:15 Discussion.

10:20 23. Application of microextraction to forensic toxicology analysis. **Y. He**

10:50 Discussion.

10:55 Intermission.

11:10 24. Use of LCMS in the pain management toxicology laboratory. **G. Milman**

11:40 Discussion.

11:45 25. Novel workflows using a Q-Tof MS for targeted and non-targeted applications for forensic toxicology. **C. Schwarz**

12:15 Discussion.

12:20 26. Application of liquid chromatography high-resolution mass spectrometry for comprehensive screening and unknown drug identification in subjects at an electronic dance music festival event. **M. Friscia**, M.L. Mohr, B.K. Logan

12:50 Discussion.

12:55 Concluding Remarks.

College of Mount Saint Vincent
304, Founder's Hall

Chemical Education

Traditional & Online

Financially supported by McGraw Hill
G. Subramaniam, *Organizer*
K. Kolack, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 27. Strategies and best practices for online teaching success. **D.P. Brown**

9:25 28. Development of a high school chemistry MOOC (massively open online course). **R.M. Savizky**

9:45 29. Investigating conceptual change in active learning environments for large enrollment chemistry courses. **G.T. Rushton**, M. Siepsiak

10:05 Intermission.

10:15 30. Technology and chemistry education. **L.C. McCann**

10:35 31. It takes a village to develop good lessons: Leaning on the interactive online network of inorganic chemists (IONiC). **F. Barrios-Landeros**

10:55 32. Creating gateway chemistry courses for at-risk students. **C.M. Evans**

11:15 Concluding Remarks.

College of Mount Saint Vincent
409, Founder's Hall

Computational/Physical Chemistry

Excited-State Materials: Perspectives from Theory & Experiment

Cosponsored by COMP, INOR and PHYS‡
Y. Small, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 33. Superconducting carbon in two dimensions. **E.R. Margine**

9:35 34. Multiple exciton generation in isolated organic molecules. **M. Sfeir**

10:05 35. Analysis of electronic couplings in photosynthetic proteins. **D. Kosenkov**, Y. Kholod

10:35 Intermission.

10:50 36. Gold nanorods and lanthanides fluoride nanocrystal assembly for enhancement of light upconversion efficiency. **D. Nykypanchuk**

11:20 37. Divide and conquer the electronic structure of condensed phases: Ground states and dynamics in real and imaginary time. **M. Pavanello**

11:50 Concluding Remarks.

College of Mount Saint Vincent
404, Founder's Hall

Drug Analysis

Z. Dai, *Organizer, Presiding*

9:00 Introductory Remarks.

9:03 38. Development and implementation of innovative high-throughput screening and analysis solutions to support discovery and development of APIs in the pharmaceutical industry. **R.M. Helmy**

9:43 39. History and nomenclature of synthetic cathinones and cannabinoids. **A. DeArmas**

10:23 40. Utilization of commercially available MIPs for illicit drugs analysis. **E.E. Mojica**

10:38 Intermission.

10:48 41. Analysis and characterization of drugs used as a preservation solution in bags of red cell concentrates. **D.M. Ferreira**, J.A. Rocha Filho, E.R. Figueira

11:18 42. Definitive metabolite identification coupled with automated ligand identification system (ALIS) technology: A novel approach to uncover structure-activity relationships and guide drug design in a factor IXa inhibitor program. **Y. Liu**

11:58 43. Analysis of synthetic cathinones and cannabimimetic agents. **M. White**

12:38 44. Detecting 1,4-butanediol in drinks. M. Nazarouk, **Z. Dai**

College of Mount Saint Vincent
302, Founder's Hall

Energy for a Sustainable Future

Financially supported by Shimadzu, Bio-Logic USA, LLC
L. M. Pratt, *Organizer*
M. Vittadello, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 45. Hidden in plain sight: Using the geometric constraints on cell geometry to exploit specific and general chemical functionality. **D. Steingart**

9:35 46. Battery material characterization as a bridge from fundamentals to applications. **J. Gallaway**

10:05 47. A key concept in magnesium secondary battery electrolytes. **M. Vittadello**, F. Bertasi, C. Hettige, F. Sepehr, X. Bogle, G. Pagot, K. Vezzù, E. Negro, S.J. Paddison, S. Greenbaum, V. Di Noto

10:35 48. Computational studies of electrochemical hotspots and ultrathin films of yttrium-doped barium zirconate. **A. Bongiorno**

11:05 Intermission.

11:15 49. Electrochemical H_2 evolution on crystalline Ni3P and its and its structural activity correlation to a series of nickel phosphide catalysts. **A.B. Laursen**, M.J. Whitaker, R.B. Wexler, E. Izett, B. Liu, A.M. Rappe, M.K. Greenblatt, G.C. Dismukes

11:45 50. High pressure NMR diffusion studies on sPEEK membranes with an organically modified titania nanofiller. C. de Bonis, C. Simari, V. Kosma, B. Mecheri, A. D'Epifanio, V. Allodi, G. Mariotto, S. Brutti, S. Suarez, **K. Pilar**, S. Greenbaum, S. Licoccia, I. Nicotera

12:15 51. Advancing knowledge of f-element separation science to close the nuclear fuel cycle. **K.L. Nash**

College of Mount Saint Vincent
310, Founder's Hall

Entrepreneur's Toolkit: Resources & True Stories

Cosponsored by SCHB‡
M. Chorghade, D. J. Deutsch, G. W. Ruger, *Organizers, Presiding*

9:00 52. Lessons learned through SCHB's Palladium Science Academy. **G.W. Ruger**

9:30 53. Entrepreneurship through STEM outreach. **C.B. Monroe**

10:00 54. Chemistry and alternative career opportunities. **C.J. Abraham**

10:30 Intermission.

11:00 55. Establishing an IP position for new life science companies. **T. Walls**

11:30 56. From dream to reality: The experiences which led to the creation of a small chemical enterprise. **L.M. Burke**

12:00 57. An entrepreneurial journey: Creating the quantified skin category. A Fitbit for your skin! **R. Mehendale**

College of Mount Saint Vincent
312, Founder's Hall

Functional Supramolecular Architectures

M. Levine, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 58. Structural analysis of extremely confined gases inside a lipophilic cage molecule. **G. El-Ayle**, K.T. Holman

9:35 59. Fine tuning dendrimers and block co-polymers for the removal of pollutants from aqueous environments. **A.M. Balija**

10:05 60. Multicomponent reactions for controlling heterofunctionality. **J.G. Rudick**

10:35 Intermission.

10:50 61. The self-assembly of periodically sequenced polypeptides confined at interfaces. **R.S. Tu**, M.L. Kubilius

11:20 62. Cyclodextrin-promoted energy transfer for non-covalent interactions and toxicant detection. **M. Levine**, D.J. DiScenza, N. Serio

College of Mount Saint Vincent
303, Founder's Hall

History of Chemistry in the New York Local Section

Cosponsored by HIST‡
J. B. Sharkey, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 63. History of Regents chemistry: An exploration of the development and impact of science education in NYS. **T. Charles**, K. Sheppard

9:35 64. Biochemistry in NY section ACS. **D.D. Clarke**

10:05 65. The Hickrill Chemical Research Foundation: A unique institution, a fascinating tale, and cutting-edge chemistry. **L. Gortler**, S.J. Weininger

10:35 66. From anonymity to Nobel recognition: Women chemists, their publications. **R. Smeltzer**

11:05 Intermission.

11:15 67. William H. Nichols entry into 19th century chemical industry. **P.W. Corfield**

11:45 68. Donald F. Othmer: His life and legacies. **R.S. Brashear**

12:15 69. A reflection on chemistry in New York over the past 125 years. **J.B. Sharkey**

College of Mount Saint Vincent
307, Founder's Hall

Microwave Chemistry: Bridging Synthetic Research & Instructional Innovation

Financially supported by Anton-Parr
A. S. Koch, S. Murphree, *Organizers*
J. H. Shin, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 70. Microwave reactors as tools in organic chemistry lab courses. **C. Kappe**

10:00 71. Necessity is the mother of invention: Development of a green undergraduate laboratory experiment demonstrating the E1 reaction utilizing a microwave reactor and resin based acid catalyst. F. Abdelnoor, Y. Fardos, M. Girges, S.K. Hussein, D. Mejia, **R.G. Aslanian**

10:30 72. Using microwave assist to stimulate a multiple component experiment to connect labs across the chemistry curriculum. **A.S. Koch**, E.H. Bresslour-Rashap, L.R. Eller, K. Neiles

11:00 Intermission.

11:15 73. Microwave-assisted esterification: A discovery-based microscale laboratory experiment. M. Reilly, R.P. King, A.J. Wagner, **S.M. King**

11:45 74. Investigations of factors controlling structures of metal-organic frameworks using microwave-assisted synthesis. **M.P. Masingale**

12:15 75. MIBLabs: A student-centered sophomore organic curriculum featuring microwave chemistry. **S. Murphree**, J.H. Shin, A.S. Koch

College of Mount Saint Vincent
308, Founder's Hall

NSF Chemistry: Funding Opportunities Symposium

Financially supported by National Science Foundation
C. Jenkins, *Organizer, Presiding*

9:15 76. National Science Foundation and broader impacts. **E. Pfeiffer**

9:45 77. Future faculty, early career faculty, and new principle investigators: Interactions with NSF chemistry. **S.L. Stoll**

10:15 Intermission.

10:30 78. NSF support for undergraduates, graduate students, and postdoctoral fellows. **M. Jenkins**

11:00 79. Faculty interactions with NSF chemistry. **L. He**

11:30 Discussion.

College of Mount Saint Vincent
306, Founder's Hall

Association for Women in Science (AWIS)

J. I. Rizzo, *Organizer, Presiding*

9:30 Introductory Remarks.

10:20 80. A personal Merck journey: Women in chemistry. **R. Ruck**

11:05 81. Promoting the growth of an inclusive and accessible STEM ecosystem: Lessons from science outreach. **J. Garbarino**

11:50 82. Notes from the presidential task force on employment: Addressing the challenges of unemployment of young graduates and mid-career chemical professionals. **P.K. Dorhout**, W.R. Ewing

College of Mount Saint Vincent
Peter Jay Sharp Athletic & Recreation Center (Gym)

General Posters

Graduate & Post-Docs

Financially supported by Rowan University, Manhattanville College, St. John's University
D. Hull, P. D. Svoronos, S. Wei, *Organizers*

10:00 - 12:00

83. Development of auto-reusable receptors for selective colorimetric recognition of fluoride. **S. Borah**, N. Gogoi

84. Analysis of conventional and organically grown strawberries for the presence of chloropicrin using GC/MS. **P. Tishion**, J.B. Soffer, K. Owens, K.K. Bagga

85. Probing inhibitor-hIAPP interactions using spectroscopic techniques: A mechanistic study. **K. Pamphille**, R. Desamero, A. Profit

86. Synthesis and characterization of CO_2 chemisorption sites in silica-based xerogels. **R. Neuweiler**

87. Determining conformation of engineered protein fibers. **C. Liu**, L. Hill, T. Jihad, S. Vawda, J.K. Montclare

88. Studying the aggregation of $hIAPP_{12-18}$ using spectroscopic and microscopic techniques. **G. Arias De la Rosa**, V. Felsen, K. Sinclair, H. Roshid, J. Tolentino, A. Profit, R. Desamero

89. Investigation of reagents for the synthesis of pentafluoro-gem-diols from perfluoropropenolates. **Q. Tran**, R. Hazlitt, D.A. Colby

90. Substitution of solvent-exposed phenylalanines to improve the stability and function of phosphotriesterase. **R. Barak Ventura**, A. Olsen, C. Yang, L. Yin, L. Halvorsen, R. Bonneau, J.K. Montclare

91. A chlorin platform for bio-medical applications. **N. Bhupathiraju**, W. Perea, H. Chu, V. Bueno, J. Gonzales, M. Yuen, W. Rizvi, N.L. Greenbaum, C.M. Drain

92. Enzymatic treatment of pyrrole and indole with soybean peroxidase (SBP). **N. Mashhadi**, K.E. Taylor, N. Biswas

93. Degradation of textile azo-dyes using enzymatic treatment with soybean peroxidase. **L.G. Cordova Villegas**, N. Biswas, K.E. Taylor

94. Design, synthesis and pharmacological evaluation of 1,3,6-trisubstituted-4-oxo-1,4-dihydroquinoline-2-carboxylic acid derivatives as selective ET_A antagonists. **N. Khadtare**, R. Stephani, V.L. Korlipara

95. Comparative studies of porphyrin C3-galactose and porphyrin C1-galactose conjugates for enhanced photodynamic therapy. **P. Pereira**, N. Bhupathiraju, W. Rizvi, R. Fernandes, J. Tomé, C.M. Drain

96. Comparative study of ether-based electrolytes for application in lithium-sulfur battery. **L. Carbone**, M. Gobet, J. Peng, M. Devany, B. Scrosati, J. Hassoun, S. Greenbaum

97. Engineered protein-based delivery of dipyridamole for the treatment of bone fracture. **A.S. Agustinus**, L. Yin, N. Schnabel, L. Witek, P. Coelho, J.K. Montclare

98. Flame retardants: New approaches to reduce exposure. **C.P. Zane**, M. Pasquinelli, N.R. Vinueza, D. Hinks, Y. Chen, N. Zhang, E. Yildirim, A. Tonelli

99. Study of chemical composition and prospecting anticholinesterase of volatile oils at *Corymbia citriodora* and *Vitex agnus castus*. **R.B. Brito Oliveira**, J. França Orlanda

100. Mechanism of diastereoselective encapsulation of tartaric acid by arylamide foldamers: A computational investigation. **M. Wujcik**, Z. Liu, V. Pophristic

101. Novel approach for the direct synthesis of nitriles from aldehydes in ionic liquids. **D.J. Quinn**, G. Haun, G. Moura-Letts

102. Semi-synthesis of a novel library of alkaloids as potential selective analgesics. **B. Gallagher**, **N. Chang**, J. Lizza, L. Filardi, A. Anthony, B. Selover, G. Moura-Letts

103. β-Galactosidase langmuir monolayer at air/subphase interface. **S.K. Sharma**, R.M. Leblanc

104. Chemical modification and biological testing of fellutamide B, a natural peptide-based proteasome inhibitor. **N. Acharekar**, L. Barasa, **S. Yoganathan**

105. Cell sensitivity and recombination repair of interstrand crosslinks in yeast strains with nonfunctional repair genes. **M. Lin**, W. Saffran

106. Evaluation of herbitóxica activity of essential oil *Corymbia citriodora* on the germination of *Allium fistulosum* and *Lactuca sativa*. **J.A. Alves**, J. França Orlanda, R.B. Brito Oliveira

107. Study of the acid-base properties of metal oxides absorbed into nanoporous silica matrices. **G.D. Ibarrola**, H.D. Gafney

108. Stepwise detection of antigens using aptamer triggered DNAzyme signal amplification. **T. Li**, J. Fu

109. Water and pH dependency of the emissivity of tungsten oxide in porous vycor glass. **D. Okamoto**, H.D. Gafney

110. Modulation of PEA-15 binding specificity by phosphorylation and possible roles of charge-triad residues in mediating conformational changes. **V. Leon**, **C. Wright**, Y. Wei

111. Spectrophotometric analysis of antioxidant activity in organic versus conventional berries. **V. Pinheiro**, K.K. Bagga

112. Surface functionalized metal-oxo polymer nanobeads as potential T_1 MRI contrast agents with dual reporting capability. **V. Dahanayake**, S.L. Stoll

113. Development of novel substrate inhibitors of bacterial phospholipid biosynthesis as new antibacterial agents. **P. Saklani**, D.P. Brown

114. Modulation of PEA-15 binding specificity by phosphorylation and possible roles of charge-triad residues in mediating conformational changes. **V. Leon**, **C. Wright**, Y. Wei

115. The counterion's role in supramolecular self-assembly. **S.J. Belh**, A. Manandhar, G. Huffman, K. Ng, A. Chowdhury, M. Patel, N. Yehya, A. des Georges, S. Loverde, D.M. Eisele

116. The structure and function of porphyrins in energy transduction: Electrochemical, optical, and quantum mechanical studies of the electronic structure of magnesium porphyrins. **G.G. Theophall**, K. Lakshmi, Y. Sun, S. Zhang

117. Streamlining the chemical synthesis of novel quorum sensing inhibitors and studies of their biological activity. **J. Capilato**, L.J. Perez

118. Copper-promoted aromatic acyloxylation: Formation of aryl esters from aryl halides using copper(II) complexes. **A. Goldstein**, F. Barrios-Landeros, S.E. Kohane

119. Scanning probe forces by rings of charge in electrolytes. **F. Zypman**

120. The harbor survey program of New York City's Division of Environmental Protection: A case study. **M. Anaya**, F. Jacques, P. Meleties, P.D. Svoronos

121. New York City's waste water and sewage treatment by the Environmental Protection Agency. **H. Shin**, E. Shin, F. Jacques, J. Villacis, P. Meleties, P.D. Svoronos

122. Synthesis and characterization of $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ ($0 \leq x \leq 1$) lithium-ion conductors. **Y. Chen**, S. Greenbaum, P. Sideris

123. Oxidative ionization under helium-plasma ionization (HePI) mass spectrometric conditions. **I. Hassan**, J. Pavlov, A.B. Attygalle

124. Role of nucleation mechanism on the size dependent morphology of organic aerosol. **M.B. Altaf**, A. Zuend, M. Freedman

125. Application of multidimensional time model for probability cumulative function to Brownian motion on fractals in chemical reactions. **M. Fundator**

126. Biochemical characterization of hemorrhagic shock after transfusion of red blood cells. D.M. Ferreira, **J.A. Rocha Filho**, **E.R. Figueira**

127. A synthetic analogue of a metallo-β-lactamase and structural characterization of a β-lactam adduct. G. Parkin, **S. Ruccolo**

128. Lanthanide complexes with fluorinated selenolate ligands: Synthesis, structure, and NIR emission. **W. Wu**, A. Kornienko, A. Kumar, T. Emge, J. Brennan

129. Fundamental understanding of binuclear alkyl hydrides of chromium and their reaction with hydrocarbons. **Y. Hung**, K.H. Theopold, G.P. Yap

130. Ligand-substituted Mn_{12} single-molecule magnet derivatives: Characterization and surface organization. **N.M. Khatri**, M.P. Lansigan, K.D. Pires, J.A. Borchers, P. Butler, D. Keavney, S.E. Lofland, K. Plass, S.L. Stoll

131. Reactivity of alkyl/aryl hydride chromium complexes supported by redox non-innocent α-diimine ligand. **L. Wang**

132. New frontiers for synthetic metalloenzymes: Imprinted nanogels with phosphatase-like activity. **M. Chernobryva**, A. Jorge, M. Resmini, M. Watkinson

133. Magnetic and electronic studies on magnetic semiconductor solid solutions. **H.A. Dalafu**, S.L. Stoll

College of Mount Saint Vincent
314, Founder's Hall

Molecular Electronics

G. M. Florio, *Organizer*
S. Wei, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 134. Impact of the diversity of single molecule junction structure on conductance and link bonds. **M.S. Hybertsen**

10:45 135. Charge transport through single molecules. **E. Borguet**

11:25 Intermission.

11:40 136. Junction conductance of fluorene molecular wires. **G.M. Florio**, S. Wei, Y. Jiang, J.M. Snaider, R. Amell

12:10 137. Bandgap engineering through controlled oxidation of polythiophene. **S. Wei**, L.M. Campos

12:40 Concluding Remarks.

College of Mount Saint Vincent
406, Founder's Hall

Nucleic Acid Chemistry

S. Zhang, *Organizer, Presiding*

10:00 138. Effect of intercalator substituent and nucleotide sequence on the stability of DNA- and RNA-naphthalimide complexes. **B. Znosko**

10:30 139. Structural and functional diversity of RNA induced by 2'-5' backbone linkages. F. Shen, R. Wang, P. Haruehanroengra, O. Levchenko, **J. Sheng**

11:00 140. Finding the environmental footprints on our genetic materials. **S. Zhang**

11:30 Concluding Remarks.

FRIDAY AFTERNOON

College of Mount Saint Vincent
307, Founder's Hall

Biospectroscopy

E. Chang, *Organizer, Presiding*

1:00 141. Conformational consequences and structural details of the self-assembly of $hIAPP_{22-29}$ and $hIAPP_{20-29}$. **J. Vedad**, R. Desamero, A. Profit

1:30 142. Correlation between membrane binding and disruption by the antimicrobial peptide Maximin 3. P. Lebron, S. Bergstresser, **E.R. Middleton**

2:15 143. The effect of N-terminal and indole amine protonation state on aromaticity and tryptophan quantum yield. A. Eisenberg, **L.J. Juszczak**

3:00 Intermission.

3:15 144. Phosphorylation study of HIV regulatory proteins using mass spectrometry. **P.N. Rathod**, H. Ho, A. Nazir, E. Nnaji, A. Chen, M. Kaur, K. Murtozaeva, L. Anti, K. Mark, X. Yu, M. Lichterfeld, E. Chang

3:45 145. ^{13}C, ^{2}H NMR studies of structural and dynamical alterations of glucose-exposed porcine aortic elastin. M. Silverstein, K. Bilici, S.W. Morgan, Y. Wang, Y. Zhang, **G. Boutis**

College of Mount Saint Vincent
304, Founder's Hall

Chemical Education

Traditional & Online

Financially supported by McGraw Hill
K. Kolack, *Organizer*
G. Subramaniam, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 146. You can have a rewarding career as an adjunct professor with the help of online media. **M.J. Castaldi**, **J.K. Murray**, Y. Badiei, J. Zhang

1:25 147. Creative design of the textbook for today's students. **J.S. Overby**

1:45 148. A student-centered approach to materials science and nanotechnology for high school students. **L.A. Avila**

2:05 Intermission.

2:15 149. Assessing the teaching and learning experience between hybrid and traditional coursework. **K.A. Baessler**

2:35 150. New chemistry experiment: Implementation of a partially online chemistry course for allied health majors at Queensborough Community College. **K. Kolack**

2:55 151. Teaching chemistry to undergraduates at the community college level: Preparing the student for the transferring process and beyond. **P.D. Svoronos**

3:15 152. Bridging low- and high-stakes in writing: Intensive chemistry and the arts. **D.A. Bruzewicz**

3:35 Concluding Remarks.

College of Mount Saint Vincent
406, Founder's Hall

Chemistry & Neutrino Physics

M. Yeh, *Organizer*
S. Hans, *Organizer, Presiding*

1:00 153. Liquid scintillator physics. **M. Yeh**

1:20 154. Neutrino detection utilizing novel metal-loaded organic and highly purified scintillators. **S.D. Rountree**

1:40 155. Cherenkov scintillation separation in liquid scintillator. **Z. Wang**

2:00 156. A sterile neutrino search in Japan using 50 tons of liquid scintillator. **J. Spitz**

2:20 157. Water-based liquid scintillator performance. **L.J. Bignell**, S. Hans, D. Jaffe, R. Rosero, E. Worcester, M. Yeh, C. Zhang

2:35 Intermission.

3:35 158. ICP MS measurements of low-level radioactivity in solid materials to be used in neutrino experiments. **M. di Vacri**, S. Nisi

3:55 159. Gadolinium-doped scintillator for reactor neutrino and dark matter search. **S. Hans**

4:10 160. Lithium-doped liquid scintillator for shore baseline antineutrino experiments. **R. Rosero**, M. Yeh, S. Hans, C. Camilo, R. Diaz Perez, A. Harris

4:25 161. Gadolinium-doped water-based liquid scintillator. **C. Camilo**, S. Hans, R. Rosero, M. Yeh, R. Diaz Perez

4:40 162. Tellurium-doped liquid scintillator for double beta decay experiments. **R. Diaz Perez**, R. Rosero, C. Camilo, S. Hans, M. Yeh

4:55 Concluding Remarks.

College of Mount Saint Vincent
314, Founder's Hall

Chemistry & the Arts

Cosponsored by CHED‡
T. Hemraj-Benny, *Organizer*
S. Karimi, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 163. Engaging students with chemistry and art hands-on activities in a large enrollment course for non-science majors. **A.C. Gaquere-Parker**

1:35 164. Inquiry at the intersection of chemistry and art. **M. Haaf**

2:05 165. Using different computational and experimental spectroscopies to demonstrate phosphate and metal interaction at different pHs. **R. Azad**

2:35 166. Non-destructive analysis of pigments on cultural heritage objects. **R.R. Hark**

3:05 Intermission.

3:20 167. Characterization of the binding medium used in Roman encaustic paintings on wall and wood. **R.M. Savizky**, J. Cuni, P. Cuni, B. Eisen, J.L. Bove

3:50 168. Synthesis of historical organic pigments: The challenge and opportunity of the nearly forgotten. **J.F. Lomax**, T.J. Moore, S.Q. Lomax

4:20 169. Pigments in antiquity: A window on a long-lost world. **M. Orna**

4:50 Concluding Remarks.

College of Mount Saint Vincent
409, Founder's Hall

Computational/Physical Chemistry

Quantum Chemical Methods for Excited-State Systems

Cosponsored by COMP, INOR and PHYS‡
Y. Small, *Organizer*
E. G. Hohenstein, *Presiding*

1:00 Introductory Remarks.

1:05 170. Configuration interaction energy between lowest pair of excited states in the circular ring model of porphyrin: Experimentally determined in metmyoglobin. **A.S. Brill**, M.L. Carlson

1:35 171. A revolutionary idea in context of x-ray quantum crystallography (QCr) and the kernel energy method (KEM). **L. Massa**, W. Polkosnik, C. Matta, L. Huang

2:05 172. Mechanisms of the lignin monomers pyrolysis: Cinnamyl alcohol. **R. Asatryan**, M. Pechagin, M. Xu, L. Khachatryan

2:35 173. Multiconfigurational quantum chemistry on graphical processing units. **E.G. Hohenstein**

3:05 Concluding Remarks.

College of Mount Saint Vincent
310, Founder's Hall

Environmental Remediation: Methods & Applications

Cosponsored by I&EC‡
S. Alexandratos, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 174. Chitin-based sorbents for mining metals from oceans: A sustainable alternative to terrestrial mining. **R.D. Rogers**, P. Berton

1:35 175. Global freshwater systems at risk: Challenges and remediation. **H.L. Taft**

2:05 176. Tailoring the surface of solid wastes for their application as adsorbents of antibiotics. **A. Navarro**, J. Silva, L. Morante, B. Llanos

2:35 Intermission.

2:45 177. Environmental remediation with polymer-supported reagents: Application to the complexing of uranium from acid mine drainage and wet process phosphoric acid. **S. Alexandratos**, X. Zhu

3:15 178. A simple extraction method for detecting the fecal indicative bacteria in urban soil. **L. Pardo**, A. Alcantara , R.K. Dhar

3:45 179. Black sand as mineral-based photocatalyst for hydrogen production under UV-Vis irradiation. **A.F. Lopez Vasquez**, G. Reyes Gomez, R. López Vásquez

College of Mount Saint Vincent
312, Founder's Hall

Functional Supramolecular Architectures

M. Levine, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 180. Dissecting electrostatic contributions to folding and self-assembly using designed multicomponent peptide systems. **V. Nanda**, A. Parmar, J. James, D. Grisham, D. Pike

1:35 181. Supramolecular block copolymers. **M. Weck**, E. Elacqua, A. Croom, K. Manning

2:05 182. Nanoscale building blocks in solid-state chemistry. **X. Roy**

2:35 Intermission.

2:55 183. Pattern formation of confined periodically sequenced polypeptides. **R.S. Tu**

3:25 184. Synthesis and characterization of poly(iodoethynyliododiacetylene) (PIEDA). **M. Freitag**, R. DeCicco, G.P. Halada, C. Young, N.S. Goroff

3:55 Concluding Remarks.

College of Mount Saint Vincent
306, Founder's Hall

Green Chemistry

R. K. Upmacis, *Organizer, Presiding*

1:00 Introductory Remarks.

1:35 185. Green chemistry outreach: Spreading science education to the national level. **G.W. Ruger**, J.R. Berk

2:00 186. An overview of biosourced and biodegradable polymeric materials: Current commercial uses and challenges for more widespread adoption. **K. Aubrecht**

2:25 187. Novel liquid-like nanoparticle organic hybrid materials with tunable chemical and structural properties for combined CO_2 capture and conversion. M. Gao, **A.A. Park**

2:50 Intermission.

3:00 188. Sustainable organocatalysis for one-pot asymmetric synthesis. **W. Zhang**

3:25 189. A mild Cu-catalyzed oxidative aromatization of indolines to indoles. **F. Peng**

3:50 190. Design and development of a greener manufacturing route for NNRTI doravirine. **Y. Cao**, D.R. Gauthier, B. Sherry

4:10 191. Towards a chemo-enzymatic synthesis of the heptapeptide antibiotic complestatin: Investigating the role of the P450 oxygenases ComI and ComJ in aryl linkage formation. **A. Mollo**

4:30 192. 3Rs in green chemistry: Resources, recycling, and responsibility. **A.E. Shinnar**

College of Mount Saint Vincent
303, Founder's Hall

Polymer Chemistry

Undergraduate Research & Teaching

R. P. D'Amelia, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 193. Synthesis and characterization of polyampholyte ionomer networks. **K.A. Cavicchi**, G. Deng

1:35 194. Factors affecting the copolymerization of α-olefin and maleic anhydride in dual solvent system. C. Tabasko, J. Arroyave, R. Sharma, **H. Kim**

2:05 Intermission.

2:20 195. Morphology of carbon nanofilled polymers. **R.E. Rivas-Sanz**, C. Seaks, V. Flaris

2:50 196. Preparation and characterization of coatings with tung-oil-based reactive diluents and linseed oil alkyd. **S. Basan**, R. Xiaofeng, P. P. Nalawade, M.D. Soucek

3:20 197. Ring-opening polymerization of ε-thionocaprolactone. **P. Datta**

3:50 Concluding Remarks.

College of Mount Saint Vincent
402, Founder's Hall

Protein Structure & Design

G. A. Caputo, *Organizer, Presiding*

1:00 198. Protein structure analysis of gonococcal cell surface protein antibody binding domains using a molecular model approach. **Y.S. Ting**

1:20 199. Detergent mediated unfolding of proteins in the presence of ionic liquids. L. Abiuso, E. Kohn, T.D. Vaden, **G.A. Caputo**

1:40 200. A retrospective and prospective view of iron-sulfur protein design. **B.R. Gibney**

2:00 Intermission.

2:15 201. Assemblies of macrocyclic peptides as functional catalysts. **Z. Lengyel**, I. Korendovych

2:35 202. Adventures in supercharging. J. Brisendine, P. Schnatz, **R.L. Koder**

2:55 203. Neutral model of subcellular pH constraints on proteome-wide isoelectric point distributions. **V. Nanda**, K. Loell

College of Mount Saint Vincent
415, Founder's Hall

Research & Education in Nuclear Magnetic Resonance & Mass Spectrometry

Financially supported by Bruker
D. S. Rovnyak, M. A. Tapsak, *Organizers*
D. E. Mencer, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 204. Educational applications of Thermo Fisher Scientific picoSpin instrumentation for NMR spectroscopy. **D. Frasco**

1:35 205. Implementation of C-13 and 2-D NMR in organic laboratory sequence. **A.J. Kiessling**

2:05 206. Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: an active-learning approach. **J. Araneda**, **S. Riegel**

2:35 207. What we discovered from providing undergraduates with high-field NMR. **S.M. Schelble**

3:05 Intermission.

3:20 208. Determination of active ingredients in analgesic drugs by thin-layer chromatography coupled with compact mass spectrometry (TLC-CMS). **C. Hao**, N. Sousou, S. Prosser, J.D. Henion

3:50 209. Resveratrol and piceid production and storage by Japanese knotweed. M. Yatison, J. Luchetta, A. Mikolon, D. Pupaza, K. Klemow, **D.E. Mencer**, W. Terzaghi

4:20 210. Nuclear magnetic resonance studies of polycarbonate films for high power thin film capacitors. **S. Lai**, D.A. Boyles, J. Fontanella, S. Greenbaum

4:50 Concluding Remarks.

College of Mount Saint Vincent
302, Founder's Hall

Energy for a Sustainable Future

Financially supported by Shimadzu, Bio-Logic USA, LLC
M. Vittadello, *Organizer*
L. M. Pratt, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 211. Fluorinated porphyrinoids as efficient platforms for new photonic materials. N. Bhupathiraju, W. Rizvi, J.D. Batteas, **C.M. Drain**

2:05 212. Light management in thin-film organic optoelectronic devices for energy efficiency and energy harvesting applications. **D. O'Carroll**

2:35 213. Fuels of the future: Using diatoms as a platform for renewable energy. **O. Levitan**

3:05 214. Enhanced gas recovery: Density functional theory computation of adsorption of CO_2, CH_4, and H_2O to shale surfaces. **L. Tribe**

3:35 Intermission.

3:45 215. Trash to treasure: Biowaste-to-energy as next fuel source. **Y. Hangun-Balkir**

4:15 216. Brown grease pyrolysis mechanism. **D. Saint Hilaire**

4:45 217. Value-added products from pyrolysis of sludges from pork production. **L.M. Pratt**, M. Vitadello, S. Groveman, D. Pham, V. Luong, N. Ngoc, P. Kim, T. Pham

College of Mount Saint Vincent
404, Founder's Hall

Medicinal Chemistry

D. D. Garver, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 218. MK-7655, A broad-spectrum β-lactamase inhibitor for combination with the carbapenem antibiotic Primaxin®: A Merck drug discovery story spanning 30 years. **H.Y. Chen**, T.A. Blizzard, J. Imbriglio, K. Young

2:05 219. Ion-charged polymers' effect on bacterial growth. **R.C. Josman**

2:35 220. Synthesis and antimicrobial activity of fullerenol and fullerenemalonic acid. **A. Pitchford**, D.D. Garver

3:05 Intermission.

3:15 221. Modeling cell permeation and proteolytic cleavage of peptides. **A.S. Bayden**, J. Audie, J. Swanson, M. Jarosinski, D.J. Diller

3:45 222. Ancient medicines wearing new disguises. **K.S. Raja**

4:15 223. Enabling capabilities in drug discovery. **P. Vachal**

College of Mount Saint Vincent
309, Founder's Hall

Analytical Chemistry & Toxicology

Financially supported by SCIEX, Waters
M. Concheiro-Guisan, *Organizer, Presiding*

2:30 Introductory Remarks.

2:35 224. Assessing ligand-induced GPCR cell signaling with dissipation monitoring of the QCM-D. **J.Y. Chen**, L.S. Penn, J. Xi

2:50 Discussion.

2:55 225. Determination of the electrochemical parameters of ferrocene in nanoemulsion. **M.O. Iwunze**

3:10 Discussion.

3:15 226. Optimization of a spectrophotometric method to determine ammonia in groundwater. **K. Aslam**, H. Kaur, S. Heralall, R.K. Dhar

3:30 Discussion.

3:35 227. Particle sizes and singlet oxygen production of silica-porphyrin-liposomes. **E.N. Doucet**, G. Fuentes , R. Spinelle, R. Gao

3:50 Concluding Remarks.

SATURDAY MORNING

College of Mount Saint Vincent
302, Founder's Hall

Biotechnology

N. Gadura, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 228. Thyroid hormone transport in the cardiac myocyte. **S. Danzi Engoron**

9:35 Discussion.

9:45 229. Neurons of the barrel cortex and their connections: A quantitative morphological analysis. **A. Tsimounis**, M. Anaya, S. Sosnowik, C.H. Tse, J. Brumberg

10:15 Discussion.

10:25 230. *Hydra* polycystins exhibit specific expression patterns and may regulate *Hydra* behaviors. **S. McLaughlin**

10:55 Discussion.

11:05 Intermission.

11:20 231. IL6-STAT3 and sphingosine-1-phosphate signaling in inflammation-induced colorectal tumor progression. **A.V. Nguyen**

11:50 Discussion.

12:00 232. CRISPR/Cas 9, a novel tool for site-specific gene targeting. **C. Roblodowski**

12:30 Discussion.

College of Mount Saint Vincent
309, Founder's Hall

Environmental Chemistry: Fate of Contaminants

Measurements, Predictions & Reactions in Water

U. Jans, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 233. Surface water discharges of disinfection byproducts from wastewater treatment plant effluent under wet weather conditions. **F.B. Dunn**, J. Wilson

9:35 234. Validation and verification of model predictions for chemical releases in estuaries. **J.P. Smith**, J.A. Cragan, M.C. Ward

10:05 Intermission.

10:25 235. Reaction of hexabromocyclododecane with reduced sulfur species in methanol/water solutions. **X. Zhang**, U. Jans

10:55 236. Investigating the photodegradability of personal care product ingredients for aquatic environmental fate assessment. **J. Lin**, M.E. Emberger

11:25 237. Occurrence of pyrethroid and organochlorine residues in human milk from Nadia, West Bengal, India. **N. Anand**, S. Ray

College of Mount Saint Vincent
308, Founder's Hall

Frontiers in Gel Chemistry

Cosponsored by COLL
Financially supported by Institute for Soft Matter Synthesis and Metrology (Georgetown University)
R. G. Weiss, *Organizer*
F. Horkay, B. Xu, *Presiding*

9:00 Introductory Remarks.

9:05 238. Functional π-organogelators based on T-shaped phenazines. **D. Lee**

9:35 239. Mechanogelation of fuel mixtures with a bioderived small molecule gellant. **J.R. Silverman**

10:05 240. Synthesis and characterization of carbohydrate-based small molecular organogelators and hydrogelators. **G. Wang**, A. Chen, I. Okafor, H. Mangunuru

10:35 Intermission.

10:50 241. At the intersection of low molecular mass organogelators and polymers. **K.A. Cavicchi**

11:20 242. Understanding molecular nuances of self-assembly of sorbitol-based molecular gelators in various solvents. **M. Rogers**

11:50 243. Gels through surfactant self-assembly and through the use of the hydrophobic effect. **V.T. John**, O.G. Owoseni, R. Zheng, J.S. Arora

College of Mount Saint Vincent
Peter Jay Sharp Athletic & Recreation Center (Gym)

General Posters

Undergraduate

Financially supported by Rowan University, Manhattanville College, St. John's University
D. Hull, P. D. Svoronos, S. Wei, *Organizers*

9:00 - 11:00

244. Development of drug-like inhibitors of Nek2 kinase. **A. Finkelstein**, S. Kumar, D. Dana

245. Use of the QuEChERS approach in the extraction of pesticides from imported fresh fruits and vegetables. **B. Um**, K. Williams, M. Iorsh, P.D. Svoronos

246. Use native plants/oils to synthesize novel antimicrobial surfaces. **K. Velez**, J.I. Rizzo

247. Determining the total amount of oxygen consumption in effluent via carbonaceous biochemical oxygen demand (CBOD) and biochemical oxygen demand (BOD). **J. Leong**, F. Jacques, P. Meleties, P.D. Svoronos

248. ArcGis: Understanding city-wide infrastructural landscape and its environmental impact. **B. Um**, **H. Shin**, **E. Shin**, J. Villacis, F. Jacques, P. Meleties, P.D. Svoronos

249. Investigation of *S*-oxidation of *m*- and *p*-substituted 2-phenyl-3-aryl-1,3-thiazolidin-4-ones with Oxone®. **K.C. Cannon**, M. Costa, M. Pepper, J. Toovy

250. A new synthesis of pyrroles using the Cadogan approach. **Y. Liu**, S. Karimi, **S. Ma**, G. Subramaniam

251. Macroporous TiO_2 photoanodes for high-efficiency PSI-based biohybrid photovoltaics. **Y. Jiang**, M. Robinson, D.E. Cliffel, G. Jennings

252. Slp1 is a key component controlling early cardiogenesis in *Drosophila*. **Y. Chen**, Y. Iwasaki, J. Gergen

253. New modes of initiating cation radical cycloaddition dimerization and polymerization reactions. **E. Shin**, B.N. Barbu, E. Webb, J.G. Gillmore

254. Molecular encapsulation of sugar alcohols by arylamide foldamers: A computational chemistry study. **E.C. Fluck**, Z. Liu, V. Pophristic

255. Treatment of wastewater samples at the New York City-Department of Environmental Protection (NYC-DEP). P.D. Svoronos, **J. Hwang**, F. Jacques, P. Meleties

256. Exploring the formation of conglomerates for optical resolution. **A. Lim**, A. Gorbenko, H.S. Barcena

257. Performance of a magnetic shape memory micropump. **Y. Chen**, S. Barker, R. Urbic, P. Mullner

258. Degradation of an azo dye by single-walled carbon nanotube-ruthenium nanoparticles composites. **N.F. Tobar**, T. Hemraj-Benny

259. Synthesis of a fluorenyl quinolone molecular switch. **K. Namjouyan**

260. Synthesis and photorelease study of glycine caged bis-1,2-(4-acetylphenylethynyl)-4,5-dimethoxybenzene, first-generation dendron phototrigger. **A. Barrella**, M. Akhter, J.I. Lee

261. Aggregation propensity of (F ® L) mutants of $hIAPP_{22-29}$. **K. Sinclair**, J. Vedad, A. Profit, R. Desamero

262. Energy of the quasi-free electron in H_2, D_2 and O_2: Probing intermolecular potentials within the local Wigner-Seitz model. **K. Krynski**, Z. Streeter, C.M. Evans, G.L. Findley

263. Adenosine/guanosine preferring nucleoside ribohydrolase: From flavonoids to fragments. **S.N. Muellers**, S. Beck, A.L. Benzie, D.W. Parkin, B.J. Stockman

264. An exploration of polycarbonate-diluent systems via FFCNMR. **C. Mallia**

265. Fabrication of core-shell, transition metal nanowires as catalysts for glucose sensors. **A. Kassotis**, C. Koenigsmann

266. Determining secondary structure and binding capacity for small molecules of cartilage oligomeric matrix protein constructs for the treatment of osteoarthritis. **N. Schnabel**, L. Yin, A.S. Agustinus, T. Kirsch, T. Minashima

267. Transition metal-based, core-shell nanowire electrocatalysts for cost-effective fuel cells. **T.J. Aimola**, C. Koenigsmann

268. Methodology testing on complex substrate, ethisterone. **J. Lee**, Y. Xing

269. The purification and analysis of distinct porphyrin molecules. **S.N. Khayyo**

270. The infrared optical measurements of hyperbolic metamaterials. **C. Harris**, S. Law, D. Wei

271. Development of cathepsin S inhibitors using Ugi reaction. **A. Ashfaq**, D. Salazar, S. Kumar

272. Cytotoxic and cytostatic effects of single-walled carbon nanotubes on triple-negative breast cancer cells. **K. Hector**

273. Tracing marine particulate organic carbon from primary production to sedimentation. **R. Wenrich**, A. Leri

274. Atomic force microscopy measurements of single-walled, carbon-nanotube treated MDA-MB 468 cells. **M. Perez**

275. Reactivity of vanadium and molybdenum oxide species on oxide supports in microwave assisted gas-phase oxidation of 3-picoline. **Y. Alkayeva**, **B. Gibadullin**, A. Gabr, A. Shutilov, G. Zenkovets

276. Characterization of the putatively heterodimeric proteinaceous ichthyotoxin of *Pterois volitans*. **Z.F. Mattes**, **N.A. Le**

277. New complexes of mes-BIAN in vanadium chemistry. **N. Tsamchoe**, **G. Risica**, **N. Onishi**, C.D. Abernethy, J.D. Gorden, J. Niklas

278. Amyloid formation of hIAPP12-18. **H. Roshid**, G. Arias De la Rosa, R. Desamero

279. Characterization of antibiotics and lipid vesicles in aqueous ionic liquid solutions. **S.L. Hanna**, K. Cook, C.A. Deleon, P. Landick, C. Chrom, G.A. Caputo, T.D. Vaden

280. The determination of gallic acid present in juice and tea beverages using high-performance liquid chromatography. **M. de los Santos**, **J. Leong**, T. Xu, S. Svoronos, P.D. Svoronos

281. Determination of the total amount of antioxidants via the Folin Ciocalteau method. **J. Leong**, **M. de los Santos**, P. Irigoyen, S. Svoronos, P.D. Svoronos

282. Novel regio- and chemoselective aminolysis of epoxides with primary amines under mild conditions. **J.R. Lizza**, G. Moura-Letts

283. Synthesis of 1,3,4,5-tetrasubstituted pyrazoles from substituted hydrazines and β-ketoesters. **I. Bakanas**, G. Moura-Letts

284. Exploration of the conformational states in EMIM FSA and EMIM BF_4 ionic liquids. **M. Hamsho**, D. Cuffari, J.F. Wishart, S. Suarez

285. Synthesis and stabilization of a protein-based magnetically-functionalized biomaterial. **S. Vawda**, L. Hill, C. Liu, T. Jihad, J. Montclare

286. Preparation of porphyrin embedded liposomes for *in vitro* cellular studies. **S. Maio**, P.K. Kerrigan, D. Amarante

287. Drug-carrying protein ferrofluid for theranostic applications. **T. Jihad**, S. Vawda, C. Liu, L. Hill, J.K. Montclare

288. Identifying the product of the reaction between chromotropic acid and formaldehyde. **K.A. Leets**, K.B. Bramble, G.D. Gibbs, L. Tribe

289. Refractive index of malonic acid measured by zoom-in method. **B. Um**, J.H. Shin

290. Determination of the refractive index of benzoic acid measured by extension method. **H. Kim**, J.H. Shin

291. Thermodynamic study of esterification using a microwave reactor. **H. Yun**, E. Shin, J.H. Shin

292. Synthesis of thiol-substituted, water-soluble phthalocyanines conjugates. **C.N. Rosamilia**

293. Detection of *Salmonella* in foods via microbiological methods. **I. Sun**, A. Lara, P.D. Svoronos

294. Cleaning and protecting the municipal water via New York City's wastewater treatment system and the DEP shoreline survey unit. **I. Sun**, F. Jacques, J. Villacis, P. Meleties, P.D. Svoronos

295. Synthesis of x-shape molecules as electron acceptors in organic solar cells. F. Caban, Y. Jiang, **S. Wei**

296. Synthesis and photorelease study of glycine caged bis-1,2-(4-acetylphenylethynyl)-4,5-dimethoxybenzene, first generation dendron phototrigger. **A. Barrella**, **M. Akhter**, **J.I. Lee**

College of Mount Saint Vincent
307, Founder's Hall

Inorganic Chemistry

G. Zhang, *Organizer, Presiding*

9:00 297. Applications of tridentate and tetradentate tripodal ligands in bioinorganic and organometallic chemistry. **G. Parkin**

9:30 298. Hydrogen bonding in reverse micelle surfactants. **M.A. Walters**, Y. Chang, A.L. Rheingold

9:50 299. Mechanistic investigation of catalytic and biocatalytic iron porphyrin carbene formation. R. Khade, **Y. Zhang**

10:10 300. Enhanced stability of heterobimetallic clusters as a driving force for cofactor assembly in dinuclear metalloproteins. **W.D. Kerber**

10:30 Intermission.

10:45 301. Heterolytic C-H and N-H/O-H activation by first-row transition metal complexes. S. Chakraborty, R. Xu, P. Piszel, C. Hayes, R. Baker, S. Bellows, **W.D. Jones**

11:15 302. Carbon monoxide activation by first-row transition metal cyano carbonyls. **J. Jiang**

11:35 303. Reactivity of low-valent iron and cobalt complexes of hydrotris(pyrazolyl)borate ligands modified with ferrocenyl substituents. **D. Cummins**, G.P. Yap, K.H. Theopold

11:55 304. New mixed-valence copper cyanide polymers.. **P.W. Corfield**, A. Sabatino, E. Cleary, J. Michalski, P. Luu

12:15 305. Versatile cobalt pincer catalysts for cross coupling reactions via a “hydrogen-borrowing” strategy. **G. Zhang**

College of Mount Saint Vincent
310, Founder's Hall

Ionic Liquids

Properties & Interactions with Biopolymers

S. I. Lall-Ramnarine, J. F. Wishart, *Organizers*

M. F. Thomas, *Presiding*

9:00 Introductory Remarks.

9:10 306. Do TFSA anions slither? Pressure exposes the role of anion conformational exchange in self-diffusion. **J.F. Wishart**, S. Suarez, A. Rúa, D. Cuffari, K. Pilar, J. Hatcher, S. Ramati

9:40 307. Structure of silicon-substituted ionic liquids. **B. Wu**, E. Castner

10:10 308. Tuning the physical properties of ionic liquid mixtures. **S.I. Lall-Ramnarine**, C. Rodriguez, E. Fernandez, E. Rosario, S. Suarez, N. Zmich, S. Dhiman, J.F. Wishart

10:40 Intermission.

11:00 309. Structures and stabilities of proteins in aqueous ionic liquid solutions: Unfolding kinetics and thermodynamics studies. **T.D. Vaden**

11:30 310. Ionic liquid solutions for dissolving cellulose. **M.F. Thomas**

12:00 311. A proton-transfer reaction and an esterification reaction in ionic liquid EMIMOAc. A. Tran, A. Miller, P. Lam, D. Walczyk, J. Tomlin, T.D. Vaden, **L. Yu**

College of Mount Saint Vincent
402, Founder's Hall

Material Chemistry

S. Dehipawala, *Organizer, Presiding*

9:00 312. Photocatalyzing multi-electron, multi-proton conversions: An excited-state acid-base process. **H.D. Gafney**, E. Look, D. Okamoto

9:20 313. Synthesis and characterization of Fe doped single-phase multiferroic. **F.A. Pearsall**, S. O'Brien

9:40 314. Reactions in individual droplets on a superhydrophobic surface: Effect of convection. **Y. Liu**, X. Chen, Q. Xu, A. Greer, Y. Zhao, A.M. Lyons

10:00 315. Nanocrystalline solar oxide perovskites derived from potassium niobate $KNbO_3$ by gel collection. **J. Lombardi**, S. O'Brien

10:20 316. Identifying corrosion protection and breakdown mechanisms of corrosion preventative compounds (CPCs), and investigating new corrosion protection technologies. **M. Brindza**, Y. Han, T. Townsend, R.K. Larsen, C. Knell, D. Durastanti

10:40 317. Co(II) containing anionic clays: Structure and particularities. **M. Jitianu**, D. Akpatsu, F. Saifan, A. Patel, A. Jitianu

11:00 318. Droplet microfluidics in industry. **J. Newhouse**, **K. Cung**, C. Holtze, R. Darji, T.W. Deisenroth

11:20 319. Origins of defects in organo-halide perovskites examined by time-resolved photoluminescence spectroscopy. **R.J. Stewart**, J.B. Asbury

11:40 320. Structural properties of iron in organic vs. non-organic *Brassica oleracea*. **U. Dewanamuni**, S. Dehipawala, H.D. Gafney

12:00 321. Melting gels and their anticorrosive properties on magnesium alloy AZ31B. **A. Jitianu**, M. Aparicio, G. Rodriguez, J. Mosa, K. Al-Marzoki, L.C. Klein

12:20 322. Determination of soil pH dependence of structural properties of iron in plants. **R.A. Ranathunga**, R. Gamage, S. Dehipawala

12:40 323. Structural investigation of Nickel oxide thin films using synchrotron x-rays. **Y. Leung**, S. Dehipawala

College of Mount Saint Vincent
301, Founder's Hall

Nano-Chemistry & Technology

Cosponsored by COLL
M. Chauhan, *Organizer*
B. P. Chauhan, *Organizer, Presiding*

F. Jaekle, *Presiding*

9:00 Introductory Remarks.

9:15 324. Self-assembly with boron-containing polymers: New luminescent, sensory and stimuli-responsive materials. G. Pawar, W. Wan, P.O. Shipman, F. Cheng, J.B. Sheridan, **F. Jaekle**

9:45 325. Scattering mediated hot-electron transfer: A new paradigm for light-driven energy transfer. **J.J. Foley**

10:05 326. Crystallite size dependency of the pressure and temperature response in nanoparticles of ceria and other oxides. **P.P. Rodenbough**, S. Chan

10:25 Intermission.

10:40 327. Synthesis of polyrhodanine-supported noble metal nanoparticles and their role in catalysis. **M. Chauhan**, T. Hong, A. Patel, B.P. Chauhan

11:00 328. Dynamic peptide libraries. **H.L. Siccardi**, C. Pappas, D. Velado, R. Ulijn

11:20 329. Nanochemistry and power technology: The design of printed nanocomposite capacitors for power electronics. L. Huang, S. Liu, S. Yang, B. Van Tassell, E. Leland, D. Steingart, I.J. Kymissis, **S. O'Brien**

College of Mount Saint Vincent
314, Founder's Hall

Organic Electronics

B. Kim, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 330. Solvent effects on the crystal structure formation of perylene diimide derivative. **J.M. Szarko**, A. Austin, X. Zhu

9:35 331. Molecular helices as electron acceptors in fullerene-free organic solar cells. **Y. Zhong**, C.P. Nuckolls

10:05 332. Effect of nanoconfinement on the crystallization and stability of metal-halide perovskites. **S. Lee**, J. Feldman, S.S. Lee

10:35 Intermission.

10:50 333. Fabrication of single crystal organic field-effect transistor using hexatriacontane as a dielectric interlayer. **B. Kim**

11:20 334. Integration of high-purity carbon nanotubes into electronic devices. **G.S. Tulevski**

11:50 335. Tuning the dynamics of triplet excitons from singlet fission in functionalized pentacene films by controlling molecular order. **C. Grieco**, A. Rimshaw, J.B. Asbury

12:20 Concluding Remarks.

College of Mount Saint Vincent
306, Founder's Hall

Photocatalysis & Solar Fuel

Cosponsored by ENFL‡ and PHYS
M. Liu, *Organizer, Presiding*

9:00 336. Catalytic reduction of carbon dioxide in artificial photosynthesis. Y. Hsieh, S.D. Senanayake, M. Ertem, **D.E. Polyansky**

9:30 337. Plasmonic photocatalysts for CO_2 conversion. **C. Wang**, S. Hammache, O.K. Ranasingha, D. Kauffman, C. Matranga

10:00 338. Surface and interface properties of photoelectrocatalysts for solar fuels. **B.E. Koel**

10:30 Intermission.

11:00 339. Stabilizing electrodeposited catalytic particles on metal-insulator-semiconductor (MIS) photoelectrodes for water electrolysis. **D. Esposito**, N. Labrador

11:30 340. Photoelectrochemical water-splitting with a $SrTiO_3$:Nb / $SrTiO_3$ n^+-n homojunction structure. **Q. Wu**, **J. Cen**, J. Tao, **D. Yan**, K. Kisslinger, M. Liu, A. Orlov

12:00 341. Super-resolution imaging of single-nanorod photoelectrocatalysis. **J.B. Sambur**

12:30 342. Hydrogen production using Ag-Pd/TiO_2 bimetallic catalysts: Is there a combined effect of surface plasmon resonance with the Schottky mechanism on the photo-catalytic activity? **M. Nadeem**

College of Mount Saint Vincent
303, Founder's Hall

Polymer Chemistry

Undergraduate Research & Teaching

R. P. D'Amelia, *Organizer*
J. Krumper, *Presiding*

9:00 Introductory Remarks.

9:05 343. Quantitative analysis of blends and copolymers of polyvinyl acetate (PVAc) using Fourier transform infrared spectroscopy (FTIR) and elemental analysis (EA). **R.P. D'Amelia**, S.M. Gentile

9:35 344. Morphological studies of ring-substituted polyanilines by first and second-year undergraduates. **D.M. Sarno**, J. Hwang, D. Perry

10:05 345. Silicone chemistry in undergraduate laboratory and research courses. K. Ryan, W. Bender, T. Longenberger, A. Krumpfer, **J.W. Krumpfer**

10:35 Interrmission.

10:50 346. PUNK: An online resource for integrating polymer science into the undergraduate curriculum. K. Aubrecht, E.B. Berda, K.A. Cavicchi, P.J. Costanzo, G.J. Gabriel, C. Goh, **S.L. Goh**, S.T. Iacono, S.E. Morgan, D. Savin

11:20 347. Industrial role-playing to replace the traditional laboratory experiment: Formulating nail polish. **N. O'Connor**

11:50 Concluding Remarks.

College of Mount Saint Vincent
304, Founder's Hall

Teaching Chemistry to Students with Disabilities

P. A. Redden, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 348. Accommodating individuals with disabilities in the chemistry lab: Focus on students accompanied by service dogs. **S. Ramp**

9:45 349. Twenty-first century digital science access tools: Opening doors of opportunity for the blind to promote hands-on learning. **C.A. Supalo**

10:25 350. Preparing students with disabilities for the challenges of graduate school: Thoughts from a REU program. **K.S. Booksh**, S. Rozovsky, J.P. Smith

11:05 351. Service dogs in the academic laboratory. **P.A. Redden**

11:45 Intermission.

11:55 Panel Discussion.

12:55 Concluding Remarks.

College of Mount Saint Vincent
404, Founder's Hall

Teaching Nanoscience

Cosponsored by CHED‡
T. Hemraj-Benny, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 352. Nanoscience in the undergraduate curriculum: Introducing students to tiny miracles. **S.M. Basu**

9:35 353. Nanomaterials education for CUNY science and engineering undergraduates. **I. Kretzschmar**

10:05 354. Integrating nanotechnology in CUNY Hostos Community College: Successes and challenges. **M. Sohel**

10:35 Intermission.

10:50 355. Introduction of a nanoscience lecture and laboratory course into an undergraduate curriculum at a community college. **T. Hemraj-Benny**

11:20 356. Involving undergraduate students in nanoscience research at a community college. **T. Hemraj-Benny**

11:50 Discussion.

College of Mount Saint Vincent
317, Founder's Hall

Organic Synthesis & Catalysis

Y. Chen, *Organizer, Presiding*

9:30 Introductory Remarks.

9:35 357. Synthesis of biologically interested heterocyclic compounds. **W. Zhang**

10:15 358. Nickel-catalyzed reductive coupling of alkyl halides with other electrophiles. **H. Gong**

10:45 Intermission.

11:05 359. Dual cross-coupling involving α-amino radicals generated from organotrifluoroborates. **M. El Khatib**, G.A. Molander

11:25 360. 'All-in-one' photodynamic device: Synthesis of a poly(ethylene glycol) galloyl sensitizer tip. **A.A. Ghogare**, A. Greer

11:45 361. A facile conversion of alkynones to enaminones and its synthetic application. **Y. Chen**

College of Mount Saint Vincent
409, Founder's Hall

Computational/Physical Chemistry

Structure & Thermodynamics in Biological Systems

Cosponsored by COMP, INOR and PHYS‡
Y. Small, *Organizer, Presiding*

10:00 Introductory Remarks.

10:05 362. The role of organized water in mediating ligand-protein interactions. **J.D. Gough**

10:35 363. Multiscale simulations to characterize the blood-brain barrier tight junctions. **S. Nangia**

11:05 364. Molecular interactions of complex biological systems in rare and orphan diseases. **K. Nguyen**, L. Tian, D. Li, M. March, R. Pellegrino, C. Kao, P. Sleiman, H. Hakonarson

11:35 Intermission.

11:50 365. A grand canonical ensemble approach to solution interfaces: Inference of the concentration gradient. **M.N. Kobrak**

12:20 366. Mag-walking Monte Carlo and quantum mechanics predictions of structures and interaction energies of ammonium halide clusters. **R.Q. Topper**, J.J. Biswakarma, V. Ciocoi

12:50 367. Water in dopamine receptors: Using solvation thermodynamics to modify a lead compound for specificity. S. Gadhiya, S. Madapa, T.P. Kurtzman, I.L. Alberts, **S. Ramsey**, N. Pillarsetty, T. Kalidindi, W.W. Harding

1:20 Concluding Remarks.

College of Mount Saint Vincent
312, Founder's Hall

Radiation Photochemistry & Photophysics

G. L. Findley, *Organizer*
C. M. Evans, *Organizer, Presiding*

10:00 368. The isotropic local Wigner-Seitz model: An accurate theoretical model for the quasi-free electron energy in fluids. **C.M. Evans**, G.L. Findley

10:20 369. Conjugate chains and bimolecular electron transfer. **J.R. Miller**, A.R. Cook, M. Bird, T. Mani, R. Holroyd, A. Sadayuki, T. Iyoda

10:40 370. Obtaining redox potentials without any electrolyte by studying one electron charge transfer equilibria with pulse radiolysi. **M. Bird**, M. Pearson, J.R. Miller

11:00 Intermission.

11:15 371. Exceptionally rapid capture of radical cations formed by pulse radiolysis. **A.R. Cook**, M. Bird, J.R. Miller

11:35 372. Photochemical and pulse radiolysis studies of intermediates involved in CO_2 reduction. **D.C. Grills**, J.J. Rochford, K.T. Ngo, S.V. Lymar, J.F. Wishart

College of Mount Saint Vincent
315, Founder's Hall

Chemical Biology

Cosponsored by BIOL‡ and ORGN‡
Financially supported by University of Texas
Y. Chen, P. Furlan, *Organizers, Presiding*

10:30 373. From epigenetic structural mechanism to targeted therapy. **M. Zhou**

11:00 374. Discovery of selective inhibitors for histone methyltransferases. **J. Jin**

11:30 375. Chemical interrogation of protein methyltransferases. **M. Luo**

12:00 376. Ubiquitin-like modifications as targets for developing cancer therapeutics. **Y. Chen**

College of Mount Saint Vincent
Peter Jay Sharp Athletic & Recreation Center (Gym)

General Posters

Faculty

Financially supported by Rowan University, Manhattanville College, St. John's University
D. Hull, P. D. Svoronos, S. Wei, *Organizers*

11:30 - 1:30

377. Photocurrent enhancement from solid-state triplet-triplet annihilation upconversion of low-intensity, low-energy photons. **C. Koenigsmann**, C. Li, F. Deng, A.L. Hagstrom, C.A. Schmuttenmaer, J. Kim

378. Design and manufacture of ICE test module to save gasoline with oxyhydrogen gas produced in alkaline electrolyzers. **R.D. Gonzalez**, B.A. Grunstein, J.M. Sandoval, L.F. Teran

379. Bio-catalyzed regioselective synthesis in undergraduate organic laboratories: Multi-step synthesis of 2-arachidonoylglycerol. **M.R. Johnston**

380. Analyzing the effect of ZrO_2 surface adsoportion on the intramolecular isomerization of azobenzene molecules. **D.C. Achey**, C. Pointer, A. Williams, K. Singewald, M. Snook, J. Alicea

381. Solar-hydrogen hybrid system integrated to a sustainable house in Mexico. **R.D. Gonzalez**, A. Yunez-Cano, M. Tufiño-Velazquez, R. Barbosa, B. Escobar

382. Stability of synthetic cathinones in preserved oral fluid samples. **B. Miller**, **M. Concheiro-Guisan**

383. Short metal-metal separations in multimetallic Au(I), Ag(I) and Cu(I) complexes. **A. Samin**

384. Fumed silica-based edible organogels and bigels. **A. Patel**

385. Synthesis, screening, and sensing applications of a novel fluorescent probe based on C-glycoside. T. Zhang, **Z. Fang**

386. Structural study of the membrane-anchored protein, hippocalcin, using reverse micelles. **K.A. Callaway**, J.M. Viviano, V. Venkataraman, N.V. Nucci

387. Electron paramagnetic resonance investigation of radiation damage and healing in Kapton. **J. Johnson**

388. Development of botulin-based small molecules as potential anti-cancer agents. S. Pathi, A. Patel, G. Jampana, **A. Vendola**, **T. Moosavi**, **S.C. Jonnalagadda**

389. Design and synthesis of functionalized benzoboroxoles as therapeutic agents. S. Pathi, D. Morgan, M.A. Rahman, J. Seay, A. Colfer, **S.C. Jonnalagadda**

390. Synthesis & spectroscopic characterization of standard long chain acyl carnitine derivatives for clinical diagnosis of fatty acid β-oxidation disorder. **H.F. Sobhi**, A. Charles, K. Ackie

391. Development of radiofluorinated analogs of abiraterone. A. Ku, A. Rodriguez, B. Huang, B.J. Punzalan, H.I. Scher, S.M. Larson, **D.R. Veach**

392. Hydroxypyridinones: Targeting HIV-1. **D. D'Alliessi Gandolfi**, H. Hanauske-Abel

393. Effect of a physical classroom demonstration on understanding of chemical equilibrium. **K. Barrett**

394. Exploring polymers through experiments in the undergraduate laboratory. J. Kral, C. McCormick, M. Castaldi, **J.L. Epstein**

395. Interaction energy of He with H_2S. **R.C. Mayrhofer**

396. Water oxidation catalysis with Ru carboxamide complexes. **Y.M. Badiei**, G. Renderos, C. Resurreccion, T. Aquino

397. Microwave-assisted synthesis of imidazolium-based ionic liquids for $LiFePO_4$ crystal engineering. **Y. Chen**, L. Cirrincione, M. Gobet, S. Greenbaum, P. Sideris

398. Hydrothermal synthesis and characterization of lithium mixed-transition-metal phosphates. **K. Lee**, P. Sideris

399. Synthesis and biological evaluation of siderophore derivatives as potential antibacterial agents. **S. Yoganathan**, J. Kong, N. Karadkhelkar

400. Differentiation of car paint chips. **Z. Dai**, F. Yu, K. Castro

401. Feasibility of remote sensing for comprehensive assessment of water quality of inland lakes in New York. **K. Barrett**, J. Curra

402. Catalytic cleavage of methylchlorosilane high boiling residue with methylimidazole: Alkyl phosphonium chloride compositions. **Y. Zhu**, K.M. Lewis, **A.T. Mereigh**, **J.D. Neely**, **D. Slick**

403. Novel ionophoric polyphenols display potent antioxidant and anti-amyloidogenic properties, and are non-toxic towards *Tetrahymena thermophila*. **A. Martinez**, T. Rahman, R. Alcendor, M. Podgorny, I. Sanogo, R. McCurdy

404. A novel way to create a crime scene for forensic chemistry. P.A. Redden, **M. Held**, **G. Patel**

405. Novel heterocyclic methodology for natural products synthesis. **S.P. Fearnley**, C. Thongsornkleeb, M.E. Domaradzki, R. Lapo, P.M. Lory

406. Assessing the fluoro-stabilization effect using *in vivo* unnatural amino acid incorporation. **C. Henkels**, C. Van Hook, R. Hohol, D. Hackford

407. Copper binding properties and antioxidant ability of multi-target compounds: Implications in the treatment of Alzheimer's disease. A. Martinez, **S. Hambleton**

408. Use of multicomponent coupling reactions for the design and synthesis of azaheterocyclic compounds as anti-cancer agents. S. Pathi, S. Fishbein, A. Kasibotla, L. Solano, K. Pandya, B. Patel, T. Gaus, **S.C. Jonnalagadda**

409. Detection of anthropogenic influences on nutrient enrichment in New York City parks. **S. Lee**, R.K. Dhar

410. Electrochemical oxidation of methanol and ethanol catalyzed by copper (I) oxide in pursuit of alcohol-based fuel cells. **A.T. Poulos**, E. Caban, A. Gobernik, M. Namer, V. Poulos, M. Sahni, N. Vaddepally, N. Yoo

411. Hybrid nanogels as recyclable catalysts. **K. Moran**, A. Patel, Q.R. Johnson, B.P. Chauhan

412. Pt/C and Pt-Ag/C nanostructured catalysts synthesized via ultrasonic irradiation for ORR: Acid and alkaline electrolyte effect. **B. Ruiz Camacho**, R. Fuentes Ramirez, R.D. Gonzalez

413. Effects of Russian propolis metal free ethanol extracts on bacterial biofilms. **C. Traba**, A. Ambi, D. Centeno, J. Bryan

414. Developing self-assembled bio-organic matrices for targeted drug delivery into tumor cells. A.M. Brown, P. Barrett, G. Knoll, **I.A. Banerjee**

415. Synthesis and anticonvulsant activity of 2'H,3H,5'H- spiro-(2-benzofuran-1,4'-imidazolidine)-2',3,5'-triones. **R. Stephani**, C. Yang

416. Probing organic solute binding in serum albumins using solvatochromic π^* indicators: Experimental and modeling studies. A. Edwards, A. Jose, N. Scafo, E. Nguyen, D. Athanasopoulos, **R. Helburn**

417. Imidazolium ionic liquids bearing symmetrical and asymmetrical cations and anions. **K. Papacostas**, E. Fernandez, E. Castner, S.I. Lall-Ramnarine

418. Synthesis and properties of asymmetric dicationic ionic liquids. **E. Fernandez**, S. Dhiman, J.F. Wishart, R. Engel, S.I. Lall-Ramnarine

419. Thio-and thio-bromo "click" approaches to carbohydrate functionalized thioglycosides. A. Mauger, **Z.J. Witczak**, R. Bielski, D.E. Mencer

420. Preparation of starch-poly-glutamic acid graft copolymers by microwave irradiation and the characterization of their properties. **J. Xu**, D. Solaiman, R. Ashby, R. Garcia, S. Gordon, R. Harry-O'kuru

421. CMDwater: A tool for ranking crystallographic waters for displacement during ligand design. **A.S. Bayden**

422. Testing of GMO foods for consumer purchase in Connecticut. **J. Pang**

423. The strengthening of polysaccharide-polyamine hybrid hydrogels by incorporating alginate. **G. Nunez**, M. Jitianu, A. Jitianu, N. O'Connor

424. Development of an organic laboratory experiment to introduce undergraduate students to olefin metathesis. **S.L. Carberry**, T. Udumulla-Arachchilage, A. Hussain, D. Richiuso, A. Hussain, H. Herrera, S. Bien-Aime

425. The relationship between osteoblast-osteoclast interaction and interleukin 6/STAT3 and sphingosine 1 phosphate signaling pathway. **S. Bong**

426. Facile fabrication of droplet patterned hierarchical microstructures by condensation of high-boiling liquids onto structured surfaces. **B.M. Jun**

427. Determination of pesticides in fruits, vegetables, and grains via the Luke method. **I. Sun**, M. Iorsh, K. Williams, P.D. Svoronos

428. Morphological characterization of supragranular neurons in the primary somatosensory cortex. **M. Anaya**, A. Tsimounis

429. Synthesis of a new α-substituted [13]-macrodilactone. **H. Shin**, K. Rutledge, J. Lawrence, M. Peczuh

430. Selenium: A potentially powerful tool to design potent anticancer molecules. **A.K. Sharma**, D. Karelia, D. Plano, S. Amin

SATURDAY AFTERNOON

College of Mount Saint Vincent
307, Founder's Hall

Activation & Transformations of Small Molecules by Metal Centers

J. M. Camara, K. E. Kristian, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 431. Mechanistic investigation of hydrogen generation by new bio-inspired Ir complexes for dehydrogenation of formic acid in water. **M. Ertem**, W. Wang, Y. Himeda, E. Fujita, J.T. Muckerman

1:25 432. Use of first-row transition-metal hydrides as hydorgen atom donors in radical reactions. **J. Kuo**, J. Hartung, A. Han, J.R. Norton

1:45 433. Polynuclear copper hydrides as catalysts for electron transfer from hydrogen. **S. Liu**, J.R. Norton, M.S. Eberhart, M.C. Neary

2:05 434. Catalytic carbon monoxide oxidation at ambient condition in basic solution. D. Shlian, J. Alboucai, M. Khaloo, A. Benhaim, M. Stock, J. Lewis, **J. Jiang**

2:25 Intermission.

2:40 435. Mechanistic considerations in water oxidation catalysis by ruthenium bipyridine-dicarboxylate and ruthenium bipyridine-phosphonate-carboxylate complexes. **D.W. Shaffer**

3:00 436. Synthesis and reactivity of a molecular titanium nitride. **M. Carroll**, L. Grant, D.J. Mindiola, P. Carroll

3:20 437. Human serum albumin-heme with proximal tyrosine ligand exhibits nitrite reductase activity. **M.I. Galinato**, E.M. Luteran, G.A. Fye, J.A. Bennett

3:40 Concluding Remarks.

College of Mount Saint Vincent
314, Founder's Hall

Ambient Mass Spectrometry for Forensic Science

E. Sisco, *Organizer, Presiding*

1:00 438. Towards development of a mass spectrometric database for the rapid identification of plant drugs of abuse by ambient ionization mass spectrometry. **R.A. Musah**, A. Lesiak, J.E. Giffen

1:25 439. Deducing the structures of amphetamine and cathinone unknowns from chemometrically processed ambient ionization mass spectral datasets of known synthetic amphetamine and cathinone structures. **K.L. Fowble**, J. Shepard, R. Musah

1:50 440. Screening of drugs of abuse using DART-MS and in-source CID reverse library search. **F. Li**, R. Beck, J. Tice, S. Shrader, B. Musselman

2:15 Intermission.

2:35 441. An overview of ambient ionization mass spectrometry efforts at NIST-STCAG. **E. Sisco**, T.P. Forbes

2:55 442. Time flies: Species identification of blow flies by direct analysis in real-time, high-resolution mass spectrometry (DART-HRMS) for postmortem interval estimations. **J.E. Giffen**, J.Y. Rosati, R. Musah

3:20 443. DART-TOF-MS analysis of personal lubricants. **M. Maric**, L. Harvey, A. Solano, M. Tomcsak, C. Bridge

3:45 444. Using APCI-MS for the screening of arson samples for the presence of accelerants. **T.H. Pritchett**, C. Fried, T. Brettell

College of Mount Saint Vincent
302, Founder's Hall

Bioinformatics

P. A. Novick, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 445. Using bioinformatics to elucidate the evolutionary dynamics of rhomboid proteases in *Streptomycetes*. **P.A. Novick**, N. Carmona, M. Trujillo

1:35 446. Using template-based modeling and bioinformatics to gain insight into the function of various protein domains/proteins. **S. Singh**

2:05 447. The evolutionary dynamics of LINE transposable elements in the vertebrate genome. **A. Sookdeo**, S. Boissinot

2:35 448. Evolutionary interpretations of mycobacteriophage biodiversity and host-range through the analysis of codon usage bias. **J.J. Dennehy**

3:05 449. Ancestors in our genome: The new science of human evolution. **E. Harris**

College of Mount Saint Vincent
306, Founder's Hall

Environment & Forensics

Financially supported by International Environmental Research Foundation
M. Miranda, R. P. Nolan, *Organizers, Presiding*

1:00 450. Lead-free ammunition. **P. Diaczuk**, T.A. Kubic

1:20 Discussion.

1:25 451. The chemical methods of gunshot residue analysis. **M. Miranda**, T.A. Kubic

1:45 Discussion.

1:50 452. Instrumental methods for the detection of gunshot residues. **T.A. Kubic**

2:10 Discussion.

2:15 Intermission.

2:25 453. Health effects of asbestos: What issues are current? **R.P. Nolan**, A. Langer

2:45 Discussion.

2:50 454. Talc and ovarian cancer. A. Langer, **R.P. Nolan**

3:10 Discussion.

3:15 455. Ion chromatography tandem mass spectrometry for ultra-trace analysis of hexavalent chromium. **V.I. Furdui**, S. Mädler

3:35 Discussion.

College of Mount Saint Vincent
309, Founder's Hall

Environmental Chemistry: Fate of Contaminants

Measurements & Reactions in Soil

U. Jans, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 456. Chemical characterization of urban soil in New York City. **A. Sarker**, R.K. Dhar

1:35 457. Bromination of soil organic particulates through abiotic mechanisms. **A.C. Leri**

2:05 458. Sorption of dioctyl sodium sulfosuccinate to coastal Gulf of Mexico sediment. **B.S. Adewale**, B.J. Brownawell

2:35 Intermission.

2:55 459. Perfluoroalkyl acid (PFAA) transport and remediation at an aqueous film forming foam (AFFF)-contaminated site. **E.R. McKenzie**, R.L. Siegrist, J.E. McCray, C.P. Higgins

3:25 460. Biochar ozonization and characterization with biochar water filtrate assays. S. Catley, O. Sacko, M. Huff, **J.W. Lee**

3:55 461. Monitoring of aquifer geochemistry to understand the mobilization of arsenic and manganese in groundwater of Chittagong, a rapidly expanding coastal city in Bangladesh. **R.K. Dhar**, A. Dhar, S. Palit

College of Mount Saint Vincent
304, Founder's Hall

Enzyme Catalysis & Inhibition

Financially supported by Enzo Life Sciences
S. Kumar, *Organizer, Presiding*

1:00 462. Development of cell-active chemical tools to study cathepsin L function. **D. Dana**

1:30 463. Mechanism and interactions of human pyruvate dehydrogenase complex with its kinase 1. **E.L. Guevara**, N.S. Nemeria, L. Yang, F. Jordan

2:00 464. Molecular docking and evaluation of small molecule inhibitors for matrix metalloproteinase-1 and 9. **I. Kumar**

2:30 Intermission.

2:45 465. Kinetic analysis and substrate binding studies of the *Escherichia coli* nitrile reductase QueF. **J. Jung**, T. Czabany, B. Nidetzky

3:15 466. Substrate specificities of the Venezuelan equine encephalitis virus nonstructural protein 2 cysteine protease. **P.M. Legler**

3:45 467. Development of drug-like inhibitory agents of Nek2 kinase. **S. Kumar**

College of Mount Saint Vincent
308, Founder's Hall

Frontiers in Gel Chemistry

Cosponsored by COLL
Financially supported by Institute for Soft Matter Synthesis and Metrology (Georgetown University)
R. G. Weiss, *Organizer*
D. Lee, M. Rogers, *Presiding*

1:00 Introductory Remarks.

1:05 468. Cartilage: A tough biological gel. **F. Horkay**

1:35 469. Supramolecular hydrogelators and hydrogels: From soft matter to molecular biomaterials. X. Du, J. Zhou, J. Li, H. Wang, Z. Feng, **B. Xu**

2:05 470. Hydrogel materials construction with peptide design and solution assembly. **D.J. Pochan**

2:35 Intermission.

2:50 471. Experimental and theoretical aspects of hydrogel-based microcantilever sensors. **H. Ji**

3:20 472. Engineering shear-thinning supramolecular hydrogels for biomedical applications. **J.A. Burdick**

3:50 Panel Discussion.

College of Mount Saint Vincent
301, Founder's Hall

Nano-Chemistry & Technology

Cosponsored by COLL
B. P. Chauhan, M. Chauhan, *Organizers, Presiding*

1:00 Introductory Remarks.

1:05 473. Nanocatalysis and the slurry-phase direct synthesis of methylchlorosilanes and alkoxysilanes. **K.M. Lewis**

1:35 474. Characterizing axial resolution while imaging $NaYF_4$:Yb,Tm nanoparticles. **P. Dawson**, M. Romanowski

1:55 475. Improving healthcare and industry: Grafting cyclosiloxane stabilized metallic nanoparticles onto various substrates. **G. Nkak**, S. Chaudhry, A. Patel, B.P. Chauhan

2:15 Intermission.

2:30 476. Microwave-assisted green synthesis of uniform ruthenium nanoparticles supported on non-functional single-walled carbon nanotube for Congo red dye degradation. **T. Hemraj-Benny**

2:50 477. The catalytic behavior of an alkene incorporated metal nanoparticle supramolecular gels via alcoholysis. **D. Artiga**, E. Castelar, A. Patel, S. Mathew, B.P. Chauhan

3:10 478. Comparative study of formation of hydroxyapatite. M. Kowaleff, N. O'Connor, **A. Jitianu**

College of Mount Saint Vincent
317, Founder's Hall

Organic Synthesis & Catalysis

Y. Chen, *Organizer, Presiding*

1:00 479. Tuning of optical, magnetic and colloidal properties of nanoparticles by dendritic ligands. **D. Jishkariani**, B. Diroll, M. Cargnello, H. Yun, J. Lee, L. Malassis, C.B. Murray, B. Donnio

1:30 480. Diastereoselective cycloadditions for the synthesis of five-membered ring nitrogen-containing heterocycles. **G. Moura-Letts**

1:50 481. 1, 3-dipolar cycloadditions of nitrile oxide with acetylenic aldehydes. **Y. Xing**

2:10 Intermission.

2:30 482. ‘Ene’ reactions of singlet oxygen at the air-water interface. **B. Malek**, W. Fang, I. Abramova, N. Walalawela, A. Ghogare, A. Greer

2:50 483. Oxazolone cycloadducts as versatile frameworks for alkaloid synthesis. **R. Lapo**

3:10 484. Heterocycle synthesis from quinols. **J. Wu**

3:30 Concluding Remarks.

College of Mount Saint Vincent
303, Founder's Hall

Organizing Research Programs at the Undergraduate Level

P. D. Svoronos, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 485. Instituting research at the community college level: Strategies that will secure the success of STEM students at the post-undergraduate level. **P.D. Svoronos**

1:35 486. Queensborough MSEIP: Using a three-tiered model to engage, retain, and graduate STEM students at a community college. **N. Gadura**

2:05 487. Engaging students in research. **P. Meleties**

2:35 Intermission.

2:50 488. The high impact practice of undergraduate research at community colleges using the CCURI model. **P. Powers**

3:20 489. Mentoring undergraduate research in different college/university settings. **E.E. Mojica**

3:50 490. Undergraduate research through laboratory experience as special projects to enrich student college experience. **A.K. Budruk**

4:20 Concluding Remarks.

College of Mount Saint Vincent
312, Founder's Hall

Radiation Photochemistry & Photophysics

G. L. Findley, *Organizer*
C. M. Evans, *Organizer, Presiding*

1:00 491. The photo-enhanced Lewis acidity of aqueous methyl viologen. **E.G. Hohenstein**

1:20 492. Near-infrared spectroscopy of ethynyl radical, C_2H. **A.T. Le**, G. Hall, T.J. Sears

1:40 Intermission.

1:55 493. Monitoring dimerization of radical anions by vibrational spectroscopy. **T. Mani**, D.C. Grills

2:15 494. EPR and NMR studies of radiation damaged polymers. **S. Humagain**, J. Johnson, D. Engelhart, J. Ho, R. Cooper, R. Hoffmann, S. Greenbaum

College of Mount Saint Vincent
310, Founder's Hall

Ionic Liquids

Radiation Chemistry & Interactions with Transition Metals

S. I. Lall-Ramnarine, J. F. Wishart, *Organizers*
M. F. Thomas, *Presiding*

1:30 495. Radiation and radical chemistry of ionic liquids for energy applications. **J.F. Wishart**, I.A. Shkrob, S. Dhiman, D.C. Grills, A.R. Cook

2:00 496. Effect of various anions of pyrrolidinium-based ionic liquids on yield of solvated electrons and reactivity observed by picosecond radiolysis technique. **S.B. Dhiman**, J.F. Wishart

2:30 497. The speciation of technetium (VII) in the presence of bistriflamidic acid in ionic liquids. **J. Hatcher**, L.C. Francesconi, J.F. Wishart

3:00 Intermission.

3:20 498. Evidence of the Hofmeister effect in the extraction of copper from aqueous to ionic liquid phase. C. Janssen, N. Macias-Ruvalcaba, M. Aguilar-Martínez, **M.N. Kobrak**

3:50 499. Surface studies of an ionic liquid on copper and gold. **A.B. Biedron**, S. Rangan, E.L. Garfunkel, E. Castner

4:20 Concluding Remarks.

College of Mount Saint Vincent
Peter Jay Sharp Athletic & Recreation Center (Gym)

General Posters

Undergraduate

Financially supported by Rowan University, Manhattanville College, St. John's University
D. Hull, P. D. Svoronos, S. Wei, *Organizers*

2:00 - 4:00

500. Self-organized organic nanoparticles of hydrophilic metalloporphyrin as a catalyst for the selective oxidation of olefins under ambient conditions. **D.N. Lema**

501. Photo-physical characterization of porphyrin conjugates. **N. Berisha**, **B. Begum**, N. Bhupathiraju, C. Farley, C.M. Drain

502. Study of multi-target directed ligands: Copper binding selectivity and inhibition of reactive oxygen species formation. **M.A. Gomez**, A. Martinez

503. Pulsed field gradient NMR study of ion transport in lithium-ion battery electrolytes for aerospace applications. **I. Diallo**

504. Measuring the nanomechanical properties of tomato cuticles using atomic force microscopy. **S.O. Smith**

505. Understanding the formation and size distribution of porous poly(*o*-toluidine) microspheres. **J. Hwang**, D.M. Sarno

506. Green and microscale flavone synthesis. **J. Pemerton**, N. Rowland, H. Avery, K. Moore, P. Powers

507. Partial sulfonation of polyaniline nanofibers. **D. Perry**, D.M. Sarno

508. Toxicity of e-juices. **J. Pemerton**, **K. Moore**, N. Rowland, P. Powers

509. Determination of elemental arsenic and leachable arsenic in aquifer sediment samples of Bangladesh. **R. Ferdous**, T. Ahmed, R.K. Dhar

510. Enantioselective synthesis of actinopolymorphol B and its analogs. **C.C. Kim**, Y. Xing, J. Lee

511. Visible light-driven energy transfer: Hybrid-engineered nanostructures versus plasmonic resonance in solar cell applications. **J. Codrington**, J. Foley

512. Hierarchical nanoparticles in photodynamic therapy. **N. Eldabagh**, J. Foley

513. Fusing a green fluorescent protein to SCO2139, a *S. coelicolor* rhomboid protease. **L. Lara**, Y. Muladjanov, M. Trujillo, N. Carmona

514. Oxidation of meso-substituted tri and tetra porphyrins. **D. Ismailgeci**, S.N. Khayyo, P.K. Kerrigan, D. Amarante, A. Novaj, S. Maio, V. Khayyo

515. Vibrational analysis of cysteine: Copper^{2+} interaction. **M. Abramova**

516. The effects of roasting on the reduction of hexavalent chromium by coffee. **R. Estevez**, **L. Cobbinah**, C. Kim

517. Interaction of catalase with nanoceramics as monitored by different spectroscopic methods. **K. Chhe**, T. Nolan, E.E. Mojica

518. Use of molecularly imprinted polymer to improve the analysis of naproxen in environmental water samples. **E. Jones**, R. Wise, E.E. Mojica

519. Comparative analyses of phenol content and antioxidant properties of Philippine tea samples. **J. Zapata**, M. Franke, E.E. Mojica

520. Binding interaction of nanoceramics (metal oxides) with human serum albumin. **T. Nolan**, E.E. Mojica

521. Antioxidant activities of different bee propolis extracts. **K. Symczak**, **A. Javornik**, **N. Evans**, E.E. Mojica

522. Effect of pH on the spectroscopic properties of several hydroxycinnamic acid derivatives. **P. Hanson**, **M. Franke**, E.E. Mojica

523. Phytochemical study and evaluation of larvicidal activity (*Aedes aegypti*) and termiticide (*Nasutitermes sp.*) of extracts *Morinda citrifolia* L. (Noni). **L. Bezerra Silva**, R.B. Brito Oliveira

524. Synthesis and characterization of silver nanoparticles and nanoprisms. **J. Hare**, M. Ghattas, C.M. Evans

525. Exploring fulgides with optoelectronic properties: Synthesis. **J. Powell**, H.S. Barcena

526. Esterification of succinic acid derivatives using dimethyl carbonate. **M. Barrie**, H.S. Barcena

527. Microwave-promoted Strecker synthesis. **K. Maziarz**, H.S. Barcena

528. Synthesis of polymers based on epoxidized soybean oil. **Y. Vvedenskiy** , **H.S. Barcena**

529. Ionic liquid solutions for cellulose and chitin dissolution. **J. Lei**, M.F. Thomas

530. Synthesis and characterization of $[Rh^{III}(NNN)(NN)L]^{n+}$. **P. Nunez**

531. Determination of the ionization constant of weak carboxylic acids using microscale freezing point depression measurements. **D. Kwun**, P. Irigoyen, P.D. Svoronos

532. Isolation and identification of antibiotic-resistant bacteria from New York City soil samples. **A. Coyotl**

533. Synthesis of pyrrolidinium ionic liquids bearing symmetrical and asymmetrical fluorous anions. **J. Ramdihal**, C. Rodriguez, E. Castner, S.I. Lall-Ramnarine

534. The effect of alkyl versus ether side chains on the physical properties of ionic liquids. **C. Rodriguez**, N. Zmich, S. Dhiman, J.F. Wishart, E. Castner, S.I. Lall-Ramnarine

535. Microbiomes associated to plant roots in NYC soil. **J. Nouel**, A. Volkova, A. Kawamura, M. Trujillo

536. Ruthenium interactions with ethanol upon microwave irradiation. **N.E. Carrero**, N.F. Tobar, T. Hemraj-Benny

537. Rapid analysis of organic micro-contaminants in complex environmental matrices using direct sample injection GC-MS. **M. Strumolo**, K.J. Bisceglia

538. Evaluating the efficacy of source reduction strategies on fecal bacteria concentrations in Mill Neck Creek, NY. **T.J. Vogel**, R.J. Brinkmann, S.J. Garren, M.A. Hunter, K.J. Bisceglia

539. Developing a pollen supplement diet for honey bees. **N. Carrasco**, J.M. Lenihan

540. Horizontal transfer of rhomboid proteases of archea. **D. Thelisima**, P.A. Novick, N. Carmona, M. Trujillo

541. Extract from *Plantago lanceolata* has an important mucolytic effect on the respiratory tract mucus. **J. Costanzo**, G. Proteasa

542. Exploration of DNA barcoding using 16S rRNA gene in invertebrates. **H. Singh**, N. Gadura, J. Stark

543. Identification of plankton species in the Hempstead harbor region. **O.J. Zagalo**, N. Gadura

544. Long-term study of the factors impacting water quality at the Hempstead harbor. **S.V. Singh**, N. Gadura

545. Exploration of DNA barcoding using the CO1 gene in invertebrates. **T. Smith**, N. Gadura, J. Stark

546. Isolation, identification, and characterization of microorganisms associated with sanitization stations. **M. Joseph**, C. Meddles-Torres, J.A. Timbilla

547. Antiphospholipid antibody and MiR106b mediated the expression of tissue factor in breast cancer cell lines. **I. Sun**, E. Lin, R. Sullivan, A.V. Nguyen

College of Mount Saint Vincent
315, Founder's Hall

Chemical Biology

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2:30 548. Structural feature and modification of keratin fiber by carbonyl-containing compounds. **M. Kadir**

2:55 549. Peptidomimetic structure and function: Synthetic peptide macrocycles with potential as anti-thrombosis agents and short artificial peptide helices and turns. **D. Guarracino**

3:20 550. Exploring the proteolytic susceptibility of peptoid oligomers. **M. Tatikola**

3:45 Intermission.

4:00 551. Phosphoproteomics of human immunodeficiency virus -1. **M. Kaur**

4:25 552. The role of calcium in the mechanism of N-methyl-4-phenylpyridirum (MPP+) toxicity toward dopaminergic cells. **V.Q. Le**, K. Wimalasena

4:50 553. Toxicity of host-guest formulations of isozyme-selective carbonic anhydrase inhibitors. **O.O. Karakus**, R.K. Sanku, U.K. Mondal, M.A. Ilies

5:15 554. Optimization of 1,2,4-triazolopyridines as inhibitors of human 11β-hydroxysteroid dehydrogenase Type 1 (11β-HSD-1): Discovery of clinical candidate BMS-823778. **J. Li**

MARM 1

Clinical diagnostics: An overview

Paul W. Dillon*, paulwdillon2@hotmail.com. Westchester Chemical Society, Valhalla, New York, United States*

Although “Classic” analytical chemistry informs much of Clinical Diagnostics, there are some important differences. Diagnostics use a limited range of sample types, most commonly blood and urine. Sample matrices have a more limited range than in general analytical chemistry.

Diagnostics are highly automated; instruments perform a wide range of analyses, randomly, with high throughput (up to 2000+ assays/hour). Typical analyses include clinical chemistries (e.g., glucose, enzyme activity), immunoassays, nucleic acid tests, and cytometry.

Not all analytes are well-defined molecular species. Some may be polymers of varying MW, some have a range of similar species, and some may have various forms (e.g., free and bound thyroxine). Assay standardization is important.

Unlike “Classic” quantitative analyses, which often drives reactions to completion, many diagnostics are kinetic with fixed times, requiring calibration with materials of known concentration.

Concentrations may be extremely low (pg/mL range) and the volume of sample for a single test may also be very low (1 to a couple of hundred µL).

In addition to analytical sensitivity and specificity, clinical sensitivity and specificity and predictive values can be crucial. Indices computed from multiple analyses are often used to ensure clinical relevance.

Clinical diagnostics are highly regulated, in the US by FDA. Clinical trials are conducted under GCP, and manufacturing follows GMP, rules. Sites may be inspected. Manufacturing systems, R&D studies, QA systems, complaint handling systems, materials, product labels, etc. will be reviewed. Reagent, calibrator, control and sample stability are all important.

MARM 2

Immunoassays in clinical diagnostics: The good, the bad, and the ugly

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While immunoassays (IAs) have been the mainstay of clinical diagnostics for the past several decades, they suffer from a number of analytical limitations. This talk will present some of the shortcomings of IAs currently used in clinical diagnostics, focusing especially on cross-reactivity, non-specific interferences, lot-to-lot variations, and heterophile antibodies. As an example of cross-reactivity, some methadone IAs produce positive results in the absence of methadone (termed a false positive) when diphenhydramine (Benadryl®) is present. Though cross-reactivity can sometimes be predicted based on molecular modeling, there are other, harder to predict interferences, that can also impact IAs; vitamin D IAs, for instance, yield falsely low results in the presence of high cholesterol levels. As an additional complication, IAs can vary substantially in the impact of these issues between different lots of reagent (presumably due to differences in the antibodies used across the different lots). Finally, the use of sandwich IAs are susceptible to heterophile antibodies which can led to substantial overestimation of an analytes concentration. The shortcomings above will all be discussed in the context of their impact on patient care and how clinical laboratories are attempting to address these issues.

MARM 3

Harmonization of vitamin D results

***Neil Parker**, neil.np.parker@siemens.com. R&D, Siemens Dx, Pawling, New York, United States*

There have been historical disparities between assays and methods which are evident from external quality assurance (EQA) schemes. Several efforts are being made to engage scientists, clinicians, manufacturers, international federations, and governmental agencies in a collaborative effort to create harmonization of measurements and methods across the world. Usually, standardization of methods requires a reference measurement procedure. The hierarchy of implementing standardization will be demonstrated by using 25(OH)Vitamin D Total, as an example, focusing on a reference measurement procedure and the Centers for Disease Control and Prevention (CDC) certification program. Such a process is being followed for other analytes, such as testosterone. The effectiveness of these efforts will be demonstrated and the need to be continuously vigilant to create harmonization with clinical laboratories, globally. Also presented will be approach a commercial manufacturer used to standardize a 25(OH)Vitamin D Total assay to align to the reference measurement procedure for this analyte.

MARM 4

Effects of overhanging analyte oligo tails in model DNA and morpholino arrays

***Ursula Koniges**, koniges@gmail.com, Rastislav Levicky. New York University, Brooklyn, New York, United States*

Hybridization of in-solution nucleic acid targets to surface-immobilized probes is a common mechanism employed in genetic analysis methods, for example DNA microarrays. In such applications, in-solution targets can be imperfect length matches to surface probes, with the resulting possibility of nucleic acid tails extending toward the surface, toward solution, or with overhangs of both orientations. We report the impact of surface- and solution-oriented tails on hybridization thermodynamics at a surface, and compare these results to a perfectly size-matched target and to solution hybridization thermodynamics. Several different probe coverages and solution ionic strengths are investigated. In addition to a DNA probe, a probe comprised of an uncharged DNA analogue, morpholino, is used to investigate the electrostatic contribution to the tail-orientation dependent biases. The reported results indicate that a surface-oriented tail markedly increases the hybridization energy penalty, whereas a solution-oriented tail has a significantly lower energy penalty effect. These results also help explain observations from a comparative study of the performance of DNA and morpholino microarrays.

MARM 5

Methods for characterization of hyaluronan from biological samples

Han Yuan[1], *hy509@nyu.edu, Ripal Amin*[1], *Xin Ye*[1], *Carol de la Motte*[2], *Mary K. Cowman*[1]. *(1) Chemical and Biomolecular Engineering, New York University, New York, New York, United States (2) Lerner Research Institute, Cleveland Clinic, Cleveland, Ohio, United States*

Hyaluronan (Hyaluronic Acid, HA) is a ubiquitous polysaccharide present in almost all tissues of vertebrates. Its molecular weight (MW) can range from several up to 25000 disaccharide repeating units, corresponding to several kilo-Daltons (kDa) to 10 Million-Daltons (MDa). HA regulates cell activity by interacting with cell surface receptor proteins, which causes signaling of a number of responses in an MW dependent manner. HA in human milk is known to mediate host responses to microbial infection via TLR4- and CD44-dependent signaling. Signaling by HA is generally size specific. Because pure low MW HA (average 35 kDa) can elicit a protective response in intestinal epithelial cells, it has been proposed that human milk HA may have a bioactive low-MW component. However, the current methods for determining the exact content and size distribution of low MW HA in actual biological tissues/fluids are under-developed, mainly because of low sample amount and isolation difficulty. This talk addresses the issues of limited sample amount and purification difficulty, and the importance of analyzing both high- and low-MW HA simultaneously. Methods for HA isolation and quantification are discussed. A method using size-dependent fractionation of HA by anion exchange on a spin column and quantification of HA in the fractions using a competitive ELISA is developed. HA size analyses for human milk samples are then conducted by this method and the results are discussed. This HA analysis method has also been performed on mammary tissues.

MARM 6

Label-free bio-sensing based on whispering gallery modes that beat the surface plasmon resonance (SPR) approach in sensitivity, analyticity, and multiplexing

Stephen Arnold, *sa1577@nyu.edu. Chemical Engineering, New York University, New York, New York, United States*

My presentation will detail the progress in the use of microcavities as Label-free biosensors, and compare their sensitivity, analyticity, and multiplexing capability to the Surface Plasmon Resonance approach.

MARM 7

Biochemical characterization of platelet-rich plasma (PRP)

Diego M. Ferreira, *diegoimeil@hotmail.com, Joel A. Rocha Filho, Estela Regina R. Figueira. Faculty of Medicine, University of São Paulo, Boituva, São Paulo, Brazil*

The development, production and characterization for new biomaterials is a great interest to regenerative medicine, many specialties in Medicine, Physics, Chemistry, Veterinary Medicine and Biology, has been dedicated to research in order to develop new biomaterials and test their possible aplicações. The new biometric data used by Doctors, Dentists and Veterinarians, this the Platelet Rich Plasma - PRP[4, 5]The production of biomaterials such as Platelet Rich Plasma – PRP, is a topic of great interest to Medical Professionals, this material has been used in regeneration processes, wound healing, bone reconstruction materials, and studied its application in cardiac surgery, plastic surgery, liver surgery, orthopedic surgery and odontology surgery.

To start a new material to be used is necessary for obtaining this known process is possible to reproduce and its properties are characterized, biological properties, physic, chemical, thermodynamic, kinetic

known, and other factors how efficacy material and economic viability of obtaining it.
The adoption of a new biometrics required extensive research before making Clinical trials in humans, the experimental design and 'necessary to avoid the waste of financial resources, time and animals. There are many experimental protocols to obtain PRP having as donor Wistars Rats, however the possible adoption of an inefficient protocol could lead to a waste of resources thus impeding the search, so we need to adopt a concise experimental procedure based on scientific evidence.
Once developed a reliable protocol for producing a biomaterial as the Platelet Rich Plasma - PRP can now make a more detailed analysis of biological properties, physic, chemical, thermodynamic and kinetic the PRP, and develop experimental animal models that will provide scientific evidence on which to base future applications or discontinuation of use for Platelet Rich Plasma – PRP.

MARM 8

Exploring new regions of polymorphic space through polymer-induced heteronucleation

***Vilmalí López-Mejías**, vilmali.lopez@upr.edu. University of Puerto Rico-Río Piedras Campus, San Juan, Puerto Rico, United States*

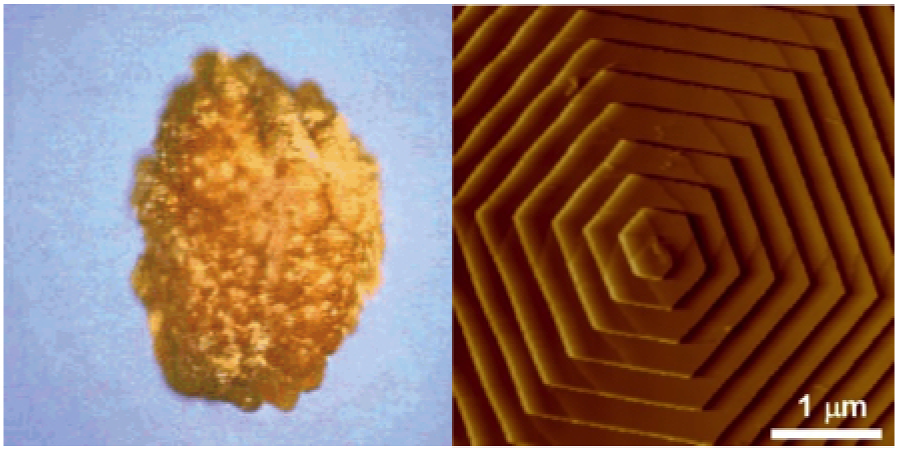
Polymorphism, the ability of molecules to exhibit multiple crystalline phases, is a phenomenon of considerable interest because it challenges the notion that molecules can arrange themselves exclusively in the thermodynamically most stable form. Moreover, the inadvertent occurrence of polymorphism has an enormous economic impact on the regulation and manufacture of crystalline materials, as their properties are intrinsic to their solid form. Therefore, it is not only important to understand the molecular structure of a compound, but also how this structure influences the packing behavior in the solid-state to control the performance of that material. Presented here is the design development of polymer-induced heteronucleation (PIHn), a powerful technique for the selective discovery and control of polymorphism that utilizes polymers as heteronucleants. The application of PIHn has allowed access to an unprecedented number of polymorphs in pharmaceuticals of the fenamic acid class. Octamorphism and pentamorphism of flufenamic and tolfenamic acid, respectively, have been established through the structural elucidation of solid forms grown using PIHn. Furthermore, a systematic investigation of the structure-polymorphism relationships in commercial, and synthesized analogues of tolfenamic acid supports the notion that an ensemble of steric and electronic features common to these structures, a “polymorphophore,” is responsible for the adoption of multiple packing modes within this molecular class. Lastly, a new design strategy for PIHn that combines favorable surface-solute interactions and geometric nanoconfinement is discussed. This strategy was able to influence the nucleation kinetics of mefenamic acid. The use of this strategy provided accesses to the metastable form, form II, exclusively on square nanopores imprinted on a biocompatible polymer surface. This strategy provides the first example of the selective crystallization of a more soluble pharmaceutical solid form on a functional polymer matrix with potential applications in drug formulation. Ultimately, the design of advanced strategies based on PIHn will help to explore new regions of polymorph space in order to experimentally derive the propensity for polymorphic behavior of a given molecular motif and perhaps provide a pathway to engineer molecular compounds with controlled properties in the presence of a functional heteronucleant.

MARM 9

Stopping crystal growth in its tracks: Pathways to therapies for pathological crystallization

***Michael D. Ward**, mdw3@nyu.edu, Laura Poloni, Alex Shtukenberg, Bart E. Kahr, Chemistry, New York University, New York, New York, United States*

The crystal growth of conventional materials like silicon has been refined for decades and has led to textbook crystal growth models. Confidence in these models quickly evaporates when considering complex inorganic solids and molecular crystals, however, despite the importance of these materials to technology, biology, and human health. In particular, many crystalline materials are associated with diseases, from malaria to kidney stones. This presentation will illustrate the beauty and complexity of crystal growth, through mechanisms often hidden and deceptive, in pathological molecular crystals, including kidney stones as well as "xenostones" that form as a consequence of active pharmaceutical ingredients that form crystals in renal spaces. Armed with an understanding of some crystal physics and crystal surface structure at the molecular level, crystal growth inhibitors can be designed that bind to specific crystal sites and prevent the formation of pathological crystals, suggesting a pathway to therapies for crystal-based diseases in general. These observations also reveal the complexity of dissymmetric surfaces of organic crystals, which stems from their inherent low molecular and crystal symmetry.



(Left) A typical cystine kidney stone. (Right) In situ Atomic Force Microscopy image revealing a macrospiral generated by a Frank-Read dislocation source on the (0001) face of a cystine single crystal.

MARM 10

Helicoidal dichroism

Bart E. Kahr*, bart.kahr@nyu.edu, Alexander Shtukenberg, Xiaoyan Cui, Shane Nichols. Chemistry, New York University, New York, New York, United States*

It has long been known that a significant percentage of molecular crystals, when grown with large aspect ratios, readily grow as helicoidal ribbons with mesoscale pitches, but general appreciation of the commonality of these non-classical crystal forms has been lost. Helicoidal crystal twisting was typically assayed by analyzing refractivity modulation. However, by growing twisted crystals from melts in the presence of dissolved, light absorbing molecules, crystal twisting can be assayed by analyzing the dichroism. *Helicoidal dichroism* is used here to describe the optical consequences of anisotropic absorbers precessing around twisted radii of helicoidal crystalline fibrils or lamellae. Two twisted crystalline compounds, hippuric acid which twists about two crystallographic axes (*a* and *c*), and *D*-mannitol which twists around singular axes, but in two polymorphic forms (*a* and *d*), are analyzed herein. These compounds, when grown from supercooled melts in the presence of a variety of histochemical stains and textile dyes, are strongly dichroic in linearly polarized light in the absorption bands of the dyes. Optical properties were measured using Mueller matrix imaging polarimetry. Hippuric acid has a large linear birefringence. That of *D*-mannitol is small by comparison permitting and analysis of the circular dichroism as well as the linear dichroism. The optical properties were simulated. They are in accord with the model of crystallites twisting developed previously and consistent with microstructural analyses. Uses of these highly structured colored films are considered.

MARM 11

Solid phase transformation during pharmaceutical processing

***Lei ZHU**, lzhu0129@gmail.com. Formulation Sciences, Merck & Co, Kenilworth, New Jersey, United States*

Active Pharmaceutical Ingredient (API) often exists in several solid forms (crystalline or amorphous). The different solid forms are known to influence the physical, chemical and mechanical properties of the API. Therefore, much effort has been put into API form screening and understanding their solid-state properties to select the most appropriate form for dosage form development and downstream processing. Even with the thoroughly studied API form, phase transformation may still occur during manufacturing processes or storage of the final dosage form. The unintentional phase transformation is often difficult to predict or control, and may have major impact on the safety and efficacy of a drug. To develop a pharmaceutical dosage form with acceptable performance and quality attributes, it is essential to understand the materials (API and excipients), the manufacturing processes, and the underlying mechanism of process induced phase transformations. This presentation will review the typical pharmaceutical processes used in solid dosage form development and their associated stresses, and the various process induced phase transformations (polymorph transition, hydration/dehydration, crystalline to amorphous or amorphous to crystalline transformation, etc.). Current theories and the most recent advancement on the underlying mechanisms will be discussed. Specifically, the recent effort on understanding dry process induced crystalline to amorphous phase transformation will be presented. Examples will be given to illustrate the impact of phase transformation. The possibility of predicting and preventing the undesired phase transformation will be discussed.

MARM 12

Precipitation-based microparticle synthesis in continuous-flow microfluidic platforms: design and application

***George Kumi**, georgekumi@gmail.com, Asma Obaid, Jinnie Anstice, Sarah Belh. Chemistry, Rutgers-Camden, Camden, New Jersey, United States*

Of the various existing microfluidic platforms, droplet-based devices are generally preferred for crystal synthesis because of the relative monodisperse size, shape and morphological distribution these devices confer onto a synthesis. In contrast, the varying crystal residence times in simple continuous-flow (i.e., non-segmented-flow) devices leads to more polydisperse crystal characteristics. However, appropriately designed continuous flow systems can reduce residence time distributions and enhance the capabilities of such systems. As a demonstration of this strategy, a non-droplet-based device that affords control of where favorable crystallization conditions occur within a device has been developed and applied to a variety of crystal syntheses, including calcium carbonate, calcium oxalate, and barium sulphate formation. The rationale for the design of these microfluidic platforms and results demonstrating the devices capabilities (e.g., morphological control) will be discussed. In addition, design improvements for the next generation of such devices will also be presented.

MARM 13

Imidazolium-based ionic liquids for the ionothermal synthesis of $LiFePO_4$

Paul Sideris*, psideris@qcc.cuny.edu. Chemistry, Queensborough Community College, Bayside, New York, United States*

$LiFePO_4$, adopting the so-called “olivine” structure, is one of the most attractive cathode materials for lithium ion batteries due to its relatively high charge capacity (~170 $mAhg^{-1}$), as well as its high thermal and electrochemical stability. Synthetic approaches which aim to the control particle-size and morphology of $LiFePO_4$ are of great interest to the community. The rationale is that by reducing the grain size and promoting the preferential growth of the crystallites along certain crystallographic directions (*a* and *c* for $LiFePO_4$), the diffusion path length of the Li^+ ion would shorten and consequently the ionic conductivity would improve. It has been shown that room temperature ionic liquids can be used as both solvents and structure directing agents in the ionothermal synthesis of cathode materials. To investigate the role of the structure of the cation in the ionothermal synthesis of $LiFePO_4$, several imidazolium-based ionic liquids, containing hydroxyl-terminated alkyl chains of various lengths, have been synthesized using microwave-assisted methods and characterized using ^1H and ^{13}C nuclear magnetic resonance (NMR) spectroscopy. These ionic liquids were used as solvents in the ionothermal synthesis of $LiFePO_4$ from various precursors. The resulting $LiFePO_4$ powders were characterized using powder X-ray diffraction, ^7Li and ^{31}P solid state NMR spectroscopy, and scanning electron microscopy. The ionic liquids were also investigated post-synthesis using NMR spectroscopy to identify any decomposition products.

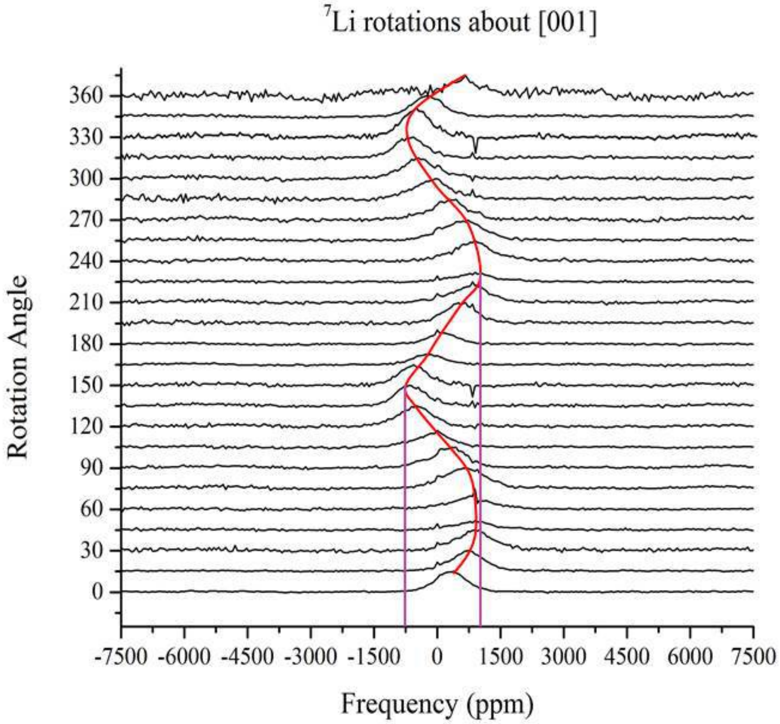
MARM 14

^7Li and ^{31}P nuclear magnetic resonance studies of single crystal LiMPO4 and $LiM_1M'_{1-x}PO_4$ (M = Mn, M’=Fe, x=0.5)

Lisa Cirrincione[1,2]*, lc647@hunter.cuny.edu, Phil Stallworth*[1]*, Steven Greenbaum*[1]*. (1) Physics and Astronomy, Hunter College, Astoria, New York, United States (2) Physics and Astronomy, The Graduate Center, CUNY, New York, New York, United States*

Li*M*PO_4 (*M*= Mn, Fe) are orthorhombic crystals, belonging to the olivine family and exhibit exceptionally high applicability for electrochemical energy storage in lithium-ion secondary batteries due to their charge storage capacity, chemical and thermal stability, and cost. Furthermore, mixed transition metal ion compounds Li(M,M’)PO_4 are particularly promising cathode materials because the redox voltage increases when Fe is substituted with Mn, Ni, or Co and the mixed compounds can be tailored for specific applications.
In these studies we used Single Crystal NMR spectroscopy as powerful tool to gain insight into the structure of Li*M*PO_4 and Li(*M,M’*)PO_4, providing us information about the local electronic and magnetic environments of the material. By measurement of the ^7Li and ^{31}P NMR frequencies with crystal orientation, we were able to determine the relative directions and magnitudes of the components of the interaction tensor giving rise to the lithium and phosphorus shifts.

In addition to the endpoints (Fe and Mn analogues), we present an NMR analysis of the mixed transition metal ion compounds $LiFe_xMn_{1-x}PO_4$,, where x = 0.25, 0.5, and 0.75 in order to shed some light on the degree of cation disorder between the lithium, phosphorus, and transition metal sites that can result in substantial degradation of cathode performance particularly with regard to reduced rate capability.



Representative ^{7}Li resonances of a single crystal of $LiMn_{0.5}Fe_{0.5}PO_4$ rotated about [001]

MARM 15

Natural abundance ^{17}O, ^{23}Na and diffusion NMR studies in carbonate-based electrolytes

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Sodium-ion batteries are of relatively new interest in the rechargeable battery field. Li-ion rechargeable batteries have been developed as comparably mature technologies; however, they still have some disadvantages, such as safety issues, short lifetime and high cost. Based on the similar chemical properties to lithium and high abundance of sodium-containing precursors, Na-based batteries might become competitive to Li-ion batteries.

In this work, we performed natural abundance ^{17}O, ^{23}Na and pulsed gradient spin-echo diffusion Nuclear Magnetic Resonance (NMR) experiments to investigate interactions between cation, anion and solvents in carbonate-based electrolytes. Electrolytes were prepared with 1M $NaPF_6$ in four different binary solvents, which are ethylene carbonate (EC)/dimethoxyethane (DME), EC/ethyl methyl carbonate (EMC), EC/propylene carbonate (PC) and EC/fluoroethylene carbonate (FEC) with three different solvent ratios 20/80, 50/50 and 80/20. All experiments were performed on a 400 SB Bruker Avance III spectrometer at 60°C. The chemical shifts of ^{17}O were compared between the 1M $NaPF_6$ electrolytes and their corresponding salt-free solvents, and ^{23}Na chemical shifts were also determined to obtain information on the Na^+ - oxygen lone pair interaction. Fig.1 shows the ^{17}O chemical shift difference between 1M $NaPF_6$ and neat solvent in EC/DME electrolytes. As with this electrolyte, the carbonyl oxygen of EC in all four binary solvent electrolytes show an obvious upfield shift, about -4ppm to -10 ppm, while the carbonyl oxygen of EMC, PC and FEC present relatively smaller upfield shift, and the other ^{17}O chemical shift mainly move to downfield after adding the $NaPF_6$ salt. The ^{23}Na, ^{19}F and ^{1}H NMR diffusion experiments were done to characterize the mobility of cation, anion and solvent respectively. These results will be combined with ongoing electrical conductivity and mass spectroscopy measurements performed at Army Research Lab.

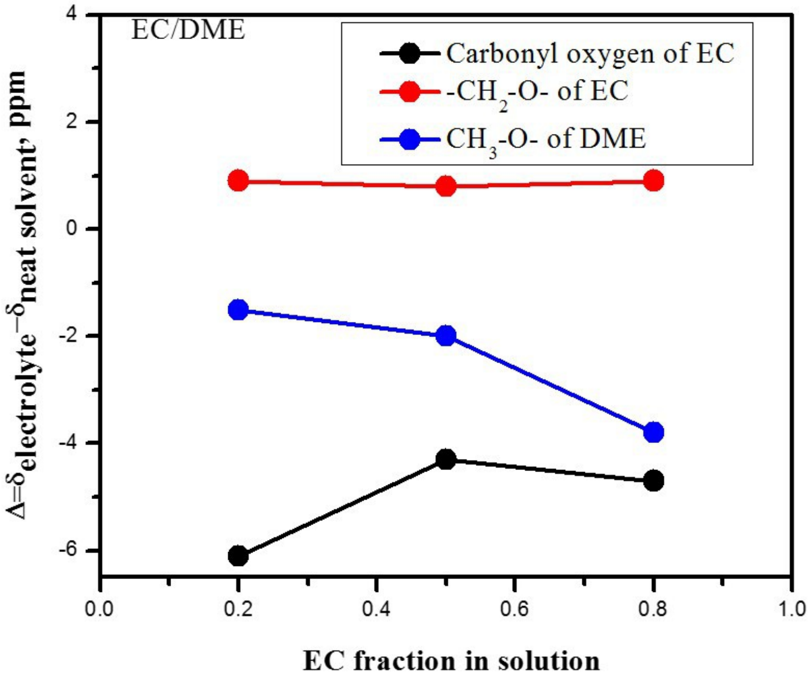

Fig.1 ^{17}O NMR Chemical shift difference in EC/DME

MARM 16

Synthesis of copper birnessite, Cu_xMnO_y nH_2O with crystallite size control: Impact of crystallite size on electrochemistry

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A novel synthetic approach for the preparation of copper birnessite, $Cu_xMnO_ynH_2O$ providing material property control was accomplished along with the detailed characterization and electrochemical measurements of varying crystallite sizes. The crystallite size which ranged from 12 to 19 nm, was inversely proportional to copper content (x) in $Cu_xMnO_ynH_2O$, $0.20 \leq x \leq 0.28$. Electrochemical evaluation showed that the higher copper content (x = 0.28) and small crystallite size (~12 nm) sample delivered ~194 mAh/g, about 20% higher capacity than the low copper content (x= 0.22) and larger crystallite size (~19 nm). This is the first electrochemical evaluation of copper birnessite in lithium based systems and demonstrates the appropriate design of synthetic parameters which enabled the preparation of $Cu_xMnO_ynH_2O$ with tunable material properties resulting in improved electrochemical performance. In addition, electrochemical testing in magnesium based electrolyte also indicated that $Cu_xMnO_ynH_2O$ is worthy of further study for magnesium based batteries.

MARM 17

The electrochemistry of the Li/$CuFe_2O_4$ system: An x-ray absorption spectroscopy study

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Mixed transition metal oxides such as the spinel ferrites, MFe_2O_4 are promising candidates for electrodes in lithium – ion batteries due to their natural abundance, benign qualities, scalable and economical preparation methods, and their capability of storing significant amounts of energy compared to conventional intercalation electrodes. $CuFe_2O_4$, for example, promises a high theoretical capacity due to the conversion mechanism which forms Cu^0, Fe^0 and Li_2O upon full electrochemical reduction. Although these materials are very promising, their use in commercial batteries is impeded by significant capacity fade. The reversibility of $CuFe_2O_4$ at various voltage ranges was studied to understand the electrochemical redox mechanism using ex–situ x–ray absorption spectroscopy (XAS). This study provided new mechanistic information with (i) observation of Cu^{2+} and Fe^{3+} reduction at distinct voltages with Cu^{2+} reducing to Cu^0 prior to the reduction of the Fe^{3+} center and (ii) demonstration that the redox couple Cu^{2+}/Cu^0 is electrochemically irreversible while the Fe^{3+}/Fe^0 redox couple is electrochemically reversible. The details of the structure of the charged (re-oxidized) $CuFe_2O_4$ structure were also elucidated, showing Fe^{3+} ions in an octahedral environment within the oxide framework and Cu^0 nanoparticles outside of the parent structure. Understanding the structure function properties of $CuFe_2O_4$ provides insight relevant to the electrochemistry of other spinel structured materials.

MARM 18

NMR studies of ion transport in ultra-concentrated aqueous lithium electrolytes

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The electrolytes currently used in lithium ion batteries are a source of many cost and safety issues, which can be mitigated by a switch to aqueous electrolyte. This was, until recently, precluded by the narrow

electrochemical stability window of the aqueous electrolyte, a problem which severely limited the practical voltage and energy density of the battery. However, recent developments have shown that it is possible to open up this stability window by increasing concentration of the salt (LiTFSI), enabling the formation of an interphase. This opens the door for a fresh focus on the properties of aqueous electrolytes. (1) Nuclear Magnetic Resonance (NMR) is a powerful tool for exploring ionic and molecular transport in electrolytes. The nuclei in question (^{7}Li, ^{19}F, and ^{1}H) are particularly well-suited to measurement by NMR, due to their gyromagnetic ratios and abundances.

We performed NMR measurements on a range of concentrations of LiTFSI aqueous electrolyte, varying from 1 m to 21 m. In particular, pulsed gradient spin-echo self-diffusion experiments were performed on a 300 MHz spectrometer. Self-diffusion coefficients for both ions and water molecules were obtained over a range of temperatures from 20°C to -60°C. As expected, we note a general trend of smaller diffusion coefficients with lower temperature, as well as smaller diffusion coefficients with higher salt concentration. Cation transference numbers were determined directly from the diffusion measurements and those results are listed in Table 1. The cation transference number increases as the temperature falls and the salt concentration rises, as well. Although this investigation focuses on the transport properties of the liquid phase, ongoing work will address SEI formation on a variety of anodes in contact with this unusual aqueous system.

1. Liumin Suo et al. "Water-in-salt" electrolyte enables high-voltage aqueous lithium-ion chemistries. Science. 350, 938 (2015).

Table 1. Transference numbers for LiTFSI aqueous electrolytes

LiTFSI (m)	Temp (?)	t^+	t^-
1	20	0.58	0.42
	0	0.63	0.37
	-20	0.60	0.40
	-40	0.54	0.46
	-60	0.76	0.24
21	20	0.70	0.30
	0	0.74	0.26
	-20	0.73	0.27
	-40	0.75	0.25

MARM 19

Characterizing dendrite growth in lithium batteries using *in situ* MRI

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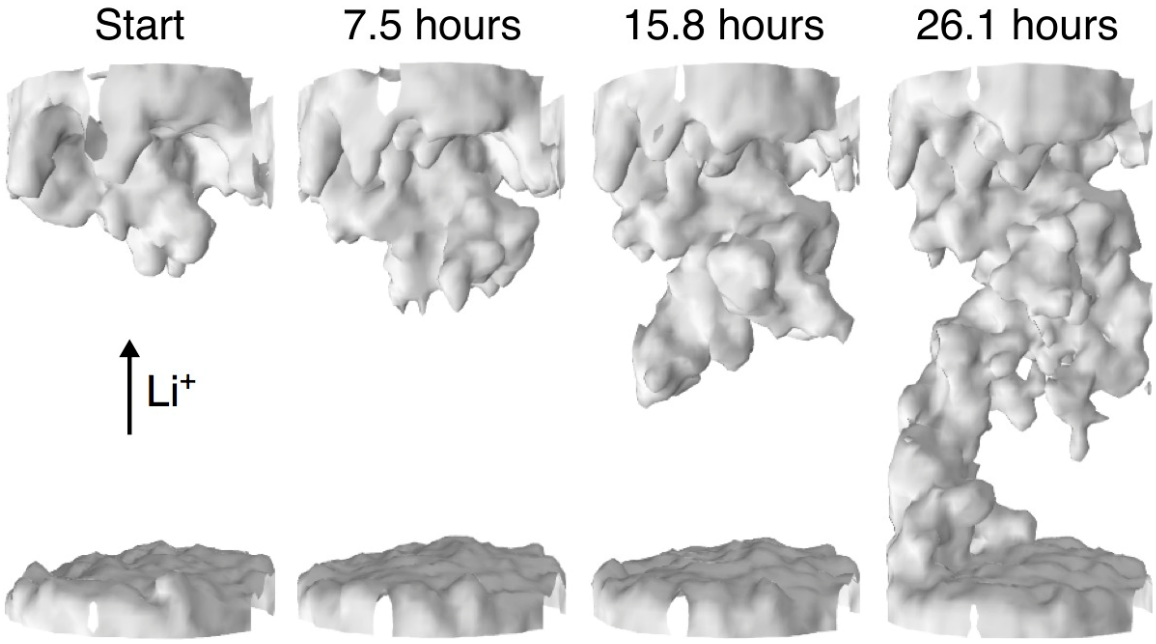
We will describe our work on the development of techniques for assessing Li-ion batteries and battery materials via magnetic resonance imaging (MRI). The goal of these studies is to analyze battery degradation and energy storage mechanisms in situ by imaging changes in both the electrolyte and the electrodes in a noninvasive fashion while a cell is charged or discharged. We have used this approach on a functioning lithium metal battery to correlate the behavior of the electrolyte concentration gradient to the type and rate of dendrite growth on the surface of the Li electrode, confirming the existence of separate growth mechanisms in different charging regimes. The methodology is extremely sensitive to Li dendrite formation, opening up the possibility of testing a broad range of materials and operating conditions to understand when dendrites grow and how they can be prevented.

The impact that the dendrites have on their surroundings through local magnetic fields also allow them to be measured indirectly using fast ^{1}H imaging techniques. The result is a real-time, 3D movie showing dendrites growing across the electrodes in the cell, shedding light on the growth behavior, rate and morphology of the structures formed (Figure 1).



^{1}H MRI performed in situ on a symmetric lithium metal battery. The images show dendrites growing from the negative (top) to the positive (bottom) electrode.

MARM 20

Silicon-based anodes for lithium-ion batteries

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The study of high energy density electrode materials is central to the development of lithium-ion batteries; alternatives to carbonaceous anodes in lithium-ion batteries are being sought in recent years. Silicon has been considered as one of the most promising anode materials for the next generation lithium-ion batteries because it would afford a much higher capacity than the commonly used graphite (~4200 mAh/g vs. 372 mAh/g). However, the major obstacle to overcome is the electrode mechanical failure caused by the excessive volume expansion of silicon on lithiation, which limits its long-term cycling performance. A nano-sized aluminum containing silicon, leached in acid, with a porous structure is shown to maintain its capacity better than pure bulk silicon or nanosized silicon. A stable capacity of 1400 mAh/g is maintained for more than 60 cycles. For the sake of alleviating the volume change impact and improving the electrochemical performance of the leached silicon, we developed a series of new silicon/silicon oxide/titanium composite anode materials, which were prepared by the ball-milling method. Powder X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), X-ray absorption spectroscopy (XAS), magnetic analysis and nuclear magnetic resonance (NMR) spectroscopy have been used to correlate the electrochemical performance with the materials' morphology and composition. The results show that the theoretical capacity of silicon in these composites can be achieved, and all the materials exhibit excellent electrochemical cyclability (with little capacity fading over 100 cycles). Such a cycling performance can be associated with the titanium particles, which are evenly distributed in these composites, buffering the drastic volume change of silicon during the electrode reaction. This research is supported by DOE-EERE-BATT, DE-AC02-05CH11231 under Award Number 6807148, and by NYSERDA

MARM 21

Oral fluid drug testing: A new look at applications, advantages, and methods

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Although urine is the most common biological matrix used in clinical toxicology, a major disadvantage is that it solely indicates past exposure to a drug. Blood is the required matrix when the impairing effects of a drug is being estimated or when attempting to establish the pharmacokinetic relationship between drug dose and drug concentration in a donor. However, blood toxicology testing requires invasive collection procedures and specially trained personnel. Thus, the development of simpler methods to assess biologically active drug levels in a person is desirable. In this study, we developed an algorithm based upon well-established drug specific pharmacokinetic variables that allowed for the estimate of a calculated steady state drug concentration range in plasma and an equivalent drug concentration window in oral fluid. This was done on an individualized, patient by patient basis. Simultaneous plasma and oral fluid samples were collected from patients that had been prescribed opiates chronically (at steady state) and analyzed by LCMSMS. An algorithm was developed that provided an estimate of the expected steady state ranges based upon the drug dose for the individual patients and the measured drug levels were compared to the calculated drug ranges. Practical application of this method could provide prescribers with a tool that indicates when a person is falling outside the calculated drug concentration range. This could be a flag of potential abuse, diversion, or non-adherence to dosing regimen, as well as individual pharmacogenomic (metabolic) differences. Other important considerations such as the impact of oral fluid contamination, oral fluid collection and salivary pH, and patient health status are also discussed. The results showed that the proper application and inherent advantages of oral fluid drug testing indicates that this biological matrix may be a promising contender as the new gold standard.

MARM 22

Quantitative analysis of licit & illicit drugs in river & wastewater samples

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Wastewater-based toxicology is an innovative and promising approach that provides information about exposure to external agents, such as drugs of abuse, in defined population groups by the analysis of human excretion products (biomarkers) in wastewater. Wastewater can provide independent, low-cost, reliable and almost real-time information compared to conventional population surveys. Marijuana is the most popular illegal drug in the USA, and the use and misuse of prescription opioids has increased dramatically in the last years.
We developed and full-validated an analytical method for the simultaneous determination of prescription opioids delta-9-tetrahydrocannabinol (THC) and its metabolites in 100 mL wastewater samples by Ultra-High Performance Liquid Chromatography-Tandem Mass Spectrometry (UHPLC-MSMS) with dual atmospheric pressure and electrospray ionization (API/ESI) source.
The samples were filtered by binder-free glass microfiber filters, and extracted by mixed mode solid phase extraction cartridges. The chromatographic separations were in reverse-phase gradient mode with 0.1% formic acid in water and in acetonitrile. Each target compound was monitored by 2 MRM transitions, one being a quantifier and the other a qualifier.
The method linearity ranged 5-1000ng/L for opioids, and 10-1000ng/L for THC and metabolites. The limits of detection were 1-5ng/L. River water, water from a sewage overflow location, and wastewater from a wastewater treatment plant were analyzed. Water was collected from different locations in Queens, Manhattan, Bronx, and Roosevelt Island into EPA certified sample containers and stored at −20 °C until analysis. River water samples tested negative. Water from the sewage overflow location tested positive for opioids (morphine 10.7ng/L, oxycodone 5ng/L), and the wastewater sample tested positive for opioids morphine, oxymorphone, hydromorphone, oxycodone, hydrocodone, and THCCOOH at concentrations 6.3-169.3ng/L.
We developed a sensitive and specific method for the simultaneous determination of prescription opioids and marijuana in wastewater samples.

MARM 23

Application of microextraction to forensic toxicology analysis

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Microextraction is a simple and fast sample preparation technique which minimizes the use of solvent in extraction. Depending on extraction medium, microextraction can be classified as solid phase based and liquid phase based. Solid phase microextraction is totally solvent free, integrating sample cleanup, enrichment and injection into one step. Liquid based microrextraction uses microliter level solvent and can be classified into single drop microextraction, three-phase liquid microextraction and dispersive liquid-liquid microextraction. Microextraction methods could be easily coupled with commonly used instruments such as gas chromatography, liquid chromatography and capillary electrophoresis for analytes separation and detection. This work reviews method development and application of microextraction technique to forensic toxicology analysis in recent years. Determination of common drugs of abuse and their metabolites in various sample matrices are discussed.

MARM 24

Use of LCMS in the pain management toxicology laboratory

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One of the aspects of pain management as a branch of medicine is medications therapies utilization to treat pain. Therapeutic drugs management requires monitoring to prevent possible addiction, tolerance, drug diversion, and abuse. Drug testing in toxicology laboratory is complex and technically challenging. Despite similar clinical goals, the analytical setup and workflow of toxicology laboratories are quite different. Analytical instrumentation plays the key role in the lab and impacts organizational, procedural, and regulatory decisions.

LCMS provide comprehensive and fast results with extreme accuracy, sensitivity and specificity. It allows analysis of the sample in its own matrix, whereas urine, blood or oral fluid. In “dilute-n-shoot” method sample is ready for analysis within a few steps. However, quick pre-analytical process can lead to analytical challenges later. Continuous injection of diluted matrix makes chromatographic column life shorter and MS source dirtier, increasing maintenance time and cost. Solid-phase extraction is a much cleaner sample preparation, although is longer and expensive, but it also decreases the maintenance needs and improves the chromatography. LC columns assortment gives labs tool to analyze diversity of various compound classes in one injection. Furthermore, rapid polarity switching in MS allows same injection analysis of compounds that would ionize in positive/negative modes. Our 52 drugs method includes amphetamines, barbiturates, benzodiazepines, opioids, cocaine, PCP, marijuana – all extracted in one method and injected as one sample. The acquisition time is 7 min. UHPLC can analyze same sample within 3-4 min, but analysis cost goes up. Throughput is an important factor for a busy laboratory and multiplexing technology can save time. This technology allows doubling the samples throughput by modification of the LC part while utilizing the same MS. This setup becomes handy once limited on space and is more cost efficient; however, its operation requires advanced technical knowledge and maintenance.

In current presentation you will learn advantages and disadvantages of different methods for samples preparation in pain management toxicology laboratory. LCMS analysis of multiple classes of drugs will be presented as well as strategies for achieving time, cost and labor efficiency of lab operation. Additionally, LCMS common issues, challenges, maintenance and validation parameters will be discussed.

MARM 25

Novel workflows using a Q-Tof MS for targeted and non-targeted applications for forensic toxicology

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Quadrupole time-of-flight mass spectrometry is becoming more acceptable in many types of mass spectrometry laboratories. Their speed, accuracy, and resolving power yield a tremendous amount of information for many applications due primarily to the advances made in electronics and computing power. In addition, the information gleaned from these hybrid systems produce more confident results faster than ever before. Here, several different types of Qtof experiments will be discussed that center around data dependent and independent workflows, including the acquisition of a digital fingerprint of each sample analyzed.

MARM 26

Application of liquid chromatography high-resolution mass spectrometry for comprehensive screening and unknown drug identification in subjects at an electronic dance music festival event

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Electronic dance music (EDM) has a strong association with a culture of recreational drug use, especially novel psychoactive substances (NPS). Over the course of two years, 126 bloods, 226 urines, 330 oral fluid samples were obtained from 396 EDM attendees at a festival event in Miami, FL, and analyzed for evidence of common therapeutic and recreational drugs as well as emerging NPS.
Analytical screening methods in blood, urine and oral fluid were developed and validated using liquid chromatography quadrupole time of flight mass spectrometry (LC-QTOF) (Waters® Acquity UPLC IClass Xevo® G2-S QTOf, with UNIFI™ 1.7 software). Structural elucidation of known and novel metabolites was also accomplished on this platform. In the course of this validation, a library of therapeutic, recreational and emerging NPS drugs and their metabolites was developed.
Using LCMSMS (Waters® Acquity Quattro- Micro®), quantitative confirmatory methods in blood and oral fluid were developed and validated for THC and metabolites, synthetic cathinones, and common drugs of abuse. All validations followed SWGTOX guidelines. Synthetic cannabinoid screening by LCMSMS (Waters® Acquity UPLC, TQS) was also employed.
Subjects participating completed surveys regarding their recent drug use. A total of 342 surveys were completed. 72% of subjects responded that they had taken a recreational or medicinal substance in the past week. The top responses for 2014 were marijuana, alcohol and cocaine, and in 2015 alcohol, marijuana and "Molly". A total of 31 subjects (21%) in 2014, and 29 subjects (15%) in 2015 said they had taken "Molly," MDMA, Ecstasy or a combination of the three. Of subjects admitting to NPS use, the most common substances found in 2014 were methylone (n=10) and alpha-PVP (n=8), compared to ethylone (n=16) and MDMA (n=13) in 2015. No alpha-PVP was found in 2015 in spite of apparently high rates of use in the Florida illicit drug market.

MARM 27

Strategies and best practices for online teaching success

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In an effort to increase student engagement and ultimately enhance student success, the approach of incorporating asynchronous learning with the traditional synchronous approach is being adopted at an accelerated pace in higher education institutions. This presentation has two primary objectives: 1) to highlight the online instructor performance expectations, which include technology access, preparation, communication, availability, course management among others, and 2) to re-iterate the evidence-based strategies for a successful online teaching-learning experience. Pertinent factors such as effective teaching strategies, learning activity ideas and assessment are addressed.

MARM 28

Development of a high school chemistry MOOC (massively open online course)

***Ruben M. Savizky**, rsavizky@cooper.edu. Chemistry, The Cooper Union, New York, New York, United States*

In this presentation I will focus on recent efforts to create a high school chemistry MOOC. The course was intended to cover the main topics in a general chemistry course, such as atomic theory and structure, stoichiometry, chemical reactions in aqueous solutions, gases, enthalpy and heat, quantum mechanics, the periodic table and periodic trends, bonding and molecular structure, hybridization and molecular orbitals, intermolecular forces, properties of liquids and solids, phase diagrams, properties of solutions, electrochemistry, acids and bases, kinetics, equilibrium and thermodynamics. I will also discuss attempts at an online laboratory component to the course. To make sure students understand the material we planned to have feedback such as guided inquiry problems, online homework and assessments in the form of quizzes and exams. This course was designed to be fast-paced and tailored to the particular strengths and weaknesses of each individual student. Preliminary results from the first airing of this course will be discussed.

MARM 29

Investigating conceptual change in active learning environments for large enrollment chemistry courses

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Recent reports have demonstrated multiple advantages of active learning in aiding students in developing a better understanding of the concepts, practices, and ways of thinking in chemistry. Efforts in chemistry education research have focused on identifying different types of alternate conceptions which students' have that may inhibit their development in chemical literary; developing instructional materials to promote conceptual change; and studying the changes in student understanding when taught using collaborative or cooperative learning methods. One area of relative scarcity is the investigation of pedagogical approaches that promote conceptual change as well as evidence that change has occurred. In this study we will discuss the relevance of studying student discourse practices in collaborative learning environments that lead to gains in student conceptual understanding. The findings should inform the development and dissemination of improved curricular resources with explicit recommendations and strategies for instructors in active learning environments at the introductory level.

MARM 30

Technology and chemistry education

Lucas C. McCann, *lucas@tophatmonocle.com. Chemistry, York University, Toronto, Ontario, Canada*

The fundamentals of second year organic chemistry have remained largely unchanged for over half a century, yet every year new versions of textbooks are published as instructors seek more effective means of teaching and gauging the learning of their students leading up to exams. The way educators present the material to students needs to shift in a manner that is more accessible and more engaging to students. Top Hat is an educational technology company that is altering the landscape of learning by bringing real-time audience response to instructors in combination with an interactive textbook. Top Hat is shifting the way students are guided and graded, both inside and outside the classroom that is complimentary to today's virtual learning style.

MARM 31

It takes a village to develop good lessons: Leaning on the interactive online network of inorganic chemists (IONiC)

Fabiola Barrios-Landeros*, barriosl@yu.edu. Chemistry, Yeshiva University, New York, New York, United States*

The Virtual Inorganic Pedagogical Electronic Resource (VIPEr) is the web-based home for a community of inorganic chemists and a repository of teaching material suitable for general or inorganic chemistry courses of different levels. This presentation will focus on strategies to adapt and implement the different types of curricular materials, or "learning objects", found on its website (www.ionicviper.org). Examples include in-class activities, problem sets, literature discussions, and laboratories. The innovative material is based mainly on research literature and is useful whether a course is being developed for the first time or an old one is getting revamped. Furthermore, instructions on how to create your own learning objects and the opportunity to share your teaching expertise with the IONiC community will be discussed.

MARM 32

Creating gateway chemistry courses for at-risk students

Cherice M. Evans*, cherice.evans@qc.cuny.edu. Queens College CUNY, Flushing, New York, United States*

General chemistry and basic chemistry are gateway freshman chemistry courses that challenge many students. (At Queens College, the pass rate in these two courses is around 50%.) Many students are under prepared for these courses. Moreover, students who have struggled in these courses tend to continue to struggle in chemistry and other science courses. This talk presents recent attempts at Queens College to use adaptive learning software and smart books to target and help at risk students.

MARM 33

Superconducting carbon in two dimensions

Elena R. Margine*, emargine@binghamton.edu. Physics, Binghamton University - SUNY, Vestal, New York, United States*

Carbon is a wonder element which underpins life on our planet, represents the vast majority of our energy sources, and arguably constitutes one of the building blocks of nanotechnology. Among its many fascinating properties, carbon has been known to exhibit superconductivity in zero, one, and three dimensions in widely diverse materials spanning fullerenes, graphite, polycyclic aromatic hydrocarbons, nanotubes, and diamond. One outstanding question in this area has been whether carbon can also superconduct in strictly two dimensions, namely in graphene and its derivatives. Very recently, two independent studies have presented the first evidence supporting the appearance of a superconducting phase in Li-decorated monolayer graphene (LiC_6) [1] and Ca-intercalated bilayer graphene (C_6CaC_6) [2].

In this talk I will review our recent computational work on the electron-phonon interaction and the paring mechanism in Li-decorated monolayer graphene [3] and Ca-intercalated bilayer graphene [4]. In both cases we provide evidence that the superconducting transition can be explained within a standard phonon-mediated mechanism and find that the low-energy vibrations associated with the alkali atoms are critical to the pairing. Finally, we predict that while a single anisotropic superconducting gap should exist in

LiC_6, it should be possible to resolve two distinct superconducting gaps in C_6CaC_6. I will conclude this talk by discussing recent advances in first-principles calculations for superconductors, in particular our recent implementation of the anisotropic Eliashberg theory using Wannier-Fourier electron-phonon interpolation [5,6].

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MARM 34

Multiple exciton generation in isolated organic molecules

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Singlet fission is a form of multiple exciton generation (MEG) in which two triplet excitons are produced from the decay of a photoexcited singlet exciton. However, practical implementations of organic MEG have been limited by the small number of organic chromophores that undergo efficient singlet fission, largely restricted to molecular crystals of oligoacenes. In these materials, the singlet fission process is highly sensitive to crystal packing and morphology, hindering the design of efficient triplet harvesting interfaces and the development of high throughput device processing strategies.

In this talk, I will discuss our recent discovery of efficient intramolecular singlet fission materials, in which two triplets are produced on an isolated molecule and in which geometric order and strong nearest neighbor coupling is no longer a design constraint. These materials, which include both small molecules and polymers, have expanded the quantity and variety of materials that undergo singlet fission and offer significant advantages in terms of their tunable molecular and electronic structure, solution processability, and the ability to form tailored interfaces. Furthermore, these materials offer a unique platform in which to study the dynamical evolution of multiexciton states, since the system can be constrained such that exactly two triplets exist on the molecule. I will discuss how the triplet yield and lifetime is affected by energetic driving force and the electronic character of the exciton states. These results allow us to gain mechanistic insight into the fission process and suggest general strategies for generating new materials that can undergo efficient fission.

MARM 35

Analysis of electronic couplings in photosynthetic proteins

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Electronic couplings are crucial for understanding the exciton dynamics and associated Förster resonance energy transfer in artificial and natural chromophores, including photosynthetic proteins. A robust computational methodology for evaluation of electronic couplings in complex molecular systems (e.g. peridinin-chlorophyll-protein) is proposed. A system is split into separate molecular fragments (e.g., chromophores), and transition dipole moments are calculated for the individual fragments with quantum chemical methods (e.g., time-dependent density functional theory). The analysis of delocalization of electronic excitations over multiple molecular fragments and their electronic couplings is presented.

MARM 36

Gold nanorods and lanthanides fluoride nanocrystal assembly for enhancement of light upconversion efficiency

***Dmytro Nykypanchuk**, dnykypan@bnl.gov. Brookhaven National Laboratory, Upton, New York, United States*

Light upconverting nanocrystals (UCNC) promise exciting advances in bioimaging, therapeutics, light harvesting and photonics. Over the last several years significant progress has been made in improving the spectral characteristics of the nanocrystals, however, the nanocrystals still suffer from reduced emission efficiency compare to larger, bulk-like particles. It has been suggested, however, that plasmonic fields may improve the upconversion by orders of magnitude. Here we explore how self-assembly of plasmonic nanorods with UCNCs can affect the upconcevrsion. Specifically, we will discuss the general strategies for the self-assembly, how the control over interparticle distance and the particle orientation can be achieved and, as the result, how these parameters affect UCNC's optical properties in this hybrid assemblies.

MARM 37

Divide and conquer the electronic structure of condensed phases: Ground states and dynamics in real and imaginary time

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We claim that a subsystem formulation of Density Functional Theory can simplify both the theoretical framework and the computational effort for calculating the electronic structure of condensed phase systems. In addition, the naturally subsystem-like form of molecular aggregates makes subsystem DFT a better descriptor of the underlying physics than regular DFT of the supersystem.

We confirm our claims by presenting simulation of dynamics of liquids and molecular crystals showing that by suppressing the inter-subsystem self-interaction error, contrary to Kohn-Sham DFT, subsystem DFT provides a physical description of the electronic structure of these systems at a fraction of the computational cost of regular (Kohn-Sham) DFT with no loss of accuracy.

Simulation of embedded excited states are also presented. We show with applications to molecular and periodic systems that subsystem DFT recovers correct non-Markovian dynamics of embedded species both in real time (for optical spectra) and imaginary time (for many-body interactions).

MARM 38

Development and implementation of innovative high-throughput screening and analysis solutions to support discovery and development of APIs in the pharmaceutical industry

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As high-throughput experimentation (HTE) emerges as an important enabling technology in the field of organic synthesis, high-throughput analysis (HTA) becomes an integralcomponent in these newly introduced HTE platforms. Without corresponding improvements in analytical throughput, HTE platforms would quickly be limited by backlogs in chemical analysis.This presentations covers high-throughput developments in traditional chromatographic techniques as well as spectroscopic and mass spectrometry methods including sensor-based approaches. Both high speed and multiparallel approaches to analysis are discussed, with a highlight on the challenges of developing methods for ‘same day analysis’ of 1536 well microplates.

MARM 39

History and nomenclature of synthetic cathinones and cannabinoids

***Adriana DeArmas**, Adriana.M.DeArmas@usdoj.gov. Northeast Laboratory, Drug Enforcement Administration, New York, New York, United States*

Synthetic cannabinoids and synthetic cathinones have been one of the latest “trends” in the field of controlled substances. Synthetic cannabinoids, also known as spice or K2, are designer drugs that are similar in structure to the compounds found naturally in the marijuana plant. They are commonly sprayed onto plant material to be smoked or smoked in liquid form via vaporizers. Synthetic cathinones, also referred to as bath salts, mimic the structure of cathinone, which can be found in the khat plant. These new psychoactive substances (NPS) are causing challenges for U.S. law enforcement officials as well as forensic chemists and the analysis involved. Certain synthetic cathinones and cathinone derivatives are banned, but the manufacturers of these drugs have found ways of synthesizing new variations of these compounds, or analogues, that are not scheduled. This presentation will focus on an introduction to synthetics; topics to be addressed include routes of synthesis, a brief history, packaging trends, and naming conventions of the compounds.

MARM 40

Utilization of commercially available MIPs for illicit drugs analysis

***Elmer-Rico E. Mojica**, emojica@pace.edu. Chemistry and Physical Sciences, Pace University, New York, New York, United States*

Analysis of illicit drugs such as amphetamines and its derivatives found in biological samples such as urine is usually done by chromatographic methods like gas chromatography (GC) and liquid chromatography (LC). The complex nature of biological samples results to the needs of using sample pretreatment methods such as solid phase extraction (SPE). There were SPE materials that were developed to improve sample pretreatment method and one of these are molecularly imprinted polymers (MIPs), a class of polymer-based recognition elements tailored to target a specific chemical or class of structurally related compounds. In this study, analysis using sample pretreatment method (SPE) with MIP was compared with analysis without treatment. In addition, the performance of two commercially available MIPs to extract amphetamine from water and synthetic urine was compared. Results showed a higher recovery of amphetamine in complex samples with the use of the sample pretreatment method (sorbents) as opposed to analysis without pretreatment. Similar results were obtained for both sorbents in terms of percent recovery of the amphetamine in both water and synthetic urine samples. An HPLC method utilizing these materials was also developed.

MARM 41

Analysis and characterization of drugs used as a preservation solution in bags of red cell concentrates

***Diego M. Ferreira**, diegoimeil@hotmail.com, Joel A. Rocha Filho, Estela Regina R. Figueira. Faculty of Medicine, University of São Paulo, Boituva, São Paulo, Brazil*

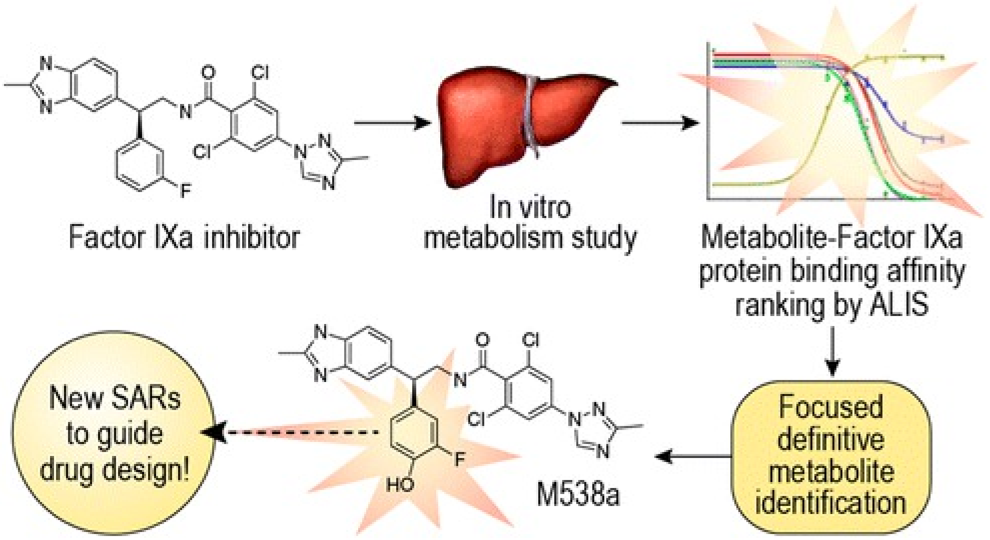
The oxygen supply to the cells need meet the metabolic demand, and have a critical effect in energy requirement in the cardiorespiratory system, this offer can be seriously affected in the case a person suffering a injury because of a surgery trauma or car accident causing blood loss, in the cases it is normal doctors recommend the transfusion of concentrates of red blood cells to help O_2 supply maintenance in the human organism. The red blood cells (CH) have a complex system[1]. For storage blood products is necessary that it be carried out at temperatures 2° C to 6° C, depending on how this occurs can lead to formation of ice crystals, causing damage to the red blood cells. To reduce effect caused because formation of ice crystals in the blood component, in the storage process is added cryoprotectant solutions such as mannitol ($C_6H_{14}O_6$), in the bags blood derived bags. Besides the natural toxicity caused by the use of cryoprotectants agents in the cryopreservation process, also observed the formation of reactive oxygen species (ROS). The development of blood preservation solutions is a big interest for medical services. Normally the bags for stored blood is CPDA-1 and CPD/SAGM. Among the parameters to measure the quality and viability of the use of red cell bags are K+, Na+, Cl-, lactate, HCO3-, ammonia, glucose and pH. On various parameters (K+, Cl-, HCO3-, glucose and lactate) solution of CPD/SAGM kept the energy metabolism of red blood cells more stable. Thus the addition of blood preservation solutions, ultimately is possible further reduce the effectiveness of blood transfusion for consume the extracted oxygen from red blood cell and aggravate symptoms as hyperkalemia.

MARM 42

Definitive metabolite identification coupled with automated ligand identification system (ALIS) technology: A novel approach to uncover structure-activity relationships and guide drug design in a factor IXa inhibitor program

***Yong Liu**, yong_liu2@merck.com. Merck, Rahway, New Jersey, United States*

A potent and selective Factor IXa (FIXa) inhibitor was subjected to a series of liver microsomal incubations, which generated a number of metabolites. Using automated ligand identification system-affinity selection (ALIS-AS) methodology, metabolites in the incubation mixture were prioritized by their binding affinities to the FIXa protein. Microgram quantities of the metabolites of interest were then isolated through micro-isolation analytical capabilities, and structurally characterized using MicroCryoProbe heteronuclear 2D NMR techniques. The isolated metabolites recovered from the NMR experiments were then submitted directly to an *in vitro* FIXa enzymatic assay. The order of the metabolites' binding affinity to the Factor IXa protein from the ALIS assay was completely consistent with the enzymatic assay results. This work showcases an innovative and efficient approach to uncover structure–activity relationships (SARs) and guide drug design via microisolation-structural characterization and ALIS capabilities.



MARM 43

Analysis of synthetic cathinones and cannabimimetic agents

Michael White, *Michael.D.White@usdoj.gov. Northeast Laboratory, Drug Enforcement Administration, New York, New York, United States*

Manufacturing formulations of synthetic cathinones and cannabimemetic agents change at a relatively rapid rate. These changes in the compounds create a challenge from a legal, as well as an analytical perspective.This presentation will cover a brief introduction to traditional federal law regarding controlled substances and the analog act, presumptive and confirmatory testing techniques, as well as helpful tools used when faced with an unknown. The primary focus of the presentation will be focus on the analysis of these compounds by mass spectrometry (MS) and an in-depth interpretation of the MS data. However, other instrumental techniques will be referenced such as LC/MS, LC-MS/MS, NMR, IR, and DART-MS. After attending this presentation, attendees will be more familiar with the legal aspects, analytical considerations and challenges presented by synthetic cathinones and cannabimimetic agents.

MARM 44

Detecting 1,4-butanediol in drinks

Maria Nazarouk[2,1], ***Zhaohua Dai***[1,2], *zdai@pace.edu. (1) Forensic Science Program, Pace University, New York, New York, United States (2) Chemistry and Physical Sciences, Pace University, New York, New York, United States*

The commodity chemical 1, 4-butanediol (1,4-BD) is a metabolic precursor for GHB (g-hydroxybutyric acid), which is an endogenously occurring neurotransmitter derived that is often used as a date-rape drug. In 2000, GHB became a banned substance by the United States Drug Enforcement Administration as a Schedule I drug and its supply is strictly regulated. However, as an industrial chemical used as a solvent and in producing some types of plastics and fibers, 1,4-BD is widely available. It can be turned into GHB by alcohol and aldehyde dehydrogenases in human body. Therefore, although 1,4-BD is not a scheduled drug in U.S., its use in consumer goods or drinks, intentionally of unintentionally, can cause serious harm, producing toxicity and clinical effects similar to those of GHB. For these reasons, facile detection of 1,4-BD may be very helpful in preventing tragedies. Here we report an easy detection method for detecting 1,4-butanediol in drinks. Using a commercially available detection tool for ketamine and GHB, we found that various amount of 1,4-BD, ranging from 1% to neat, in aqueous solutions of ethanol, can induce a quick and durable color change, similar to reported changes induced by GHB. Detection of GHB in real beverages and alcoholic drinks, as well as in-depth investigation of the mechanism of such detection and endeavor to improved detection tools will also be presented.

MARM 45

Hidden in plain sight: Using the geometric constraints on cell geometry to exploit specific and general chemical functionality

Daniel Steingart, *steingart@princeton.edu. Dept of MAE, Princeton University, Princeton, New Jersey, United States*

Endeavors in electrochemical energy storage are industrial masochism for the same reason they are academic hedonism: a working, rechargeable battery represents a tight coupling of multiphase phenomena across chemical, electrical, thermal and mechanical domains. Despite these couplings, most treatments of batteries in the academic literature emphasize the material challenges and opportunities as opposed to the system level workings. There are at least three good reasons for this: 1) to date, tools for examining the structure of “real” cells in operando are largely limited to synchrotron x-ray and neutron methods, 2) full cells are products engineered for application demands and not platonic ideals and 3) material improvements can have enormous impact on battery performance.

Yet understanding and examining the physical dynamics of cells in a “scaled context” is still a worthwhile academic endeavor. The battery as a system presents problems that are difficult to decouple, but the study of such problems can introduce new opportunities and inform electrochemical reactor designs and material utilization strategies.

By studying full “scaled” cell behaviors we have learned how to compensate for certain material disadvantages and to create batteries and components that can meet performance targets which challenge traditional materials-first strategies. First, I will show that the “dendrite” may not be the universal anathema it is made out to be (at least in a water stable system). Second, I will show what we can learn from the many reasons it is difficult to cycle a traditional “bobbin” AA cell. Finally, I will examine a “stupid battery trick” unique to the zinc alkaline bobbin that can teach us something (perhaps) universally applicable to all closed batteries.

MARM 46

Battery material characterization as a bridge from fundamentals to applications

Joshua Gallaway, *joshuagallaway@gmail.com. Chemical Engineering, City College of New York, New York, New York, United States*

Electricity generation by solar and wind power will be limited until reliable, economical, and safe electrical storage is also available at the grid scale. Due to their flexibility, electrochemical storage systems such as batteries are a likely candidate. However, the benchmark cost of 2 ¢/kWh-cycle is extremely demanding, excluding the use of a wide swath of the periodic table except in trace amounts. The search for new battery materials is underway as researchers target sodium, magnesium, and calcium ions, and many older chemistries are reconsidered and reconfigured to achieve the cost and safety targets. The best chemistry for grid scale batteries remains undecided.

A fundamental feature of electrochemistry is that it by necessity involves the interplay of two electrodes, an anode and a cathode. Techniques exist to test electrodes in isolation, but in practical devices the electrodes usually interact. Device performance is determined not only by the performance potential of each electrode, but also by the effect of each electrode on the other. Because of this and the need to maximize interface, battery design is hierarchical: (i) active materials are chosen due to their voltages and rate capabilities; (ii) the active materials are formed into useful electrodes, which may have high surface area; (iii) the two electrodes are integrated into a device; and (iv) devices are connected to form a system, if needed. This hierarchy requires specialized characterization at every level. True device-level characterization is only now coming into its own as techniques are developed to collect microscopic data from within sealed batteries, and this promises to advance understanding into the complex mechanisms that occur inside cycling batteries. An overreliance on materials-level characterization ignores conditions arising from device-level aspects. There is also the danger for a *fallacy of composition*, in which remarkable capabilities of the materials are inferred to the device without justification, based on a misunderstanding of battery design principles.

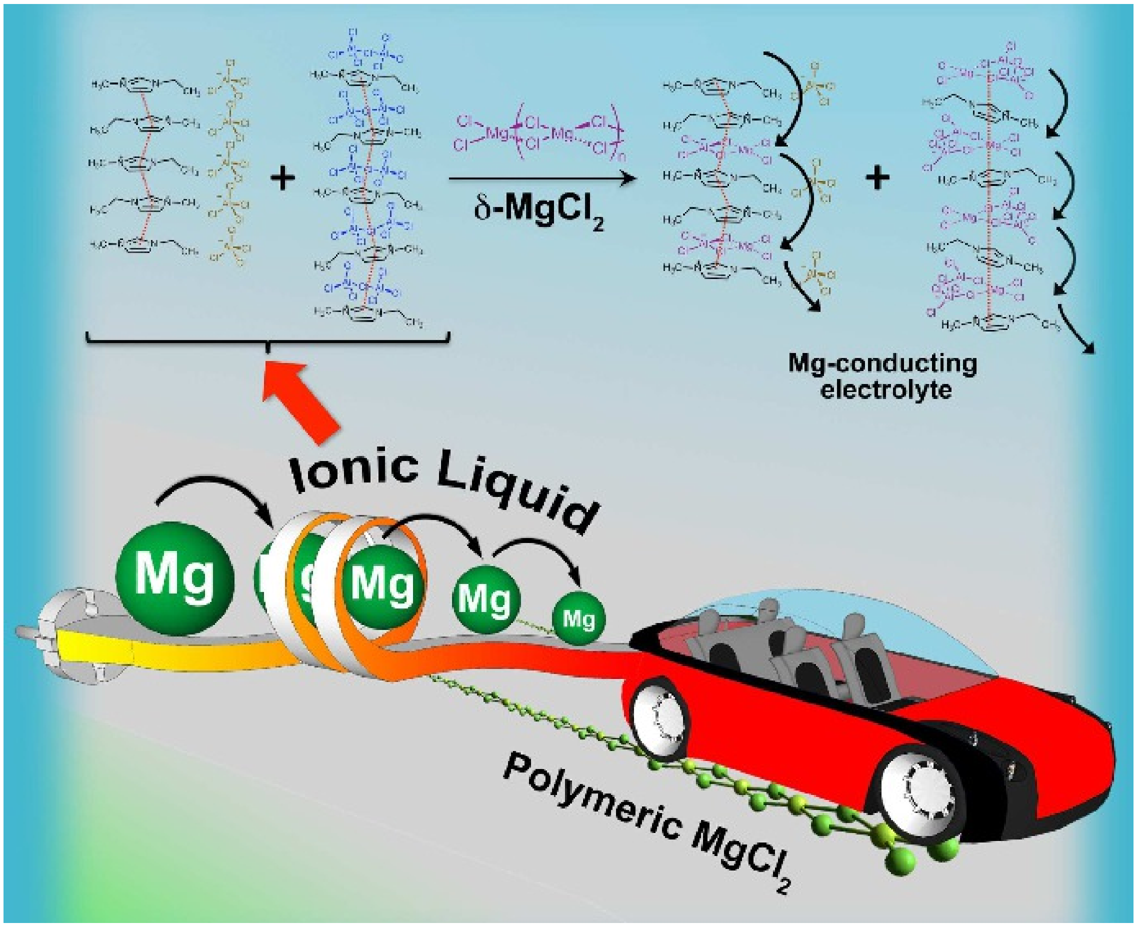
In this talk I will demonstrate that fundamental discharge mechanisms can be impacted by the manner in which materials (i) are integrated into electrodes and devices (ii and iii). This is especially true because achieving goals such as high energy density require materials to be pushed into regimes far from those at which the basis materials are often characterized, such as high concentrations and mass loadings.

MARM 47

A key concept in magnesium secondary battery electrolytes

Michele Vittadello[2]*, mvittadello@mec.cuny.edu, Federico Bertasi*[3]*, Chaminda Hettige*[2]*, Fatemeh Sepehr*[1]*, Xavier Bogle*[4]*, Gioele Pagot*[3]*, Keti Vezzù*[3]*, Enrico Negro*[3]*, Stephen J. Paddison*[1]*, Steven Greenbaum*[4]*, Vito Di Noto*[3]*. (1) Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, Tennessee, United States (2) Chemistry and Environmental Science, Medgar Evers College, Brooklyn, New York, United States (3) Chemical Sciences, University of Padova, Padova, Italy (4) Physics, Hunter College, New York, New York, United States*

A critical roadblock toward practical Mg-based energy storage technologies is the lack of reversible electrolytes that are safe and electrochemically stable. Here we report on high-performance electrolytes based on 1-ethyl-3-methylimidazolium chloride doped with $AlCl_3$ and highly amorphous d-$MgCl_2$. The phase diagram of the electrolytes reveals the presence of four thermal transitions that are strongly dependent on salt content. High-level DFT-based electronic structure calculations substantiate the structural and vibrational assignment of the coordination complexes. A 3D Chloride-Concatenated Dynamic network model accounts for the outstanding redox behaviour, the electric and magnetic properties, with insight into the conduction mechanism of the electrolytes. Mg-anode cells assembled with the electrolytes were cyclically discharged at a high rate (35 mA/g) exhibiting an initial capacity of 80 mAh/g and a steady-state voltage of 2.3 V.



MARM 48

Computational studies of electrochemical hotspots and ultrathin films of yttrium-doped barium zirconate

Angelo Bongiorno, *angelo.bongiorno@csi.cuny.edu. Chemistry, College of Staten Island - CUNY, Staten Island, New York, United States*

Yttrium-doped barium zirconate (BZY) is a proton-conducting electrolyte forming a class of novel materials for a new generation of solid oxide fuel cells (SOFCs). In this presentation, I will report on two recent density functional theory (DFT) studies of BZY. The first investigation focuses on the proton transfer reaction occurring at triple phase boundary (TPB) regions formed by BZY, a metal catalyst, and a hydrogen-rich gas phase. This study shows that the spilling process of hydrogen atoms from the surface of the metal catalyst onto the electrolyte surface is energetically favored at peripheral sites of the metal-electrolyte interface, and that the proton incorporation process into the sub-surface region of the electrolyte involves energies of the order of about 1 eV. At the TPB, the energy cost associated with the proton transfer reaction is controlled by both the chemical congruence and the Schottky barrier at the metal-electrolyte interface. In the second study, I will discuss our recent computational effort to interpret a set of experimental observations to elucidate the structure and fast proton transport properties of strained ultrathin films of BZY grown by pulsed laser deposition on $NdGaO_3$ substrates. This study shows that the BZY films incorporate a significant amount of Y dopants substituting for Ba^{2+}, and that in regions rich in Y substitutions for both Zr and Ba, the proton transfer process involves nearly zero-energy barriers. These results, together with the experimental observations, indicate that A-site cation substitutions by Y lead to fast transport pathways in BZY and hence they are responsible for the experimentally observed enhanced values of the proton conductivity of these oxide films. I will conclude this talk by presenting an outlook of our computational research on solid electrolytes.

MARM 49

Electrochemical H_2 evolution on crystalline Ni3P and its and its structural activity correlation to a series of nickel phosphide catalysts

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Electrochemical water splitting has more than an order of magnitude larger energy density than even the most powerful batteries (~142MJ/kg H_2 vs ~9MJ/kg Li-ion batteries). The former, therefore, promises to be essential for the development and application of renewable energy sources, like solar and wind, in a future sustainable energy society. In addition to storing energy, hydrogen (H_2) from water splitting also offers an environmentally friendly source for sustainable fertilizer production. On the laboratory and industrial scale, the archetypical electrocatalyst for acidic H_2 evolution is platinum (Pt), a scarce and globally unevenly distributed element. Over the past decades, several transition metal compounds (nitrides and sulfides) have shown good activity for H_2, but a huge gap remained in activity to match Pt. Since 2013, many transition-metal phosphides have been reported as potential replacements for Pt. Recently, we reported a nickel phosphide compound, Ni_5P_4 with electrical efficiency comparable to Pt (based on electrode area) and with excellent corrosion resistance in both strong acid and alkali during H_2 evolution. Here, we present the synthesis and benchmarking of Ni_3P, another member of the extensive nickel phosphide family of stoichiometric crystalline compounds. Due to instability of pure nickel in strong acid and alkali, nickel-rich electrocatalysts (or low phosphorus) are expected to be unstable in acidic electrolytes. By contrast, here we demonstrate that crystalline Ni_3P shows high activity and excellent stability in both acid and alkaline solution. We have used structural analysis, with a basis in the previously published DFT calculations, to offer insights into the systematic trends in both electrocatalytic efficiency and corrosion stability of the extended nickel phosphide series. Additional new insights in surface reconstructions, based on DFT calculations, show great promise in rationalizing the activity trend across the nickel phosphide series (Wexler, R. B. , Rappe, A. M., et al under preparation). Supported by a joint DOE-EERE/NSF-CBET grant, NATCO, DOE-BES, DOE, NSF, NERSC, & Rutgers.

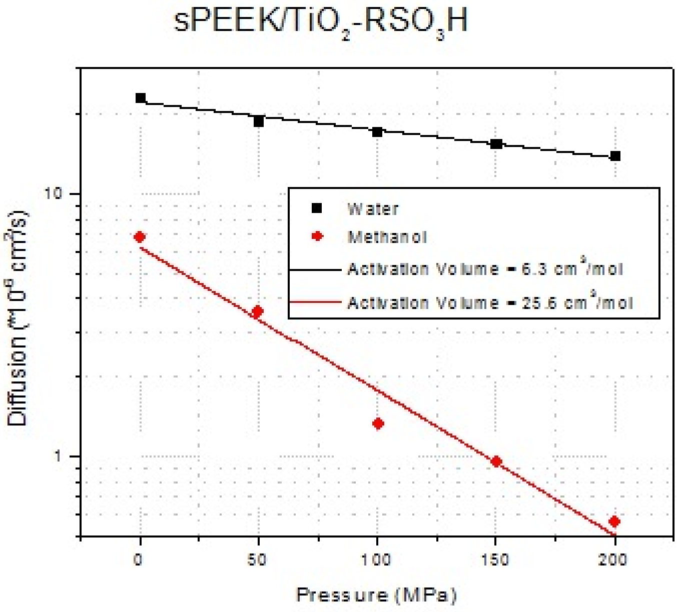
MARM 50

High pressure NMR diffusion studies on sPEEK membranes with an organically modified titania nanofiller

Catia de Bonis[5]*, Cataldo Simari*[6]*, Vasiliki Kosma*[6]*, Barbara Mecheri*[5]*, Alessandra D'Epifanio*[5]*, Valentina Allodi*[8]*, Gino Mariotto*[8]*, Sergio Brutti*[2]*, Sophia Suarez*[1]*,* ***Kartik Pilar***[7,4]*, kp383@hunter.cuny.edu, Steven Greenbaum*[7]*, Silvia Licoccia*[3]*, Isabella Nicotera*[6]*. (1) Brooklyn College of CUNY, Brooklyn, New York, United States (2) Dip.Scienze, Un Basilicata, Potenza, Italy (3) Univ of Rome Tor Vergata, Rome, Italy*

(4) Physics and Astronomy, CUNY Graduate Center, New York, New York, United States (5) Chemical Science and Technologies, University of Rome, Rome, Italy (6) Chemistry and Chemical Technologies, University of Calabria, Cosenza, Italy (7) Physics, Hunter College, New York, New York, United States (8) Informatica, Universita di Verona, Verona, Italy

Nuclear magnetic resonance (NMR) diffusion measurements were obtained for three types of sulfonated Poly Ether Ether Ketone (sPEEK) membranes, which show potential for use as an electrolyte in direct methanol fuel cells (DMFCs). sPEEK membranes were either kept pristine, contained 10% TiO2 nanofiller, or contained 10% organically functionalized titania nanofiller, TiO2-RSO3H. Membranes were fully hydrated with either 2M H2O/CD3OD or 2M D2O/CH3OH, allowing us to observe diffusion rates of water and methanol separately. Measurements were completed at 303 K and 328 K at variable pressure between ambient pressure and 200 MPa. Measurements were taken in the static field gradient, measured to be 21 T/m, of a 7.3 T Chemagnetix NMR magnet as a pulsed field gradient can't be used in combination with the high pressure Cu-Be NMR probe. Self-diffusion activation volumes were calculated for each set of pressure measurements. The results indicate that the nanofillers decreased the activation volume for water at both temperatures, with the organically modified titania nanofiller having the smallest activation volume. The nanofillers were also found to increase the activation volumes associated with methanol diffusion, with the organically modified titania nanofiller showing the largest activation volume here. This indicates there is a larger barrier to methanol diffusion in sPEEK membranes containing the organic nanofiller, while the nanofillers simultaneously reduce the barrier to water diffusion. These properties show that sPEEK membranes may be an attractive alternative electrolyte, to the more commonly used Nafion, in DMFCs.



Graph depicting both water and methanol diffusion in sPEEK membranes with organically modified titania nanofiller at 55°C

MARM 51

Advancing knowledge of f-element separation science to close the nuclear fuel cycle

***Kenneth L. Nash**, knash@wsu.edu. Washington State University, Pullman, Washington, United States*

The existential challenges to life, liberty, and the pursuit of happiness that could be imposed by a changing global climate strongly encourage careful consideration of all varieties of low emission power production for the increasingly crowded planet Earth. Every option that reduces greenhouse gas emissions that can be exploited or expanded must and should be considered. Arguably, the most controversial option is still fission-based nuclear power. Despite its high energy density, captured and contained waste products, high reliability of power generation, near zero greenhouse gas emissions and comparatively compact footprint, opposition to expanding nuclear power continues (outside of a few countries) based principally on 1) memory of three power reactor accidents, 2) fear of the spread of nuclear weapons and of a return of Cold War international tensions, and 3) the multiple thousand year radioactive half-lives of a small suite of by-products of fission. The comparative scarcity of fissionable uranium and thorium resources is another factor less frequently discussed. These several issues could be intelligently addressed by adopting a closed loop fuel recycling system dedicated to maximum utilization of the resources available. Born of the Cold War emphasis on the production of weapons-usable materials by a small number of countries and decades of complementary research on advanced systems to support transmutation, the basic separation science and technology needed to close the nuclear fuel cycle is generally available. Contemporary global research and development on advanced nuclear fuel cycles targets improving the utilization of this resource while enhancing waste management options and minimizing the potential for weapons diversion of weapons-usable materials. In this presentation, selected features of ongoing research supporting advanced recycling options for nuclear fuels will be discussed. Portions of the work discussed have been supported by the U.S. Department of Energy, Office of Nuclear Energy, Fuel Cycle Research and Development program under several Nuclear Energy Research Initiative, Nuclear Energy University Programs, and the Sigma Team for Minor Actinide Separation projects.

MARM 52

Lessons learned through SCHB's Palladium Science Academy

***George W. Ruger**, gruger@nicepak.com. Palladium Science Academy, Modena, New York, United States*

The Small Chemical Business Division offers numerous resources for helping entrepreneurs realize their full potential. Using some of the tools that the Division offers has helped me to turn my idea into a reality. I will talk about what techniques were successful and which ones were not as I developed my business plan and started to implement my ideas. Some areas of value that I will discuss are social media tools for spreading my message to increase leads and how to plan a realistic budget and time frame. The Division also offers mentoring through the Chemical Angel Network (CAN). Using the mentoring has helped me focus my ideas and use resources that I would otherwise not have access to.

MARM 53

Entrepreneurship through STEM outreach

***Christin B. Monroe**[1,2], monroe@princeton.edu. (1) Chemistry, Princeton University, Princeton, New Jersey, United States (2) Christin Monroe and Associates, Flemington, New Jersey, United States*

Entrepreneurship boils down to creating businesses to solve problems. A problem our country faces is a lack of undergraduates majoring in Science, Technology Engineering and Mathematics (STEM) careers. In fact, only 5% of undergraduates earn college degrees in STEM fields. We present herein a design of a unique STEM outreach program that will bring together selected high school students, graduate students and professional scientists from the triad of academia, industry and government. We will expose all students to the vast array of opportunities in STEM fields, stimulate entrepreneurship, via professional development workshops.
Workshop topics will include: 1) networking strategies, 2) interview strategies, 3) resume building/ LinkedIn profiles, 4) how to be a mentee and mentor, 5) navigating primary literature and presentation strategies and 6) scientific entrepreneurship. The career seminar will give students a vision of the future for careers in STEM. Selected participants will research a significant discovery in science and assemble a final assignment. We will bring a community of scientists of all experience levels and backgrounds to showcase the vast opportunities that exist in STEM. **This program represents the first steps in creating my own business** that centers on encouraging more students to pursue careers in STEM to build the workforce of the future.

MARM 54

Chemistry and alternative career opportunities

Carl J. Abraham[1,2], *cjabraham1@aol.com. (1) Scientific Advisory Svc Ltd, Great Neck, New York, United States (2) ForceField (NA), LTD, Great Neck, New York, United States*

Chemistry majors have a limited number of opportunities in pursuing a career after receiving their academic degrees. They can pursue careers in teaching, industry or the government. Other opportunities exist in consulting and inventing if one is capable of adding a few related disciplines and credentials to the basic training in chemistry.

After ten years of working in industry and teaching, the author has pursued a career in consulting and inventing products for the last forty-five years. Most of the products that were invented were first patented, and then manufactured and placed in the stream of commerce. They involved the use of the author's background in chemistry and many of its applications. The products ranged from sports and recreational activities to industrial and consumer products.

The consultation aspect of the author's career over the last forty-five years has been very rewarding. The subject matter involved has expanded to many subject areas beyond chemistry and are not taught in any university. They are self taught or learned from other specialists in other disciplines.

The presentation will cover the alternative opportunities for scientists in the areas of inventions and consulting.

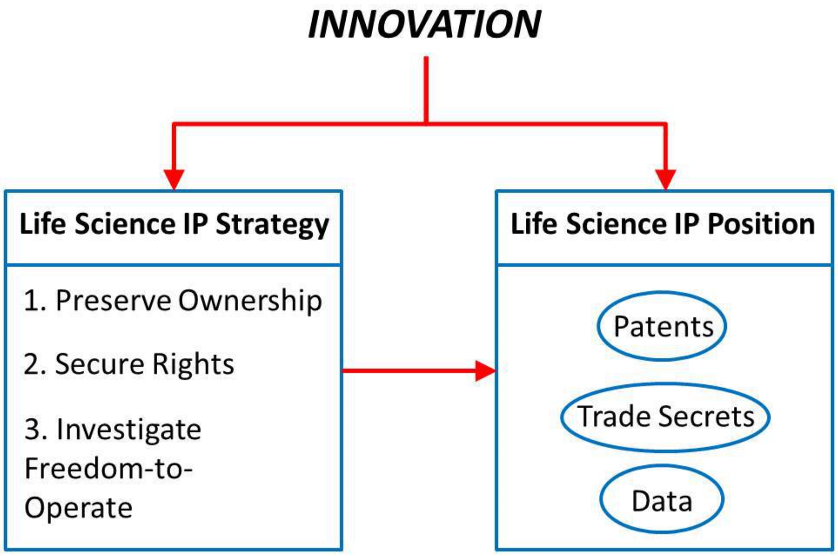
MARM 55

Establishing an IP position for new life science companies

Thomas Walls, *Thomas.walls@morganlewis.com. Morgan Lewis & Bockius LLP, Philadelphia, Pennsylvania, United States*

Intellectual property and preclinical/clinical data are the lifeblood of the pharmaceutical and biotech industry. However, new life science companies should think about more than just filing patents.

Cultivating a robust intellectual property position means securing legal protection for marketable research while developing an intellectual property strategy for shepherding new developments on their way to the marketplace. Along the way, a company should also be mindful of protecting both preclinical and clinical data associated with new developments. This talk will discuss certain aspects of a life science company's intellectual property strategy. With respect to potential commercial products, an intellectual property strategy should include: (1) establishing intellectual property and data exclusivity, (2) securing data use rights and intellectual property protection for potential commercial products of sufficient scope and duration, and (3) investigating or clearing potential freedom-to-operate issues for commercial products.



MARM 56

From dream to reality: The experiences which led to the creation of a small chemical enterprise

Lagree M. Burke, *mburkephd@cox.net. ASIR Materials Corporation, Bronx, New York, United States*

ASIR Materials Corporation was launched, in 2015, as a small business which specializes in materials primarily for the electronics industry. In addition to servicing this niche market, ASIR also provides contract research consulting and assistance for other markets as well. The genesis of ASIR Materials started as the investment in corporate R&D activities declined. Moreover, the Small Chemical Business Division (SCHB) of the American Chemical Society was a instrumental influence, providing sound insight, which led to the formation of the company. The chronicles, that enabled the formation of this entity will be discussed.

MARM 57

An entrepreneurial journey: Creating the quantified skin category. A Fitbit for your skin!

Rahul Mehendale, *Rahul@myskininc.com. mySkin Inc, Jersey City, New Jersey, United States*

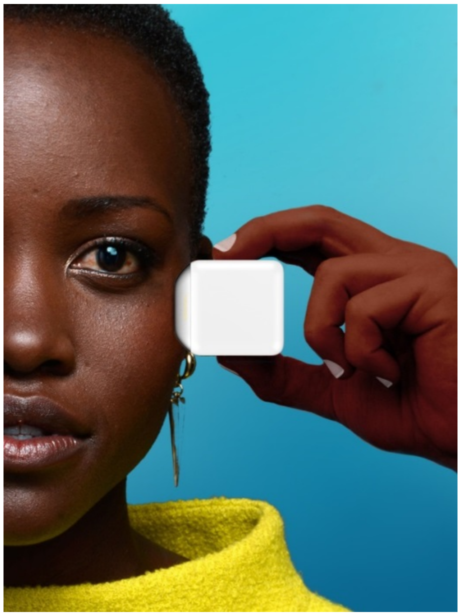
mySkin is creating the quantified skin category - we are using Sensors + Data + Great Software to transform skin and beauty.

Ours is a story of a guy who grew up in India teaming up with his Harvard friend - a US Army Ranger and both getting into the pursuit of cracking the code on skin health. We founded mySkin in 2007.

We recently announced OKU: the first personal skin coach – it is like a FitBit for your face and connects to the mobile phone. This is a category creator like Kindle, iPAD, Clairsonic, each of which has become a huge franchise.

A recently completed consumer test showed that women could not live without OKU, gained insight into their skin, and effected behavior changes along the dimensions of Lifestyle, Diet and Product usage.

https://www.youtube.com/watch?v=qkEjo5Dazw4



MARM 58

Structural analysis of extremely confined gases inside a lipophilic cage molecule

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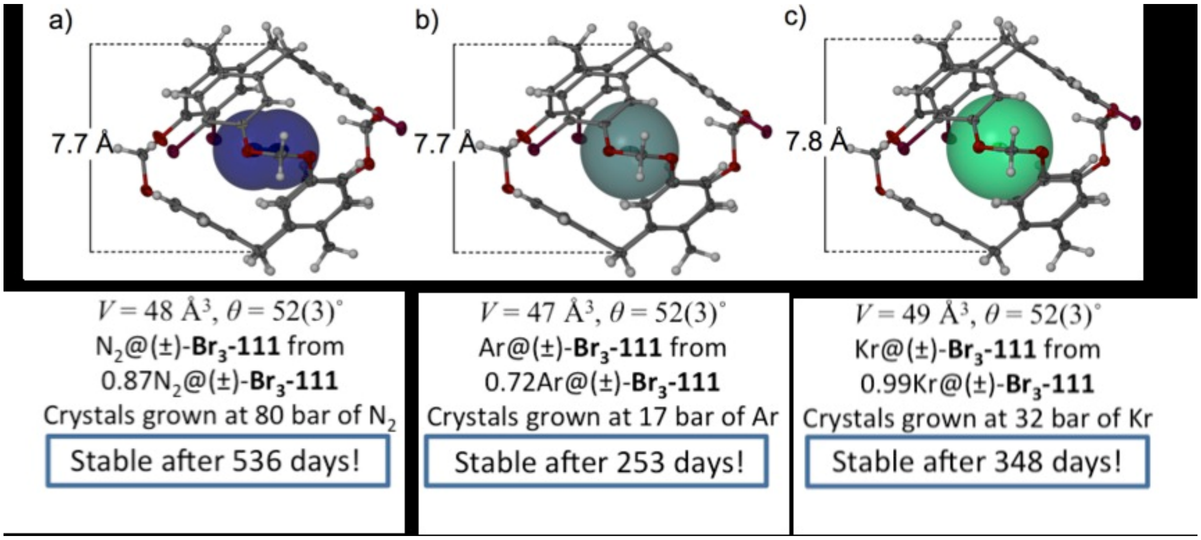
Porous host-guest complexes and assemblies have been developed in the past decades for the study of interactions based on hydrogen bonds, van der Waals forces, and hydrophobic interactions for a wide range of applications including gas storage, separations, and sensing. Discrete molecules with [ultra]microcavities are not formally defined as being porous, however possess molecule-sized void spaces allowing the formation of inclusion complexes similar to ultramicroporous materials. In 1981, Andre Collet introduced macrocycles with a defined hydrophobic cavity where the guest can be entirely "contained" inside. Cryptophanes have been extensively studied related to their ability to selectively

encapsulate small molecules and gases. The smallest cryptophane, known as cryptophane-111 (**111**), has a cavity size limited to ~ 73 Å^3, thus allowing it to be an excellent host for small gases like H_2, CH_4, Xe, C_2H_4, and C_2H_6. In fact, **111** exhibits the highest affinity for Xe (V_{vdW} = 42 Å^3) in organic solvents with a binding constant of 1×10^4 M^{-1}at 293 K and a very slow decomplexation rate. We envision that cryptophanes may have intriguing properties towards materials that exhibit porosity “without pores” or display extreme confinement of gaseous species purely by van der Waals forces. A functionalized derivative of **111**, trisbromocryptophane-111, (±)-**Br_3-111** was successfully synthesized by the heterocapping of (±)-**CTP** with trisbromocyclotriphenolene (±)-**Br_3-CTP**. Single crystal X-ray diffraction data were obtained for the guest free (±)-**Br_3-111** host as well as for complexes of N_2, Ar, Kr, and Xe in order to better understand gas confinement.



$V = 48$ Å^3, $\theta = 52(3)$°
N_2@(±)-**Br_3-111** from
0.87N_2@(±)-**Br_3-111**
Crystals grown at 80 bar of N_2
Stable after 536 days!

$V = 47$ Å^3, $\theta = 52(3)$°
Ar@(±)-**Br_3-111** from
0.72Ar@(±)-**Br_3-111**
Crystals grown at 17 bar of Ar
Stable after 253 days!

$V = 49$ Å^3, $\theta = 52(3)$°
Kr@(±)-**Br_3-111** from
0.99Kr@(±)-**Br_3-111**
Crystals grown at 32 bar of Kr
Stable after 348 days!

Thermal ellipsoid plots of small gas complexes of **Br_3-111**

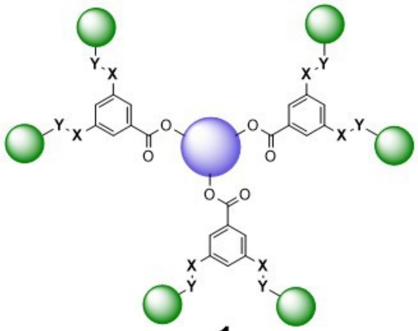
MARM 59

Fine tuning dendrimers and block co-polymers for the removal of pollutants from aqueous environments

Amy M. Balija, *amy.balija@gmail.com. Chemistry, Fordham University, Fair Lawn, New Jersey, United States*

The growing global population in combination with increasing amounts of environmental pollutants has increased the need for improved methods of removing organic pollutants from water supplies and the environment. Polymer-based strategies for water purification offer advantages over activated carbon, the standard absorbent for removing organic pollutants. However, many polymer-based water purification systems utilize a “patching” approach in which the periphery of a known architecture is modified with specific functionalities to encapsulate small molecules. Research in our group targets new macromolecules for water purification by altering the monomers, not just by modification of a known scaffold. Two types of macromolecules are of particular interest: dendrimers (**1**) and biodegradable block co-polymers (**2**). Optimization of these structures is underway to discover new systems capable of more efficient removal of organic pollutants from water. In this presentation, the design, synthesis and

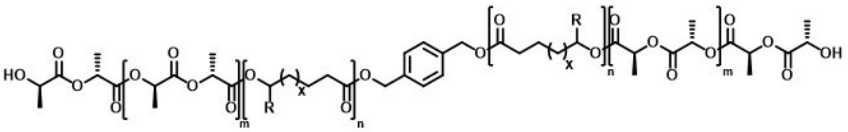
evaluation of these systems will be discussed. Initial studies indicate that small changes in composition has led to drastic changes in the ability for the macromolecule to remove model aromatic pollutants.



1

X = CH_2 or O 🟢 = Phenyl or C_6H_{11}

Y = O or CH_2 🔵 = Core



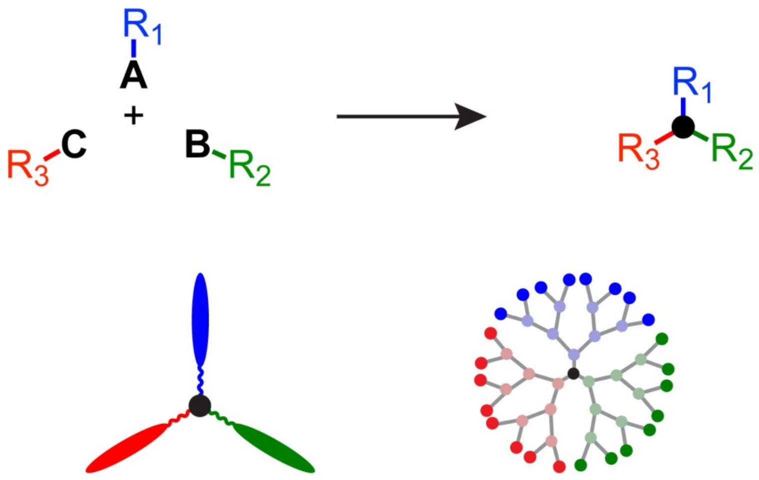
2

MARM 60

Multicomponent reactions for controlling heterofunctionality

Jonathan G. Rudick, *jon.rudick@stonybrook.edu. Chemistry, Stony Brook University, Stony Brook, New York, United States*

Multivalent display is a privileged tool for enhancing interactions between weakly self-assembling groups. Because they are conveniently synthesized, monolithic arrays presenting a discrete number of a single self-assembling unit have established the role that multivalency plays in binding of receptors through to stabilization of liquid crystalline mesophases. Heterolithic arrays that combine several different self-assembling units are less well characterized because controlling heterofunctionality adds significant synthetic complexity. Comparisons have revealed that well-defined heterolithic materials can exhibit properties that are unique from those of materials obtained though random multifunctionalization strategies. This presentation will discuss in the context of self-organizing liquid crystalline materials how multicomponent reactions have been employed to create well-defined heterolithic multivalent architectures.



MARM 61

The self-assembly of periodically sequenced polypeptides confined at interfaces

Raymond S. Tu, *tu@ccny.cuny.edu, Matthew L. Kubilius. Chemical Engineering, The City College of New York, New York, New York, United States*

Periodically sequenced peptides can be confined to interfaces and assembled into patterns that present chemical functionalities with exceptional spatial precision. These rationally designed peptides and polypeptides are rapidly becoming useful components in nanostructured materials for applications ranging from drug delivery to energy storage. This presentation will examine several fundamental aspects of self-assembly and pattern formation of well-defined sheet forming peptides confined at interfaces (see figure). Our approach involves three steps. (1) We design and synthesize simple periodic peptide sequences, yielding surface-active b-strands that self-organize into aggregates to form patterns as a function of the peptide sequence. Rational peptide design allows us to systematically explore the role of hydrophobicity, electrostatics and molecular size on materials properties. (2) We use a set of interfacial characterization tools to examine in intermolecular assembly and supramolecular mechanics of the self-assembled structures. (3) We apply two-dimensional equations of state that define both the phase behavior and the critical surface concentrations of nascent aggregates at the interface. Subsequently, we can apply these parameters to predict the dimensions of pattern formation and to determine the potential of the peptide assemblies as biomimetic materials.

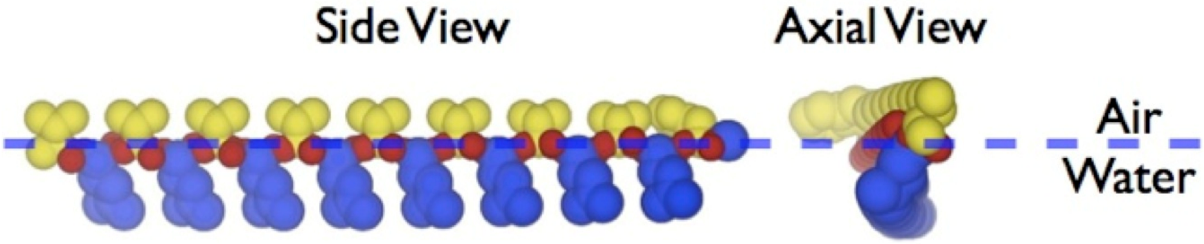


Figure. A periodically sequenced peptide confines a b-strand structure to the air-water interface, hydrophobic (yellow) and hydrophilic (blue) amino acids.

MARM 62

Cyclodextrin-promoted energy transfer for non-covalent interactions and toxicant detection

Mindy Levine[1], *mindy.levine@gmail.com, Dana J. DiScenza*[2], *Nicole Serio*[1]. *(1) University of Rhode Island, Sharon, Massachusetts, United States (2) Chemistry, University of Rhode Island, Pomona, New York, United States*

Research in the Levine group focuses on macrocycle-promoted, non-covalent energy transfer from small molecule toxicants to high quantum yield fluorophores. This research includes fundamental investigations of the structure-property relationships that govern how molecules interact when they are in close proximity but not covalently attached, and it also includes applications of these systems in the detection of carcinogens in biological fluis and in the environmental remediation of oil spills.

MARM 63

History of Regents chemistry: An exploration of the development and impact of science education in NYS

Thea Charles, *thea.charles@stonybrook.edu, Keith Sheppard. Institute for STEM Education, SUNY Stony Brook, New York, New York, United States*

Science has a long and important history in American education and society, but few realize how long and important because little historical research is reported (Bybee, 1982). Not only is there an abundance of missing historical research, even reference in current publications to the historical research that has been conducted is limited. The K - 12 science education field has been in a “crisis” driven reform period for decades. Science education has a long history and many occasions to repeat the past. If the field does not continue to evolve then the work done by the pioneers in the field could go to waste and future generations could stand to lose an immense and critical opportunity for intellectual development. Regents Chemistry is an interesting lens through which one can explore science education because it was established in NYS, currently the largest and most diverse K - 12 education system in America. In addition, an exploration of the system can reveal insight into the origin and impact of many aspects of high school Chemistry that we still see today.

MARM 64

Biochemistry in NY section ACS

Donald D. Clarke, *clarke@fordham.edu. Chemistry, Fordham Univ, Bronx, New York, United States*

Biochemistry in the modern sense is generally attributed to Eduard Buchner who got the Nobel Prize in chemistry in 1907 for study of fermentation in cell-free yeast preparations. Digestive enzymes had been known well before that but were considered to be extracellular ferments. This was a European development that eventually spread to the U S A. Another track for such developments was the use of isotopic labeling of substrates to trace metabolic pathways. This was primarily a US development, which got its real start with Urey’s isolation of Deuterium at Columbia University that earned the Nobel Prize for Chemistry in 1934. National ACS designated the Chemistry department there as a National Historical Chemical Landmark. The biochemistry department of Columbia’s College of Physicians and Surgeons followed up on this by using D labeled fatty acids and amino acids to trace the path of metabolism of such

substrates. Under the leadership of Hans T Clarke, the 1947- 48 chair of the NY section of the ACS this department became one of the premier biochemistry departments in the USA. Biochemistry was taught most often in Medical schools and the emphasis there was on measuring levels of metabolites to establish normal vs disease states. The most notable individual in this area was D D Van Slyke at the Rockefeller Institute. This group grew away from the NY section to form the American Association of Clinical Chemists in 1948.

MARM 65

The Hickrill Chemical Research Foundation: A unique institution, a fascinating tale, and cutting-edge chemistry

Leon Gortler[1], *leonselma@gmail.com, Stephen J. Weininger*[2]. *(1) Chemistry, Brooklyn College, Brooklyn, New York, United States (2) Chemistry, Worcester Polytechnic Institute, Brookline, Massachusetts, United States*

A conversation, in 1946, between Ruth Alice Weil, a Columbia graduate student, and her mentor, William Doering, resulted in the formation of a small laboratory in Katonah, New York that had a significant impact on the development of organic chemistry. The laboratory, which only lasted for 10 years, made important contributions to aromatic chemistry and to carbene chemistry. This paper will review the formation of the laboratory, its major contributions, and the important players in its development and success.

MARM 66

From anonymity to Nobel recognition: Women chemists, their publications

Ronald Smeltzer, *rksmeltzer@verizon.net. Ronald Smeltzer, Princeton, New Jersey, United States*

New York's Grolier Club, the nation's leading society for bibliophiles, has highlighted the history of chemistry in three exhibitions since the organization's founding more than 130 years ago. Very recently, a major exhibition focused on the contributions of women to the physical sciences. Based upon the research done, and the discoveries made, for this recent exhibition, the publications of five chemists—Marie Meurdrac (1610?–1680), Marie-Geneviève-Charlotte Thiroux d'Arconville (1720–1805), Elizabeth Fulhame (fl. 1780–1794), Dorothy Crowfoot Hodgkin (1910–1994), and Rosalnd E. Franklin (1920–1958) will be described to highlight aspects of publication history over four centuries.

The most curious feature of this publishing history is that until the late eighteenth century most women apparently preferred to not have their names associated with their publications, although their identities were known to their contemporaries. Title pages sometimes have only initials or an oblique reference to the identity of the author. The transition from books to periodicals as the primary medium for publication will be evident as the publishing histories of the five women are described.

Aspects of printing history and methods will be invoked in descriptions of some of the publications of the five women. In the case of Meurdrac, for example, a previously unnoticed typesetters error was shown—from both the printed text and the paper of the title page—to be the origin of first editions wrongly dated 1656 instead of 1666. Aspects of the development of methods of printing, especially for illustration work, will be described.

MARM 67

William H. Nichols entry into 19th century chemical industry

***Peter W. Corfield**, pwrc@earthlink.net. Chemistry, Fordham University, Briarcliff Manor, New York, United States*

William H Nichols was a remarkable man who had great influence on the young New York chemical industry. He and his friend Charles Waters started manufacturing mineral acids when he was only eighteen. He eventually founded the General Chemical Company, which after many mergers and acquisitions became the Allied Chemical Corporation. He was noted for his entrepreneurial spirit, for bringing scientific principles into manufacturing, and for high ethical standards. As a mature industrial chemist, Nichols funded the gold medal for the New York Section's new annual research award in 1902. This became the first national award of the American Chemical Society, now known as the William H. Nichols Medal Award. The presentation will explore Nichols' contributions in the context of the state of chemical industry in New York during the latter part of the nineteenth century.

MARM 68

Donald F. Othmer: His life and legacies

***Ronald S. Brashear**, rbrashear@chemheritage.org. Chemical Heritage Foundation, Philadelphia, Pennsylvania, United States*

Donald F. Othmer (1904–1995) had a profound impact on chemistry and chemical engineering during his life, from his early work at Kodak, through his work and students at Brooklyn Polytechnic University, through the *Kirk-Othmer Encyclopedia of Chemical Technology*, to his consulting work and numerous patents. His shrewd investments also allowed Othmer and his wife and inseparable companion, Mildred Topp Othmer, to have a great impact on many institutions after their deaths in 1995 and 1998, respectively. This paper will follow the life and career of Donald Othmer starting with his education, primarily at the Universities of Nebraska and Michigan. After receiving his Ph.D. in chemical engineering, he went to work with Kodak in Rochester, NY, but with the Great Depression and not being able to recoup much benefit from the patents he obtained for Kodak, he went into academia, obtaining a position in the newly-independent chemical engineering department at Brooklyn Polytechnic which allowed him to have a private consulting practice. Othmer consulted for hundreds of companies and traveled to many countries with Mildred and claimed some 150 patents for improvements on a wide variety of chemical processes. Othmer was involved in diverse projects such as the distillation of kerosene in Burma/Myanmar, on desalination for the U.S. Department of Commerce, and the publication of the *Kirk-Othmer Encyclopedia* with his colleague at BPU, Raymond Kirk. By the end of their lives, Donald and Mildred Othmer had an estate valued at $800 million and left much of it to several institutions that were important in their lives. One of those is the Chemical Heritage Foundation in Philadelphia, PA, which now houses the Donald F. and Mildred Topp Othmer Library of Chemical History.

MARM 69

A reflection on chemistry in New York over the past 125 years

***John B. Sharkey**, johnbsharkey@me.com. Chemistry, Pace University, Mountainside, New Jersey, United States*

Once can trace the start of chemistry in New York, or New Amsterdam as it was then called, to the distillation of brandy in 1640. The first chemical activities of the new colony involved the production of such commonplace articles as leather, beer, distilled liquors, tile and brick, whale oil, stoneware, sugar and the other numerous needs of everyday life. As we celebrate the 125th anniversary of the New York Section of the American Chemical Society, this presentation will review some highlights in chemistry in more recent times, through the National Historic Chemical landmarks Program. Since 1993 there have been seven such Chemical Landmarks within the New York Section.

MARM 70

Microwave reactors as tools in organic chemistry lab courses

***C Kappe**, oliver.kappe@uni-graz.at. Institute of Chemistry, University of Graz, Graz, Austria*

High-speed microwave synthesis has attracted a considerable amount of attention in recent decades. Since the first reports on the use of microwave heating to accelerate organic chemical transformations by the groups of Gedye and Giguere/Majetich in 1986, more than 10000 articles have been published in the area of microwave-assisted organic synthesis (MAOS). The initial slow uptake of the technology in the late 1980s and early 1990s has been attributed to its lack of controllability and reproducibility, coupled with a general lack of understanding of the basics of microwave dielectric heating. The risks associated with the flammability of organic solvents in a microwave field and the lack of available systems for adequate temperature and pressure controls were major concerns. Since the late 1990s the number of publications related to MAOS has therefore increased dramatically to a point where it might be assumed that, in a few years, most chemists will probably use microwave energy to heat chemical reactions on a laboratory scale. Not only is direct microwave heating able to reduce chemical reaction times from hours to minutes, but it is also known to reduce side reactions, increase yields and improve reproducibility. Therefore, many academic and industrial research groups are already using MAOS as a forefront technology for rapid reaction optimization, for the efficient synthesis of new chemical entities, or for discovering and probing new chemical reactivity.

In this lecture we will highlight the use of a novel and easy-to-use lab scale microwave-type reactor as tool in organic chemistry labs.

MARM 71

Necessity is the mother of invention: Development of a green undergraduate laboratory experiment demonstrating the E1 reaction utilizing a microwave reactor and resin based acid catalyst

*Feiby Abdelnoor, Youssef Fardos, Monica Samy Girges, Sara K. Hussein, Diana Mejia, **Robert G. Aslanian**, raslanian@njcu.edu. Chemistry, New Jersey City University, Jersey City, New Jersey, United States*

The discussion of E1 and E2 reaction mechanisms is an integral part of the undergraduate Organic I curriculum, and the theory is usually illustrated with a hands-on experiment in the Organic I laboratory. Typically, the students perform an acid-catalyzed E1 elimination of a substrate like 4-methylcyclohexanol by refluxing the alcohol in the presence of a strong acid catalyst system like sulfuric acid and phosphoric acid. We recently faced a dilemma at NJCU during the construction of our new science building when we could not run the elimination reaction in the usual manner due to a lack of suitable lab space. We addressed this problem by developing a new, green elimination protocol utilizing a resin based acid catalyst to replace the strong mineral acid catalyst and microwave heating to eliminate the need for a reflux condenser and running water. This presentation will outline the procedure we developed and its application to several secondary and tertiary alcohols.

MARM 72

Using microwave assist to stimulate a multiple component experiment to connect labs across the chemistry curriculum

Andrew S. Koch[1], *askoch@smcm.edu, Elan H. Bresslour-Rashap*[1], *Leah R. Eller*[2], *Kelly Neiles*[1]. *(1) St Marys Coll of Maryland, Saint Marys City, Maryland, United States (2) Patuxent River Naval Air Station, Lexington Park, Maryland, United States*

With the recent renewed interest in biodiesel and the search for catalysts that decrease waste and come from renewable sources, we have designed a series of undergraduate chemistry labs that follow the production of catalyst, synthesis of biodiesel, and analytical and thermo study of the final product. The production of calcium oxide from calcium carbonate, obtained from eggshells, makes for a great general chemistry lab that demonstrates conservation of mass, and teaches students to view all materials as natural resources. These students then contract the organic chemistry lab students to test their catalyst in the production of biodiesel. In the organic lab students prepare biodiesel using the catalyst provided by the general chemistry lab, and compare the quality of that biodiesel relative to biodiesel prepared by conventional methods using NMR spectroscopy. Using microwave-assisted synthesis of biodiesel allows time for student design, which fosters scientific method. The biodiesel samples can be further tested in the physical chemistry lab. The traditional bomb calorimeter lab in physical chemistry can serve as a second contract sources for students. The organic students send written reports back to general chemistry with their finding on biodiesel production, and contract the physical chemistry students to compare the energy content by mass and volume of their new fuel to that of regular diesel. This sort of multi-lab experience helps demonstrate the interdisciplinary nature of work in chemistry, helps foster good reporting habits, and demonstrates the relevance of standard techniques in solving current problems.

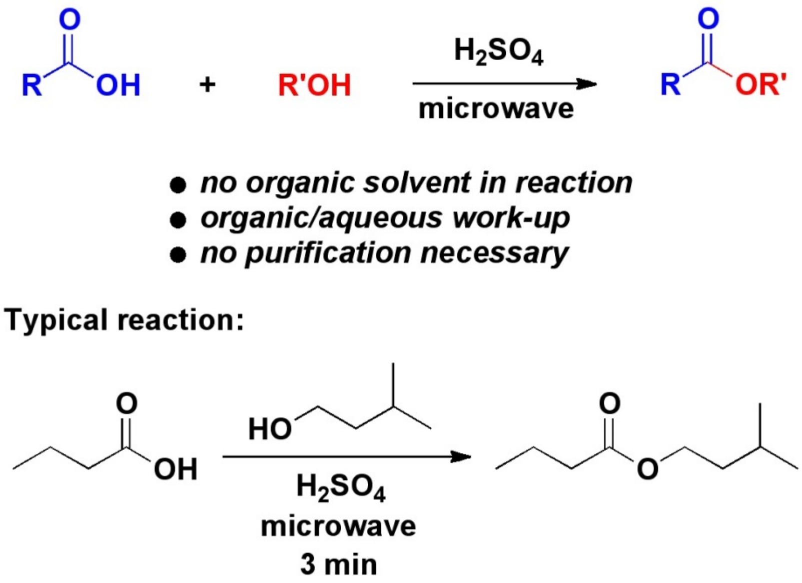
MARM 73

Microwave-assisted esterification: A discovery-based microscale laboratory experiment

Maureen Reilly[1], *Ryan P. King*[4], *Alexander J. Wagner*[3], ***Susan M. King***[2], *s3king@uci.edu. (1) Department of Chemistry, University of California Irvine, Irvine, California, United States (2) Chemistry, University of California, Irvine, Huntington Beach, California, United States (3) Chemistry, Scripps Research Institute, San Diego, California, United States (4) Chemistry, Massachusetts Instutute of Technology, Cambridge, Massachusetts, United States*

An undergraduate organic chemistry laboratory experiment has been developed that feautures a discovery-based microscale Fischer esterification utilizing a microwave reactor. Students individually synthesize a unique ester from known sets of alcohols and carboxylic acids. Each student identifies the best reaction conditions given their particular reagents (either excess alcohol or excess carboxylic acid) as well as the ideal work-up procedure for their reaction. Products are analyzed using ^{1}HNMR spectroscopy, IR spectroscopy, and scent. This modern adaptation of the classic Fischer esterification provides the

opportunity for discussion of important chemistry concepts, including acid catalysis, Le Chatelier's Principle, and green chemistry.



- *no organic solvent in reaction*
- *organic/aqueous work-up*
- *no purification necessary*

Typical reaction:

MARM 74

Investigations of factors controlling structures of metal-organic frameworks using microwave-assisted synthesis

Michael P. Masingale, *masingal@lemoyne.edu. Le Moyne College, Syracuse, New York, United States*

Student researchers designed and carried out projects whose purpose was the examination of factors that control the structures found for a variety of Metal-Organic Framework (MOF) compounds. The time savings that accompany the use of microwave assisted syntheses enabled students, for whom curricular demands left few contiguous hours for laboratory work, to carry out scientifically meaningful investigations. Investigations of the role of the metal ion, the metal-to-ligand mol ratio, solvent, temperature, microwave power, and time of synthesis on the structure of MOFs were investigated. The syntheses of two organic molecules used in the preparation of MOFs, and the incredible time saving achieved via microwave assisted synthesis, will also be described.

MARM 75

MIBLabs: A student-centered sophomore organic curriculum featuring microwave chemistry

S. Murphree[1], *smurphre@allegheny.edu, Jun H. Shin*[2], *Andrew S. Koch*[3]. *(1) Chemistry, Allegheny College, Meadville, Pennsylvania, United States (2) Chemistry, Queensborough Community College, Oakland Gardens, New York, United States (3) St Marys College of Maryland, Saint Marys City, Maryland, United States*

A laboratory curriculum has been developed for the sophomore Organic curriculum taking advantage of the rapid reaction times afforded by microwave-assisted organic synthesis (MAOS). A series of modules have been constructed to explore various types of chemistry (e.g., nucleophilic substitution, reduction, electrophilic aromatic substitution, etc.) embedded within a context of experimental design and data analysis, with the intent of providing a more authentic laboratory experience. Instructional materials have been developed and curated using an open-source web hosting service. The collection (MIBLabs) and individual modules will be presented.

MARM 76

National Science Foundation and broader impacts

***Eric Pfeiffer**, eripfeif@nsf.gov. National Science Foundation, Arlington, Virginia, United States*

At the National Science Foundation, all research proposals must address both the Intellectual Merits and the Broader Impacts criteria. The area of broader impacts may include scientific broader impacts, educational innovations, novel and/or far-reaching plans for dissemination, outreach activities and efforts to broaden participation, particularly efforts to engage women and members of traditionally underrepresented groups in the STEM disciplines. This presentation will highlight examples of broader impacts activities and staff will answer audience questions.

MARM 77

Future faculty, early career faculty, and new principle investigators: Interactions with NSF chemistry

***Sarah L. Stoll**, sls55@georgetown.edu. Georgetown University, Washington, District of Columbia, United States*

NSF Program Officers and Administrative Staff will provide a special session especially for future faculty, early career faculty, and new principle investigators. This session will focus on NSF basics: understanding the NSF Merit Review Criteria and review mechanisms. Presenters will give an overview of the NSF Division of Chemistry core research programs. Special emphasis will be given to submitting a Faculty Early Career Development Program (CAREER) or Research at Primarily Undergraduate Institutions (RUI) proposal.

MARM 78

NSF support for undergraduates, graduate students, and postdoctoral fellows

***Michelle Jenkins**, mjenkins@nsf.gov. National Science Foundation, Arlington, Virginia, United States*

This presentation focuses on NSF funding opportunities for undergraduates, graduate students and postdoctoral fellows. NSF Program Officers and Administrative Staff will discuss finding and applying for Research Experiences for Undergraduates programs. We will also discuss the Graduate Research Fellowships Program (GRFP) and international opportunities for graduate students, giving tips on how and when to apply. Finally, we will talk about Postdoctoral Fellowship Opportunities across the National Science Foundation.

MARM 79

Faculty interactions with NSF chemistry

***Lin He**, lhe@nsf.gov. National Science Foundation, Arlington, Virginia, United States*

This presentation is designed for faculty members at all institutions. NSF Program Officers and Administrative Staff will walk through several NSF solicitations and types of funding opportunities. We will focus on: Early Concept Grants for Exploratory Research (EAGER), Grant Opportunities for Academic Liaisons with Industry (GOALI), Major Research Instrumentation (MRI), Research Experiences for Undergraduates Site Proposals (REU Sites) and current initiatives: INFEWS, DMREF, BRAIN, SI2. We will also talk about supplemental funding opportunities for those investigators who already have NSF awards.

MARM 80

A personal Merck journey: Women in chemistry

***Rebecca Ruck**, rebecca_ruck@merck.com. K15-3MN3, Merck Co., Inc., Kenilworth, New Jersey, United States*

There is tremendous interest paid to increasing diversity and inclusion across STEM subjects. This emphasis has resulted in diverse career opportunities for talented female chemists across the pharmaceutical industry. This presentation will focus on my personal career progression within the Merck Process Chemistry organization. It will include scientific highlights from my time in the lab and from team members under my supervision. It will highlight the accomplishments of women and demonstrate my passion to recruit and retain women in chemistry. This has been achieved by building relationships with female graduate students and providing mentorship and sponsorship for these women as they enter the organization and grow into roles of increasing responsibilities.

MARM 81

Promoting the growth of an inclusive and accessible STEM ecosystem: Lessons from science outreach

***Jeanne Garbarino**, jgarbarino@rockefeller.edu. Science Outreach Program, The Rockefeller University, New York, New York, United States*

Advances in science and technology are happening at incredible rates, providing insights into complex and previously unfathomable concepts. As these science fictions transition into reality, our society is being shaped in new ways, carving paths for a new technology-driven workforce. Yet, despite the need for high quality STEM education in a competitive global economy, US students are continually outperformed in science and math by other developed nations. While some progress is being made, there is a stark contrast when it comes to access to STEM opportunities, particularly for women and people of color. Here I will discuss how The Rockefeller University Science Outreach Program is working to improve accessibility to scientific opportunity for multiple audiences, drawing on my personal experiences as a women in STEM.

MARM 82

Notes from the presidential task force on employment: Addressing the challenges of unemployment of young graduates and mid-career chemical professionals

Peter K. Dorhout[1], *dorhout@ksu.edu, William R. Ewing*[2]*. (1) College of Arts Sciences, Kansas State University, Manhattan, Kansas, United States (2) Committee on Economic and Professional Affairs, Yardley, Pennsylvania, United States*

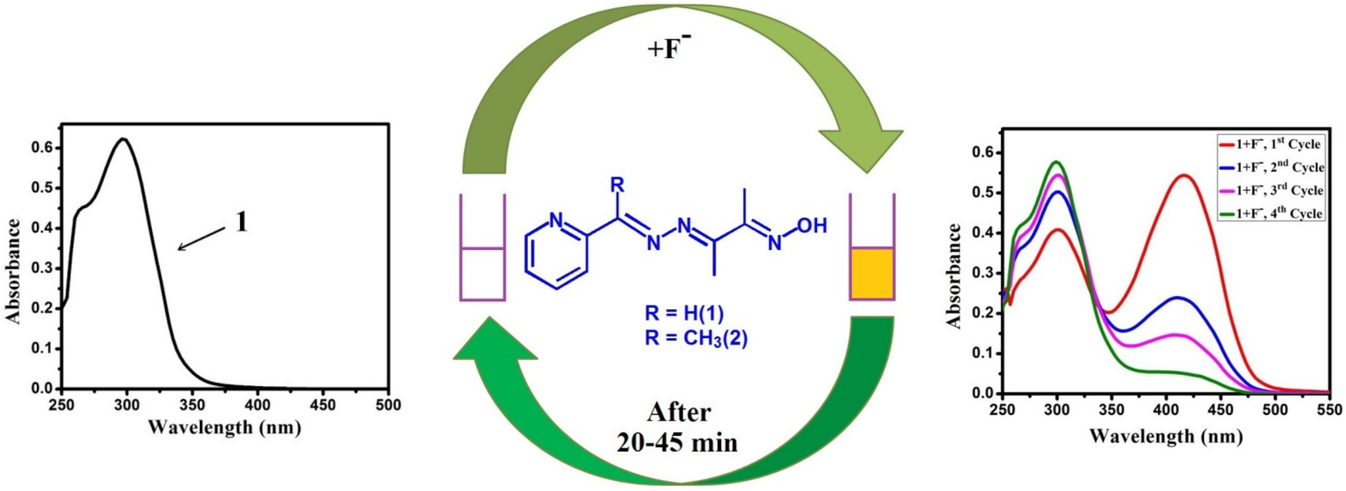
The supply and demand of chemists is affected by many interrelated factors such as the strength of the economy, the types of jobs available, the number of graduates, globalization and the prices of raw materials. There is a growing gap in unemployment percentages between established chemists and mid-career relative to recent graduates. Starting with the most recent recession in the late 2000's, that gap has been widening and not recovering, and the overall unemployment among chemists at all career stages has not fully recovered to pre-recession lows. Data suggest that the nature of the chemical industry is changing, which affects how we educate future practitioners, professionals, and non-chemists. This talk will present analyses of recent employment and industry data and how ACS has responded in the past to similar challenges along with suggestions as to how ACS could take the lead at changing professions to promote diverse learning opportunities and broaden the career sustainability of current and future ACS members.

MARM 83

Development of auto-reusable receptors for selective colorimetric recognition of fluoride

Suchibrata Borah*, s.borah1991@gmail.com, Nayanmoni Gogoi. Chemical Sciences, Tezpur University, Sivasagar, Assam, India*

A proof of principle study to devise auto-reusable colorimetric receptors for fluoride recognition based on H-bonding interaction is described. The design of receptors capable of binding fluoride ion efficiently and selectively in water *i.e.* for real-life applications is consequently a meaningful, however challenging task. Four new aliphatic oximes featuring additional aromatic ring are reported among which three are highly selective colorimetric receptors for fluoride ion recognition. The interesting part of the story is that two of the receptors are auto-regenerated after a short interval of binding with fluoride. However, H-bonding mediated binding of fluoride ion to both the receptors are reasonably labile, this allows reuse of both the receptors for colorimetric fluoride recognition upto three cycles without any need for reactivation.



MARM 84

Analysis of conventional and organically grown strawberries for the presence of chloropicrin using GC/MS

Patrick Tishion[1], *ptishion318@gmail.com, Jonathan B. Soffer*[3]*, Kevin Owens*[3]*, Kishore K. Bagga*[2]*. (1) Graduate School of Biomedical Sciences and Health Studies, Drexel University, Philadelphia , Pennsylvania, United States (2) Graduate School of Biomedical Sciences and Health Studies, Drexel University, Philadelphia, Pennsylvania, United States (3) Chemistry, Drexel University, Philadelphia, Pennsylvania, United States*

Chloropicrin is a fumigant pesticide used in many fruit and vegetable crops including strawberries. Acetonitrile extracts from conventional and organic strawberries were analyzed for chloropicrin residue from the fumigation process. Samples were prepared using an optimized pesticide extraction technique referred to as QuEChERS. Dispersive solid phase extraction removed potential interferences from sample extracts. Preliminary data from this work through method development indicates chloropicrin is detectable at concentrations of 0.01 ng/ml in standard solutions. Detector response suggests chloropicrin is detectable at 2-3 orders of magnitude lower than 0.01 ng/ml. Ongoing work to determine the lowest limit of detection and the concentration of chloropicrin (if any) in strawberry extracts will be discussed in this paper. Final data from this investigation carries potential public health implications.

MARM 85

Probing inhibitor-hIAPP interactions using spectroscopic techniques: A mechanistic study

Kendra Pamphille, *kendra.pamphille@yorkmail.cuny.edu, Ruel Desamero, Adam Profit. Chemistry, CUNY York College, Jamaica, New York, United States*

The human islet amyloid polypeptide (hIAPP)/amylin has been studied for decades primarily due to its correlation with blood glucose homeostasis. In recent decades hIAPP aggregation has been known to contribute to the onset of type II hyperglycemic diabetes. In fact, studies involving the examination of pancreatic tissue from cadavers with known Type II diabetes diagnosis have proven that there is a stark correlation between Type II diabetes and β-amyloid deposits. The primary structure of the hIAPP is the same in both diabetic and non-diabetic patients; hence peptide aggregates are caused by environmental factors or deviations in peptide activation. In order to, characterize and understand the assembly mechanisms and factors that drive fibril formation, and consequently β-amyloid deposits; a peptide database is constructed from hIAPP fragments. The wild and modified $hIAPP_{(30-37)}$ peptide fragments are then probed and monitored via various spectroscopic methods to assay peptide aggregation kinetics. In particular the $hIAPP_{(30-37)}$peptides each exhibit parallel beta sheet characteristics indicated by the presence of peaks at ~1675 cm^{-1} in Raman and ~1625 and ~1675 cm^{-1} in Infrared Radiation spectroscopic measurements.

MARM 86

Synthesis and characterization of CO_2 chemisorption sites in silica-based xerogels

Robert Neuweiler, *robert.neuweiler38@qmail.cuny.edu. Chemistry and Biochemistry, CUNY Queens College, Island Park, New York, United States*

Photocatalyzed reduction of carbon dioxide to methane occurs in nanoporous silicas doped with metal oxides. Carbon-13 isotope labelling shows that only chemisorbed carbon dioxide is reduced to methane, while diffuse reflectance FTIR (DRIFT) spectra suggest that chemisorbed carbon dioxide is first converted to a formic acid like species and then this species is reduced to methane via the Fischer-Tropsch sequence. The availability of these chemisorption sites, which in the case of porous Vycor glass (PVG), are formed during the manufacturing process. This is a major limitation on the conversion efficiency, characterizing the nature of these chemisorption sites, and their role in converting carbon dioxide to methane. Water, also involved in the conversion process competes with carbon dioxide by adsorbing to the hydroxylated surface of the silica matrix is another limiting factor in the efficiency of the conversion process. The presence of water in the glass matrix is monitored using near infrared (NIR) spectroscopy and quantified by thermal gravimetric methods. Since the conversion also occurs in metal oxide doped, base catalyzed tetramethoxysiliane/methanol/water (TMOS/CH_3OH/H_2O) xerogels, experiments have been undertaken to explore synthetic routes to increasing the number of chemisorption sites in these silica matrices. Here, we describe the syntheses of TMOS/CH_3OH/H_2O xerogels and the synthetic approaches and experimental conditions to increasing the number of carbon dioxide chemisorption sites within these nanoporous xerogels matrices.

MARM 87

Determining conformation of engineered protein fibers

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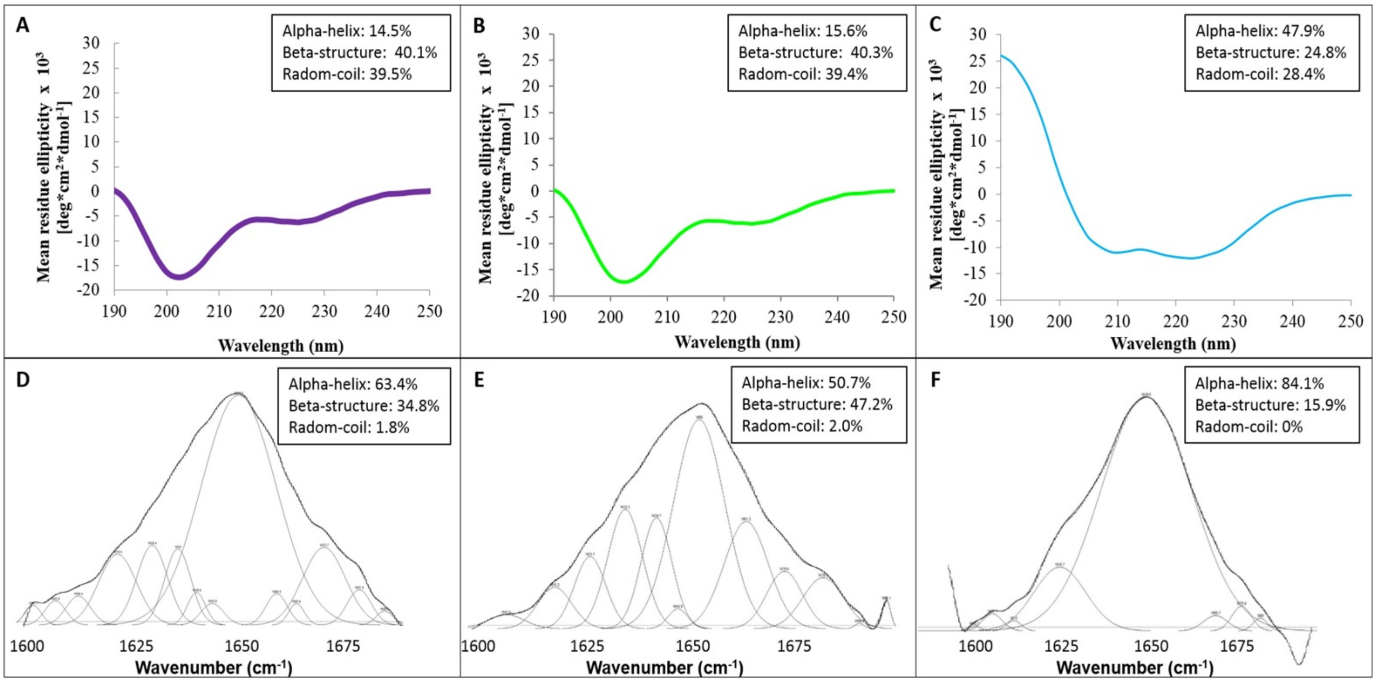
Because of their biocompatibility, proteins have become appealing drug delivery vehicles. Development of these therapeutics, however, relies on assessment of protein secondary structure and conformational characteristics to ensure suitable engineering for drug delivery. The N-terminus of the Cartilage Oligomeric Matrix Protein, COMPcc, is a pentameric coiled-coil motif. Our group has engineered this domain to create the protein Q, which maintains patches of positive and negative surface charges, allowing for lateral nanofiber assembly. Upon binding to the small molecule, curcumin, the protein Q further assembles into microfibers, which are subsequently stabilized by the chemical crosslinking agent bis(sulfosuccinimidyl)suberate (BS3). Both circular dichroism (CD) spectroscopy and attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) are employed to characterize the secondary structure of Q protein assemblies. We have found that ATR-FTIR and CD provide drastically different results and hypothesize that FTIR has improved accuracy given the that protein Q assembles into solid fibers. Using FTIR, we evaluate structural changes upon drug binding and crosslinking to ensure the maintenance of the coiled-coil structure which is optimal for drug delivery.



Comparison of protein Q nanofibers' secondary structure assessed by Circular Dichroism (CD) and Attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR). Insets reveal secondary structures calculated from the concentration-independent Raussens et al method for CD (**A-C**) or from the areas of the deconvoluted ATR-FTIR peaks (**D-F**). CD wavelength spectrum (**A**) and ATR-FTIR (**D**) were assessed for 10µM Q nanofibers at 25°C, revealing drastically different results between the two techniques. CD and FTIR analyses were also performed on Q fibers at 20µM after 100µM curcumin binding (**B,E**) and after subsequent crosslinking with BS3 reagent (**C,F**).

MARM 88

Studying the aggregation of hIAPP$_{12-18}$ using spectroscopic and microscopic techniques

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Alzheimer's disease, Prion disease, and Type II diabetes are characterized by the production of amyloid fibrils. However, there is still much to know about the mechanism behind amyloid fibril formation. We studied the process of amyloid formation using the 12-18 fragment (LANFLVH) of the human islet amyloid polypeptide (hIAPP), which is secreted by the pancreatic-β-cells and aggregates in Type II diabetes. The aromaticity of the amino acids in this fragment and in the regions 20-29, and 30-37 of hIAPP are considered to cause fibrillization. Previous work in our lab on the hIAPP$_{22-29}$ fragment has indicated that the π-electron distribution on the side chain of the phenylalanine residue modulates aggregation. The rate of aggregation increases when the aromatic ring of phenylalanine is electron poor, but it is decreased or eradicated when this ring is electron rich. In order to study the effect of π-electron distribution on fibrillization, we synthesized phenylalanine analogs and mutants of the LANFLVH fragment with electron donating and withdrawing groups. We employed transmission electron microscopy (TEM), Circular dichroism (CD), turbidity, fluorescence, Raman and Fourier Transform

Infrared measurements to study the mechanism of fibrillization on the phenylalanine analogs and mutants of LANFLVH.

MARM 89

Investigation of reagents for the synthesis of pentafluoro-gem-diols from perfluoropropenolates

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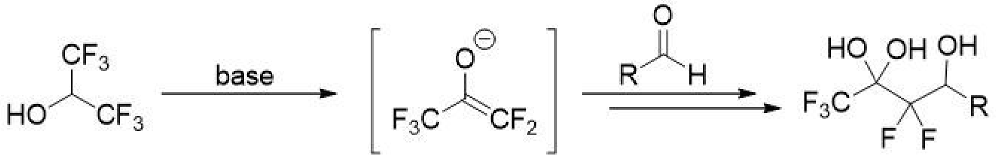
The incorporation of fluorine into organic molecules is an important strategy in drug development, because it improves metabolic stability of the compound and increases lipophilicity. Difluoromethylenes are difficult to install in complex molecules, because there are few methods to install the difluoromethylene unit and they often require harsh reaction conditions. One of the most common ways of installing a difluoromethylene unit is by use of a difluoroenolate.

Recently, our laboratory has reported that difluoroenolates can be generated from pentafluoro-gem-diols through the release of trifluoroacetate. Currently there is only one method to prepare the pentafluoro-gem-diols, which requires four steps from aldehyde. We have investigated two new approaches to produce pentafluoro-gem-diols: one using indium-mediated difluoro-allylation and another utilizing a perfluoropropenolate derived from hexafluoroisopropanol. The latter method reduces the overall number of synthetic transformations to two steps. One existing problem with producing perfluoropropenolates is that two equivalents of n-BuLi are required. We have investigated alternative types of reagents to generate these reactive intermediates from hexafluoroisopropanol and overcome the existing limitation. The two synthetic strategies as well as studies to produce perfluoropropenolates under mild conditions will be presented.



MARM 90

Substitution of solvent-exposed phenylalanines to improve the stability and function of phosphotriesterase

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Phosphotriesterase (PTE), an enzyme that naturally occurs in the soil bacteria *Pseudomonas diminuta,* can be used to catalyze the hydrolysis of organophosphates (OPs). It is the most efficient of available OP hydrolases and has the potential to detoxify dangerous OP-based substances such as commercial insecticides and weaponized nerve agents. PTE is characterized by a dimeric TIM-barrel structure, which is coordinated in part by seven phenylalanine residues on its dimer interface. While PTE seems to be a promising detoxifier, its poor stability, short half-life and activity limit its practical use. Seeking to improve PTE structure and function, we designed eight variants by mutating the enzyme's remaining eight solvent-exposed phenylalanine residues. We evaluated the variants using Rosetta, a computational software developed to predict macromolecular interactions. The stability and activity of the variants were further characterized through circular dichroism, differential scanning calorimetry, and kinetic assays. Here, we demonstrate the stability and activity of the variants.

MARM 91

A chlorin platform for bio-medical applications

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Porhyrinoids such as porphyrins, phthalocyanines and chlorins serve as good theranostic agents in biomedical applications. Among these porphyrinoids, chlorins have a good balance between singlet oxygen quantum yields for photodynamic therapy (PDT) and fluorescence quantum yield for diagnosis of different diseases (theranostics). Chlorins have one double bond less than porphyrins and a strong red absorption around 650 nm. Chlorins were studied previously as an antiviral and antibacterial agents in addition to cytotoxic agents for cancer. Here we present the synthesis of chlorin possessing polyethylene glycol (O-PEG) with a carboxylate linker followed by the conjugation to three different molecules lysozyme enzyme, single strand DNA and bovine serum albumin (BSA).

MARM 92

Enzymatic treatment of pyrrole and indole with soybean peroxidase (SBP)

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Contamination of soil and water by N-heterocyclic aromatics such as indole and pyrrole is of great environmental concern. Indole is detected at levels as high as several mg/L in liquid manure from swine farms (Schüssler *at al.,* 1999). It also can be discharged to the ecosystem from coking plants and refineries (winters *et al.,* 1976). Indole is highly toxic to aquatic life and is considered carcinogenic and mutagenic and has a strong odor (Schüssler *at al.,* 1999 & Sharma *et al.,* 2010). Along with other refractory compounds, indole can have a negative effect on biological treatment of coking wastewater (Xu *et al.,* 2015). Pyrrole has been found along with several other heterocyclics in µg/L concentration, in ground water contaminated by creosote (Johansen *et al.,* 1997). In recent years formation of halogenated pyrroles in drinking water has been reported by several researchers. Some of these halopyrroles are strongly cytotoxic and genotoxic towards mammalian cells (Richardson *et al.,* 2003 & Yang *et al.,* 2014). The aim of this study was to investigate an alternative treatment technique using soybean peroxidase as a catalyst in aqueous solution at ambient temperature. Experiments were conducted in batch reactors with reaction initiated by addition of hydrogen peroxide and run to completion (3 hours). Parameters affecting

the reaction including enzyme concentration (in standard catalytic units, U/ml), hydrogen peroxide concentration, pH and reaction time were optimized. The effectiveness of the treatment was measured by decrease in the area of the corresponding HPLC peak with UV detection. The optimal conditions were pH 1.6, 0.45 U/mL of enzyme along with 1.5 mM hydrogen peroxide for more than 95% removal of 1 mM initial indole concentration. The time course showed almost 90% of the substrate is removed during the first hour of the reaction. In case of pyrrole pH 1.6, 4.5 U/mL of enzyme and 1 mM hydrogen peroxide led to 84% removal of 1 mM pyrrole. Increasing enzyme concentration beyond 4.5 U/mL only gave a very small increase in percent removal of pyrrole and is considered economically infeasible

MARM 93

Degradation of textile azo-dyes using enzymatic treatment with soybean peroxidase

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In several industries such as the textile dye industry, azo-dyes account for the majority of the dyestuffs produced (Chivukula *et al.,* 1995). The discharge of dyes represents an environmental problem and is a public health concern. They can alter the pH, increase the biochemical oxygen demand and chemical oxygen demand, reduce the photosynthetic capability of aquatic plants and microorganisms also they are also considered toxic and carcinogenic. Enzymatic treatment using peroxidase might be useful for the decolorization and degradation of dyes and an environmental friendlier technique compared to conventional ones (Kumar *et al.,* 2006; Chacko & Subramaniam, 2011).

In the present investigation, two representative azo-dyes were treated with soybean peroxidase (SBP) in the presence of hydrogen peroxide (H_2O_2) in order to decolorize and degrade the dye solution: Acid Blue 113 (AB113) and Direct Black 38 (DB38). Several parameters were optimized for maximum decolorization: H_2O_2 concentration, pH, enzyme concentration (as catalytic activity in standard units, U/mL), and reaction time. Batch reactors were run in triplicate with initial concentrations of 1 mM AB113 and 0.5 mM DB38, varying the different parameters during 3 hours reaction. Decolorization was measured by the decrease of light absorbance at each dyes maximum wavelength using a spectrophotometer; the dye degradation was measured by high performance liquid chromatography (HPLC) analysis and total organic carbon (TOC) removal.

Enzymatic treatment of azo-dyes using SBP is an effective method for color reduction and dye degradation .The optimal pH for AB 113 and DB 38 were found to be 4 and 3.6, respectively. For AB 113, 1.5 U/mL of enzyme and 2.5 mM of H_2O_2 were needed for a maximum color removal of 93% along with 10% TOC removal and 97% dye degradation. On the other hand, higher concentrations were required for DB 38, achieving higher color removal, 3 U/mL of enzyme and 2.5 mM of H_2O_2 for 97% color removal, 51% TOC removal and more than 95% dye degradation.

MARM 94

Design, synthesis and pharmacological evaluation of 1,3,6-trisubstituted-4-oxo-1,4-dihydroquinoline-2-carboxylic acid derivatives as selective ET_A antagonists

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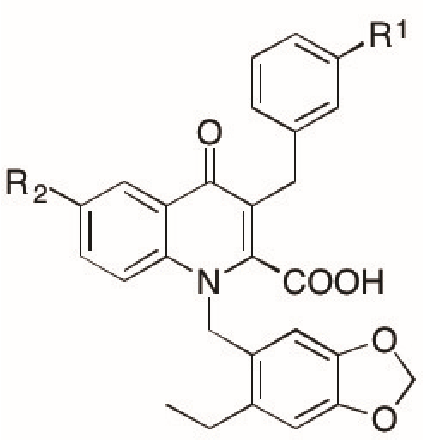
Endothelin receptor antagonists, both selective ET_A antagonists and non-selective $ET_{A/B}$ antagonists, are under investigation for the treatment of various diseases such as pulmonary arterial hypertension, chronic

heart failure, vascular remodeling, renal failure and cancer. Previous work in our lab has shown that 1,3,6-trisubstituted-4-oxo-1,4-dihydroquinoline-2-carboxylic acid derivatives exhibit endothelin receptor antagonist activity. The most potent compound (R_1 = -COOH, R_2 = $-OCH_2CH_2CH_3$) exhibited an IC_{50} value of 4 nM against ET_A receptors and an IC_{50} value of 2870 nM against ET_B receptors ($ET_{B/A}$ selectivity ratio of 717). A series of substituted quinolone analogues was designed to further understand the structure activity relationship. Alkyloxy groups of varying chain lengths at position 6 of the quinolone core and an acidic moiety at meta position of the side chain benzyl ring were substituted to optimize the inhibitory activity against $ET_{A/B}$ receptors. The potential endothelin receptor antagonist activity will be determined by *in vitro* Förster resonance energy transfer (FRET) using GeneBLAzer® assay technology.



MARM 95

Comparative studies of porphyrin C3-galactose and porphyrin C1-galactose conjugates for enhanced photodynamic therapy

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The protein family of galectins is defined by their ability to bind specific carbohydrates, including galactose. Due to the overexpression of galectins (such as galectin-1 protein) in cancer cells, the conjugation of galactose with a porphyrinoid has demonstrated to be a valuable strategy to improve selectivity of cancer photodynamic therapy. Additionally, galactosylation provides porphyrinoids amphiphilicity or even water solubility.

Galactosylated photosensitizers have been developed *via N*-, *S*-, *C*- and *O*-galactosylation by attaching the anomeric carbon or carbon-6 of the sugar to the macrocycle of the porphyrinoid. To gain affinity for galactose-binding proteins, the galactosylated porphyrinoids have been also developed by using galactose sugar in a multivalent format. Besides this, optimization of monovalent galactose by derivatization of the galactose carbon-3 yielded compounds with high affinity to galectin-1.

In an attempt to increase the affinity of porphyrinoids to galectin-1 protein, we have attached galactose units through carbon-3 to a porphyrin by click conjugation (**Por-C3-Gal4**). Furthermore, to validate the potential of **Por-C3-Gal4,** the same tetrapyrrolic macrocycle was also attached to the carbon-1 of galactose sugar (**Por-C1-Gal4**). The aim of the present study was to investigate the photophysical properties, uptake and photodynamic efficiency of **Por-C3-Gal4** and **Por-C1-Gal4** in *in vitro* cancer models. *In vitro* studies were performed in monolayers of cancer cells containing high and low levels of galectin-1 protein. Attempting to mimic the several heterogeneous treatment effects found *in vivo*, *in vitro* studies were also performed in the corresponding three-dimensional spheroid cancer cell cultures. **1)** Liu, F. T.; Rabinovich, G. A. *Nat. Rev. Cancer* 2005, 5, 29–41. **2)** Singh, S.; Aggarwal, A.; Bhupathiraju, N. V. S. D. K.; Arianna, G.; Tiwari, K.; Drain, C. M. *Chem. Rev.* 2015, 115, 10261–10306. **3)** van Hattum, H.; Branderhorst, H. M.; Moret, E. E.; Nilsson, U. J.; Leffler, H.; Pieters, R., J. *J. Med. Chem.*, 56, 1350-1354. **4)** Pereira, P. M. R.; Silva, S.; Cavaleiro, J. A. S.; Ribeiro, C. A. F.; Tomé, J. P. C.; Fernandes, R. *PLoS One* 2014, 9, e95529.

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MARM 96

Comparative study of ether-based electrolytes for application in lithium-sulfur battery

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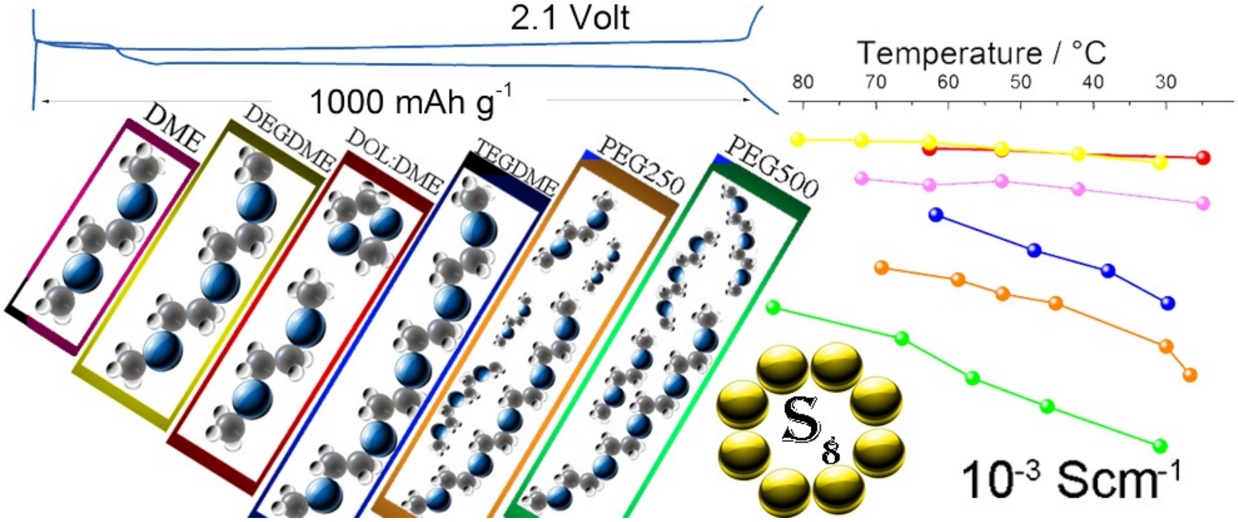
Herein we report the characteristics of electrolytes using various ether-solvents with molecular composition CH3O[CH2CH2O]nCH3, differing by chain length, and LiCF3SO3 as the lithium salt. The electrolytes, considered as suitable media for lithium−sulfur batteries, are characterized in terms of thermal properties (TGA, DSC), lithium ion conductivity, lithium interface stability, cyclic voltammetry, self-diffusion properties of the various components, and lithium transference number measured by NMR. Furthermore, the electrolytes are characterized in lithium cells using a sulfur−carbon composite cathode by galvanostatic charge−discharge tests. The results clearly evidence the influence of the solvent chain length on the species mobility within the electrolytes that directly affects the behavior in lithium sulfur cell. The results may effectively contribute to the progress of an efficient, high-energy lithium−sulfur battery.



MARM 97

Engineered protein-based delivery of dipyridamole for the treatment of bone fracture

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In the United States, it has been estimated that more than 1.5 million individuals experience bone fracture caused by diseases in addition to incidences. Bone morphogenetic protein (BMP-2) has been employed in current clinical setting as a treatment besides autologous and cadaveric graft. However, it has been recently discovered that BMP-2 leads to several adverse effects, such as vertebral osteolysis, ectopic bone formation, radiculitis, and cancer proliferation. Stimulation of adenosine A2A receptor (ADORA2A) has been reported to exhibit significant reduction in bone pitting and porosity, which motivates the development of stimuli as alternative treatments. Dipyridamole has been observed to indirectly stimulate ADORA2A by preventing reuptake of the ligand adenosine, and has shown promising *in vivo* and *in vitro* results on par with conventional treatment of BMP-2. Nevertheless, injection on a daily basis is required due to rapid clearance of dipyridamole, and this administration causes discomfort to patients. Here, we proposed the coiled-coil domain of cartilage oligomeric matrix protein (COMPcc) as a carrier to deliver dipyridamole with provision of protection and sustained release. COMPcc when self-assembled into homopentamer bears a hydrophobic cavity, that can effectively binds to a variety of hydrophobic molecules such as vitamin A, vitamin D_3 and curcumin. In this study, we assess binding capacity of COMPcc to dipyridamole in order to further optimize the formulation for the treatment.

MARM 98

Flame retardants: New approaches to reduce exposure

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In 2013 the National Fire Protection Agency reported 1.24 million fires, which attributed to 3,200 deaths, 15,925 injuries and $12 billion in property damage. Flame retardants (FRs) play a significant role in fire protection by delaying the ignition or spread of a fire. These chemicals tend to be either organohalogenated or organophosphorous based compounds, which some studies have indicated can cause adverse health effects, such as endocrine disruption. It was recently demonstrated that a common FR, triphenyl phosphate (TPP), can form an inclusion complex (IC) with β-cyclodextrin (BCD) to help reduce toxicity. The goal of our work is to use a combination of experiments and molecular modeling to characterize these ICs. Mass spectrometry results indicate that TPP forms an IC with BCD, while molecular dynamics simulations suggest a 2BCD:1TPP crystal structure. In addition, we are working to identify other potential FRs that can form ICs with BCD and other CDs.

MARM 99

Study of chemical composition and prospecting anticholinesterase of volatile oils at *Corymbia citriodora* and *Vitex agnus castus*

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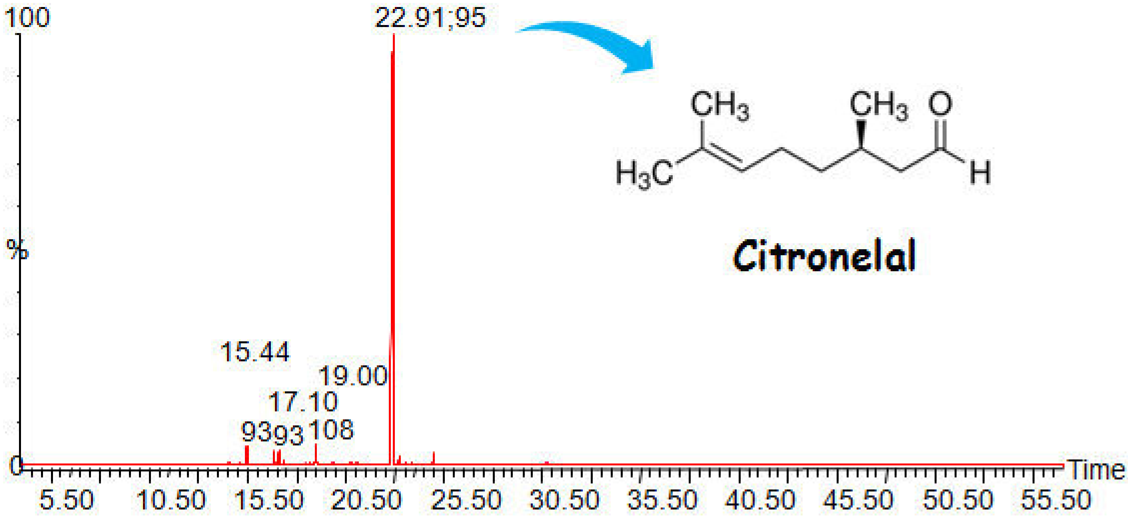
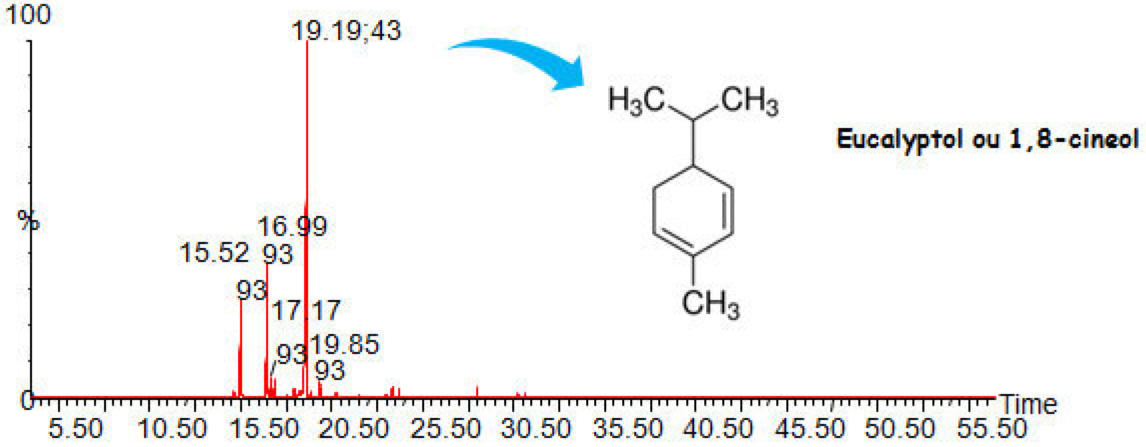
Alzheimer's disease has raised a considerable interest from the scientific community , since this neurodegenerative disease affects a considerable part of the population aged between 60 and 65 years. The current treatment is the use of cholinesterase inhibitors , which act directly on the cholinergic deficit caused by the disease. The Acetylcholinesterase (AChE) inhibitors impede that acetylcholine from being metabolized, thus increasing its availability in the nerve synapse. However, these drugs are very costly and cause various side effects, being required the search for new candidates for the treatment of Alzheimer's disease. The herbs in their diversity have volatile oils with great therapeutic and pharmacological potential. Thus the present study evaluated the anticholinesterase ability of volatile oils of *Corymbia citriodora* and *Vitex agnus castus* . The results showed that the yield of oil essential *Corymbia citriodora* was 3.5 % , while *Vitex agnus castus* presented 0.35 %. For the classification of chemical species in the samples of the oils ,was performed Gas chromatography–mass spectrometry (GC-MS). Was identified in the volatile oil of *C. citriodora* ten chemical compounds, having citronellal as the major constituent. The *Vitex agnus castus* oil presented nine compounds with 1,8- cineol as major constituent. In the qualitative chromatographic assay on silica plates, was observed the appearance of white stains or halos on a yellow background, thus indicating anticholinesterase activity. These results demonstrate that terpenoids classes affects the inhibition of acetylcholinesterase and therefore should be investigated as a prospective treatment to Alzheimer's .

Keywords: *C. citriodora* ; *V. agnus Castus* ; Alzheimer's



Chromatogram of the volatile oil of *Corymbia citriodora.*



Chromatogram of the volatile oil of *Vitex agnus castus* .

MARM 100

Mechanism of diastereoselective encapsulation of tartaric acid by arylamide foldamers: A computational investigation

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Arylamide foldamers are synthetic polymers consisting of alternating aromatic and peptide units that fold into stable secondary structures in solution. They have a variety of applications in biochemistry, medicine, and material science. One promising application uses arylamide helices to encapsulate ligands and isolate them from the environment and has potential in drug delivery. Huc et al. synthesized foldamer capsules that diastereoselectively encapsulates tartaric acid and other small chiral molecules. Their studies have shown that the left handed helix prefers to bind the L-tartaric acid. Using molecular dynamics simulations, we have determined the mechanism of stereoselectivity for encapsulation of tartaric acid by arylamide foldamers. The knowledge gained from this study will aid in the rational design of foldamer capsules.

MARM 101

Novel approach for the direct synthesis of nitriles from aldehydes in ionic liquids

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Nitriles are a very important functional group and their synthesis from simple substrates under mild conditions a continuous focus in the organic chemistry field. In our efforts to assess the chemical properties of hydroxylamine sulfonic acids we found that at elevated temperatures and ionic liquids, aldehydes undergo an unusual oxidative pathway to form nitriles with high conversions and selectivities. We found that aromatic and aliphatic aldehydes undergo this transformation with high yields and not traces of other potential side products. We have also devised a proposed mechanism for this transformation.

MARM 102

Semi-synthesis of a novel library of alkaloids as potential selective analgesics

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Alkaloids are natural products with a variety of pharmacological properties, including selective binding to opiate receptors. The natural abundance of these molecular scaffolds, sometimes (although rarely) allows for the amplification of structural features towards the enhancement of their pharmacological properties. We were able to activate a relatively unfunctionalized skeleton into a highly reactive amino ester alkaloid. With that in hand, we have built a series of libraries via Strecker/alkynylation reactions on the amine as one diversification point and ester to amide coupling reactions on the ester as a second diversification

point. These libraries will be assayed against a battery of opiate receptors for the assessment of their pharmacological profile as potential selective analgesics.

MARM 103

β-Galactosidase langmuir monolayer at air/subphase interface

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The interfacial properties of β-galactosidase were studied through surface chemistry and spectroscopic techniques. β-galactosidase interacted with X-gal to give the galactose as well as blue colored organic moiety. We investigated the β-galactosidase Langmuir monolayer in absence and presence of X-gal of varying concentration to the sodium chloride subphase. It was found that the limiting molecular area as well as the monolayer breaking point surface pressure kept on decreasing with the increasing amount of X-gal. In accordance to the data obtained from the isotherm it was also found that β-galactosidase forms a stable monolayer that does not aggregate at the air-subphase interface. The stability of the monolayer at the air-subphase interface was studied by using compression-decompression cycles with and without X-gal at varying concentration and different surface pressures. The infrared reflection-absorption spectroscopy (IRRAS) and Brewster angle microscopy (BAM) of β-galactosidase Langmuir monolayer was also investigated for pure and mixed β-galactosidase at the air-subphase (X-gal dissolved in limited amount of DMF and further diluted with 0.1 M NaCl solution). The objective of this article is to investigate the surface chemistry of β-galactosidase on air-subphase interface using Langmuir monolayer technique.

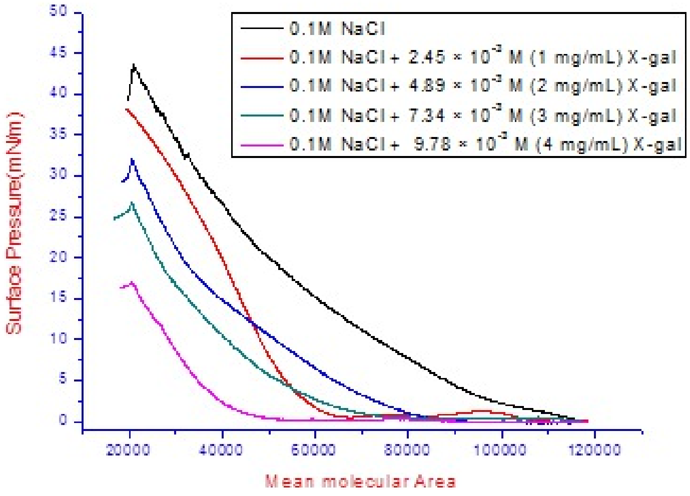
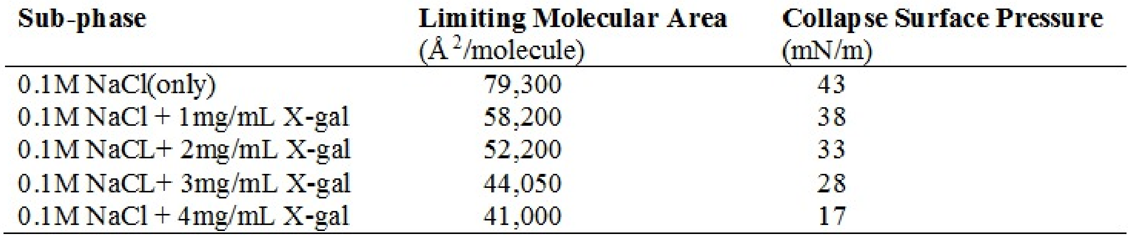


Figure: Surface pressure versus mean molecular area isotherms for 3.7×10^{-7} M β-Galactosidase spread on 0.1M NaCl and (2.45, 4.89, 7.34 and 9.78) × 10^{-3} M of X-gal



Sub-phase	Limiting Molecular Area (Å ^{2}/molecule)	Collapse Surface Pressure (mN/m)
0.1M NaCl(only)	79,300	43
0.1M NaCl + 1mg/mL X-gal	58,200	38
0.1M NaCL+ 2mg/mL X-gal	52,200	33
0.1M NaCL+ 3mg/mL X-gal	44,050	28
0.1M NaCl + 4mg/mL X-gal	41,000	17

Table: Data showing limiting molecular area and collapse surface pressure for different subphases.

MARM 104

Chemical modification and biological testing of fellutamide B, a natural peptide-based proteasome inhibitor

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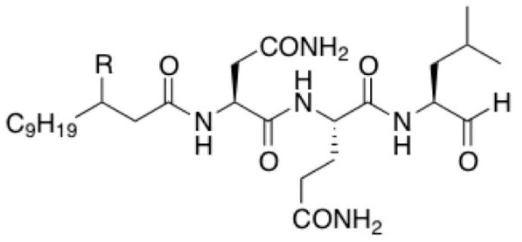
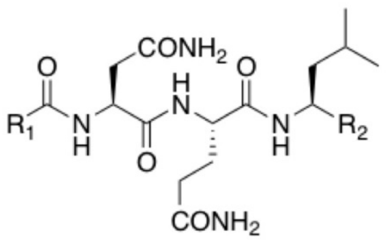
Fellutamides (A-D) are a unique class of lipopeptides from a marine fungi, and exhibit promising proteasome inhibitory activity. Drug leads that inhibit proteasome activity has emerged as promising candidates for the treatment of cancer, inflammatory diseases, and many other disorders. Fellutamide B (**1**) is a tripeptide natural product with a lipidated *N*-terminal Asn, and C-terminal leucinal residue. It has been shown to be the potent member of this class of natural products, and exhibits anticancer activity against several types of cancer cell lines. To date, very limited structure activity relationship (SAR) studies has been done on **1**, hence our research group has initiated a program to synthesize a library of structural analogs of **1**. Our goal is to better understand the role of lipid-chain as well as the electrophilic aldehyde motif. Additionally, we envisioned substituting the aldehyde motif with a more stable analog to limit the extent of epimerization of the *C*-terminal leucinal residue. We have synthesized a series of analogs of fellutamide B (**2** - **9**) by modifying the *N*-terminus with a C-10, C-12 or C-14 acyl chain. Current efforts are focused on synthesizing an aldehyde bioisostere (nitrile or benzimidazole) analog of leucinal, and synthesizing the analogs **6** - **9**. These synthetic analogs will be evaluated for cytotoxicity against a panel cell lines. The results from this study will aid in the design of a new series of analogs with improved chemical stability and pharmacological profile, and perhaps allow us to better understand the mechanism of action of this unique class of natural product.



Fellutamide B (**1**): R = OH
Deoxyfellutamide B (**2**): R = H



3: $R_1 = C_9H_{19}$, , R_2 = CHO
4: $R_1 = C_{11}H_{23}$, , R_2 = CHO
5: $R_1 = C_{13}H_{27}$, , R_2 = CHO
6: $R_1 = C_9H_{19}$, , R_2 = CN
7: $R_1 = C_{11}H_{23}$, , R_2 = CN
8: $R_1 = C_{13}H_{27}$, , R_2 = CN
9: $R_1 = C_{13}H_{27}$, , R_2 = benzimidazole

MARM 105

Cell sensitivity and recombination repair of interstrand crosslinks in yeast strains with nonfunctional repair genes

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Saccharomyces cerevisiae, or baker’s yeast, has a eukaryotic genome and has the ability to reproduce quickly; for this reason it’s used as a model organism in human research, particularly for the study of genetics. The treatment of DNA with psoralen and ultraviolet light leads to interstrand crosslinks (ICLs) that covalently link two individual strands of DNA. This treatment prevents replication and transcription and causes cell cytotoxicity. To establish cellular sensitivity to ICLs, we must target and disrupt a nonessential gene within the yeast genome. Nonfunctional genes are removed from the yeast cells and replaced with a different gene such as KanMX, a marker which codes for resistance to the antibiotic Geneticin. We are studying several genes to assess their functions in ICL repair and recombination. *PSO2* (ORF: YMR137C), *SHU1* (ORF: YHL006C), and *SLX4* (ORF: YLR135W).). The product of the *PSO2* gene plays roles in joining hairpin ends in ICL repair. The *SHU1* protein is a component of the *SHU* complex, which contains *PSY3, CSM2,*and *SHU2.* It is important for error-free DNA repair and necessary for promoting pairing of homologs during meiotic homologous recombination. The *SLX4* gene encodes an endonuclease that is involved in DNA processing. It acts upon the recombination and repair pathways, which promotes a template switch during break-induced replication. We will investigate the roles of the *PSO2*, *SHU1*, and *SLX4* genes in the maintenance of genome stability by characterizing the products of ICL-induced recombination in strains with deficiencies in those genes. All of these three genes have been found to be disrupted, *SHU1* deficient strains are not more sensitive than repair proficient cells to ICLs. These disrupted genes will be placed into yeast strains with *his3* gene repeats to study ICL-induced recombination. In *SHU1* – deficient yeast cells ICLs Induced high levels of recombination. Survival experiments will be done with these genes to see the cell sensitivity and recombination to ICL.

MARM 106

Evaluation of herbitóxica activity of essential oil *Corymbia citriodora* on the germination of *Allium fistulosum* and *Lactuca sativa*

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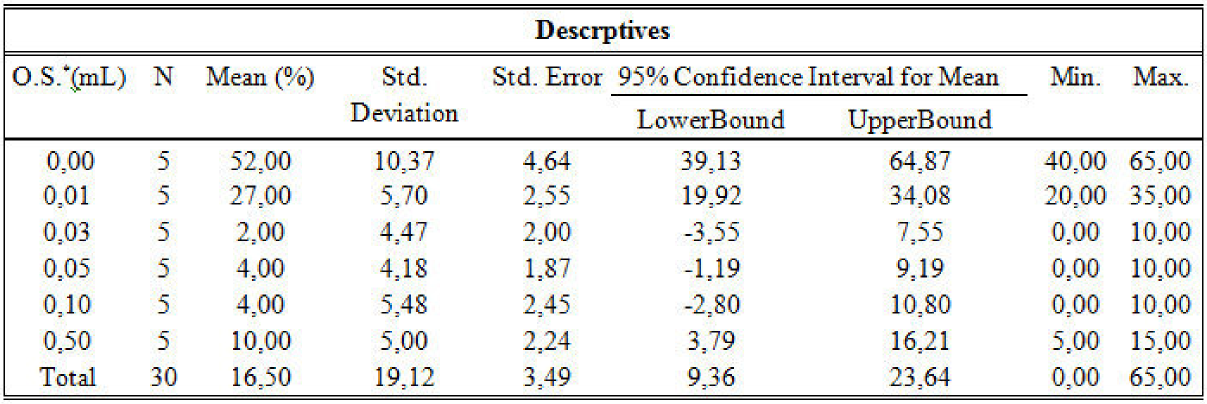
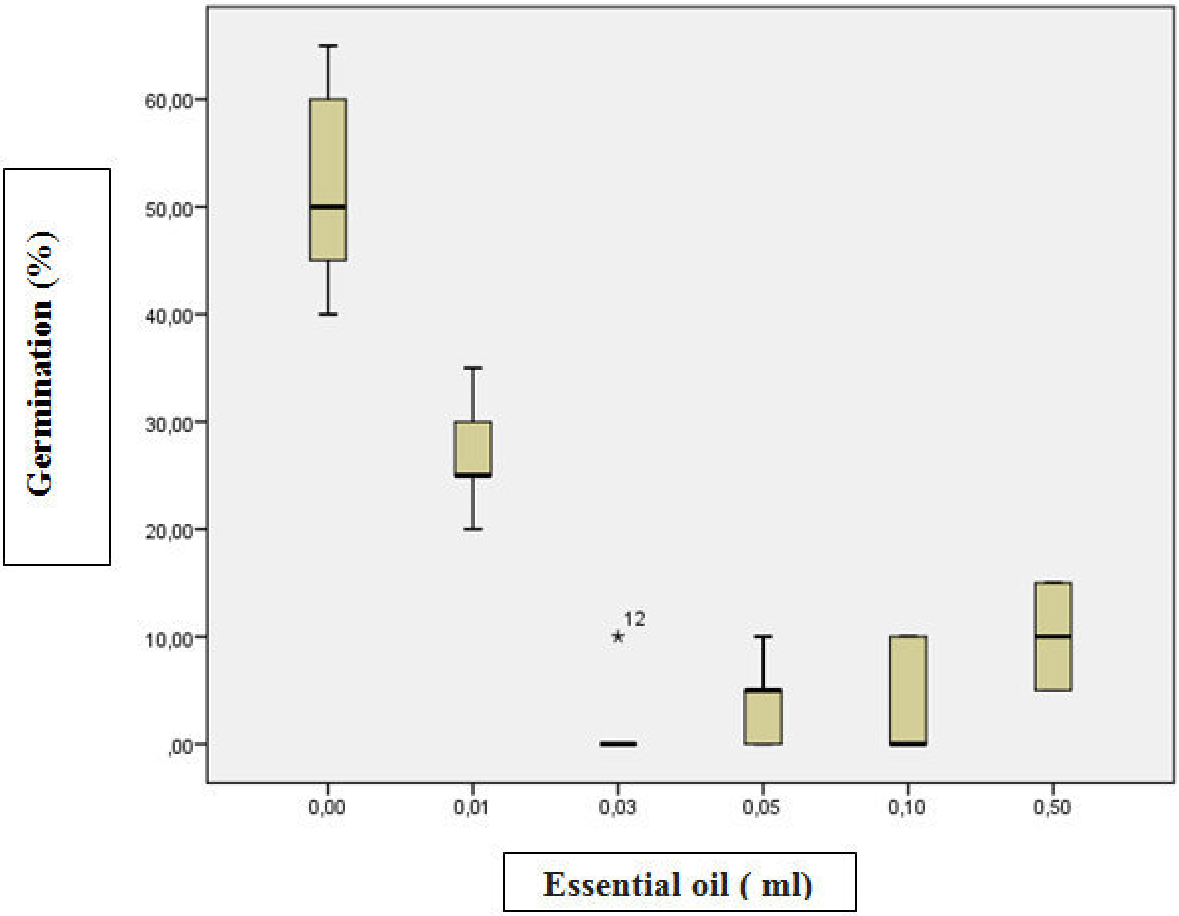
The use of volatile oils derived from plants of the secondary metabolite have been reported as potential seed germination inhibitors and cause intoxication of plant species, associated with the loss of photosynthetic capacity. The aim of this study was to evaluate the effects of the essential oils from *Corymbia citriodora* (Eucalyptus) by hydrodistillation method of vapor, through Clevenger apparatus, to develop herbitóxicos tests on selected samples of Allium fistulosum seeds (chives) and *Lactuca sativa* (lettuce). The identification of chemical compounds present in the essential oil of *Corymbia citriodora* by gas chromatography technique coupled to Mass Spectrum (GC-MS), indicated the citronellal as major constituent. The analyzed concentrations were 0,01ml ; 0,03ml ; 0.05ml ; 0.1ml ; 0.5ml. The results were very satisfactory, particularly for analyzes in *Lactuca sativa* seeds where the results were 100 % inhibition of germination and consequently root development in all the tested concentrations. In the germination tests and root development of seed Allium fistulosum there was a significant inhibition of both germination and root development, especially the concentration of 0,03ml, with the percentage of 2% germination whereas for the other concentrations effective results were obtained both for the inhibition of germination and blockage for root development. The tests show that the volatile oil *Corymbia citriodora*, has potential for bioherbicida in the seed germination control and combat of subsequent weeds.

Keywords: Corymbia ciotriodora, Essential oil, herbitoxica activity

Table. **Analysis descriptive data for the percentage of germination medium of chives.**



Descrptives								
O.S.*(mL)	N	Mean (%)	Std. Deviation	Std. Error	95% Confidence Interval for Mean		Min.	Max.
					LowerBound	UpperBound		
0,00	5	52,00	10,37	4,64	39,13	64,87	40,00	65,00
0,01	5	27,00	5,70	2,55	19,92	34,08	20,00	35,00
0,03	5	2,00	4,47	2,00	-3,55	7,55	0,00	10,00
0,05	5	4,00	4,18	1,87	-1,19	9,19	0,00	10,00
0,10	5	4,00	5,48	2,45	-2,80	10,80	0,00	10,00
0,50	5	10,00	5,00	2,24	3,79	16,21	5,00	15,00
Total	30	16,50	19,12	3,49	9,36	23,64	0,00	65,00



Box- polt Graph chives germination data in different essential oil volumes.

MARM 107

Study of the acid-base properties of metal oxides absorbed into nanoporous silica matrices

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Photocatalyzing multi-electron, multi-proton reactions with low-cost, abundant, thermodynamically-robust materials lies at the heart of converting solar energy into energy rich fuels, utilizing visible light to drive the reduction of CO_2 to CH_4. Different metal oxides have been known to photocalyze the conversion for more than a quarter of a century, yet these systems continue to require UV excitation and methane yields remain small. Recent experiments with WO_3 have led to a new excited-state acid-base (ESAB) model, suggesting that the metal oxide does not act as a source of electrons, but instead creates an acid-base gradient in which the reduction of CO_2 and oxidation of H_2O occur exergonically at different pH.

MARM 108

Stepwise detection of antigens using aptamer triggered DNAzyme signal amplification

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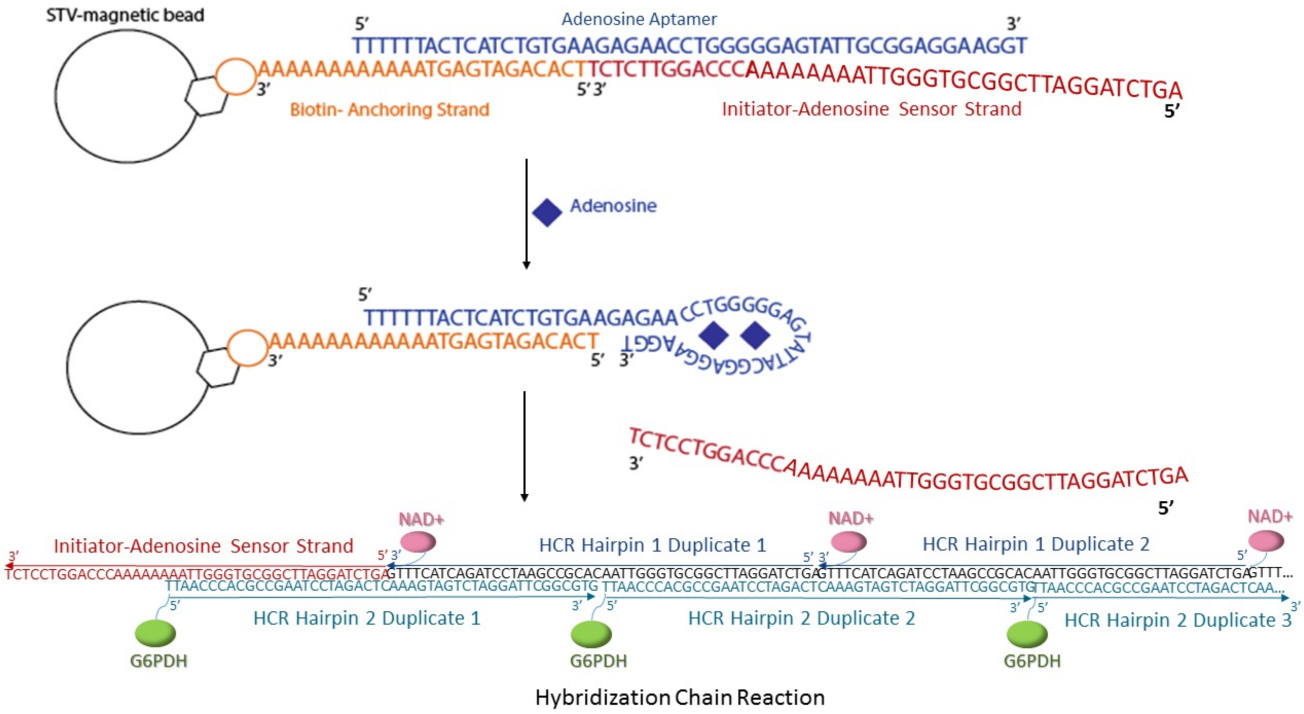
DNA aptamers are target-specific duplex sequences which change conformation after binding to target. Such property could be applied to engineer stepwise bio-sensing reaction cascades, for instance, introducing the releasing of the target sensing strand while the conformational change of aptamer-complement duplex is triggered from aptamer-to-target binding followed with triggered hybridization chain reaction (**Figure 1**). On the streptavidin bead surface, sequential assembled localized adenosine aptamer changes conformation after binding to adenosine or cocaine, thus releases the initiator-sensoring strand which is semi-complementary to the aptamer strand. The released initiator-sensing strand could act as the initiator of a hybridization chain reaction via binding to the sticky end of HCR hairpin 2 probe strand which is partially complementary to the initiator and the pre-conjugated to one unit of the glucose-6-phosphate dehydrogenase (G6PDH) and remains stable without initiator. The HCR hairpin 2 strand is then opened up and its newly exposed end nucleates at the sticky end of HCR hairpin 1, conjugated to the cofactor nicotinamide adenine dinucleotide (NAD+), and opens the hairpin to expose the end of it. As conjugated hairpins propagate to form an elongated nicked double helix, the G6PDH and NAD+ are brought together thus form complete DNAzymes with amplified enzymatic signals. Such a DNAzyme chain reaction initiated by the released initiator-sensing strand, could potentially be used to sense target molecules in low concentrations with promising output.



MARM 109

Water and pH dependency of the emissivity of tungsten oxide in porous vycor glass

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Tungsten Oxide adsorbed onto porous vycor glass (PVG) have been observed to convert CO_2 into CH_4 with the aid of visible light, yet the reducing potential of an electron in the WO_3 (+0.2V vs. NHE) is not capable of the reduction of CO_2 (-1.90V vs. NHE). The excited-state acid-base (ESAB) model proposes that the metal oxide does not act as a source of electrons, but instead creates an acid-base gradient in which the reduction of CO_2 and oxidation of H_2O occur exergonically. Recent UV-VIS absorption and Raman experiments have confirmed that tungsten oxide forms different polyoxometalates in solution and also in PVG dependent on the pH of the solution. Additionally, experiments have shown that Tungsten Oxide in PVG emission intensities are dependent with the level of hydration present in the glass in a parabolic manner and not exclusively the pH.

MARM 110

Modulation of PEA-15 binding specificity by phosphorylation and possible roles of charge-triad residues in mediating conformational changes

Victor Leon, *landmarkvictor@gmail.com,* ***Chanel Wright***, *cwright@njcu.edu, Yufeng Wei. Chemistry, New Jersey City University, Bayonne, New Jersey, United States*

Phosphoprotein enriched in astrocytes or PEA-15, is a small, non-catalytic protein that involves in regulation of a variety of remotely related biological pathways. It contains an N-terminal death effector domain (DED) folded into a six-helix bundle and an unstructured C-terminal tail. Also, PEA-15 possesses a characteristic surface feature, termed charge-triad, which is formed among three highly conserved charged residues. PEA-15 can inhibit death receptor-mediated apoptosis (or programmed cell death) by interacting with the adapter protein, Fas-Associated protein with Death Domain (FADD), blocking the recruitment of procaspase-8 to the death-inducing signaling complex (DISC) and preventing caspase-8 activation. The specific binding of PEA-15 to FADD is regulated by phosphorylation of two C-terminal serine residues, S^{104} and S^{116}, which switches PEA-15 from a tumor suppressor to a tumor promoter by inhibiting apoptosis.

We are studying the interaction of $S^{104}D/S^{116}$ D double mutant PEA-15 (PEA-15DD), mimicking the doubly phosphorylated state, with FADD using NMR spectroscopy. We have found that PEA-15 DED may adopt additional conformations in the DED with rearranged relative helical orientations among the six helices in $S^{104}D$ and $S^{116}D$ mutant. The interactions between the FADD DED and PEA-15DD DED are mostly electrostatic, and the binding site of PEA-15 on FADD seems to coincide with the binding site procaspase-8, and thereby blocking the recruitment and activation of procaspase-8 at the DISC. Future studies will include investigation of PEA-15 and protein-protein interactions using differential scanning calorimetry and fluorometric assays.

MARM 111

Spectrophotometric analysis of antioxidant activity in organic versus conventional berries

Vanessa Pinheiro, *pinheiva@gmail.com, Kishore K. Bagga. Graduate School of Biomedical Sciences and Professional Studies, Drexel University College of Medicine, Philadelphia, Pennsylvania, United States*

Research data is still unclear as to whether organic food contains a higher nutritional value than conventional foods. One such nutritional value that can be studied is the antioxidant levels in conventional versus organic berries. The null hypothesis states that there is no significant difference in antioxidant levels between the two types of fruit. Assays to determine total antioxidant capacity, total phenol concentration, total flavonol concentration, and total flavonoid concentration were run on strawberries, raspberries, blueberries, and blackberries. Upon completion of data analysis, results shall be presented.

MARM 112

Surface functionalized metal-oxo polymer nanobeads as potential T_1 MRI contrast agents with dual reporting capability

VIdumin Dahanayake*, vd153@georgetown.edu, Sarah L. Stoll. Chemistry, Georgetown University, Washington, District of Columbia, United States*

Magnetic Resonance Imaging (MRI) is one of the foremost non-invasive diagnostic imaging tools available today. Most MRI scans utilize paramagnetic substances known as contrast agents (CAs) to enhance the MR signal. Gadolinium chelates and super paramagnetic iron oxide particles have been the CAs of choice for this purpose. However toxic effects, environmental concerns and lack of T_1 contrast have made these CAs to become obsolete. Our previous studies have identified a biologically benign poly nuclear metal-oxo cluster,$[Mn_8Fe_4O_{12}(O_2CCH_3)_{16}(H_2O)_4]$ or Mn_8Fe_4 as a potential CA. Exploiting its proneness for ligand exchange, the acetate groups were replaced for the polymerizable ligand, 4-vinylbenzoate.The substituted cluster was then subsequently incorporated into polystyrene latex beads by way of the miniemulsion polymerization process resulting in monodispersed nanobeads (70.9 ± 9.4 nm in diameter) with positive T_1 contrast agent.

Herein we have included hydrophobic fluorescent dyes within the matrix for effective identification once introduced into a biological system. A polymerizable pyrene derivative PyMMA (1-pyrenylmethyl methacrylate) was copolymerized within the polymer matrix. Appearance of florescence was noted under UV irradiation at 365nm after purification via dialysis. A polymerizable fluorescein derivative, fluorescein *O*-methacrylate was also used that excites at 485nm enabling it to be used with an abundantly available argon laser in biological systems.

Acrylic acid was used as a carboxylic functionalized monomer to yield covalently bound surface charges on the aforementioned nanobeads bearing florescent dyes as a marker. Well-formed beads were acquired by SEM (Fig.1). We have also investigated the possibility of obtaining sulfonate and phosphate functionalized beads by using a polymerizable surfactant and a hydrophilic cross linker respectively.These surface modified fluorescence marked beads were found to be non-toxic to cells by preliminary cytotoxicity assays carried out on LNCap and PC-3, two types of human derived cancer cell lines.

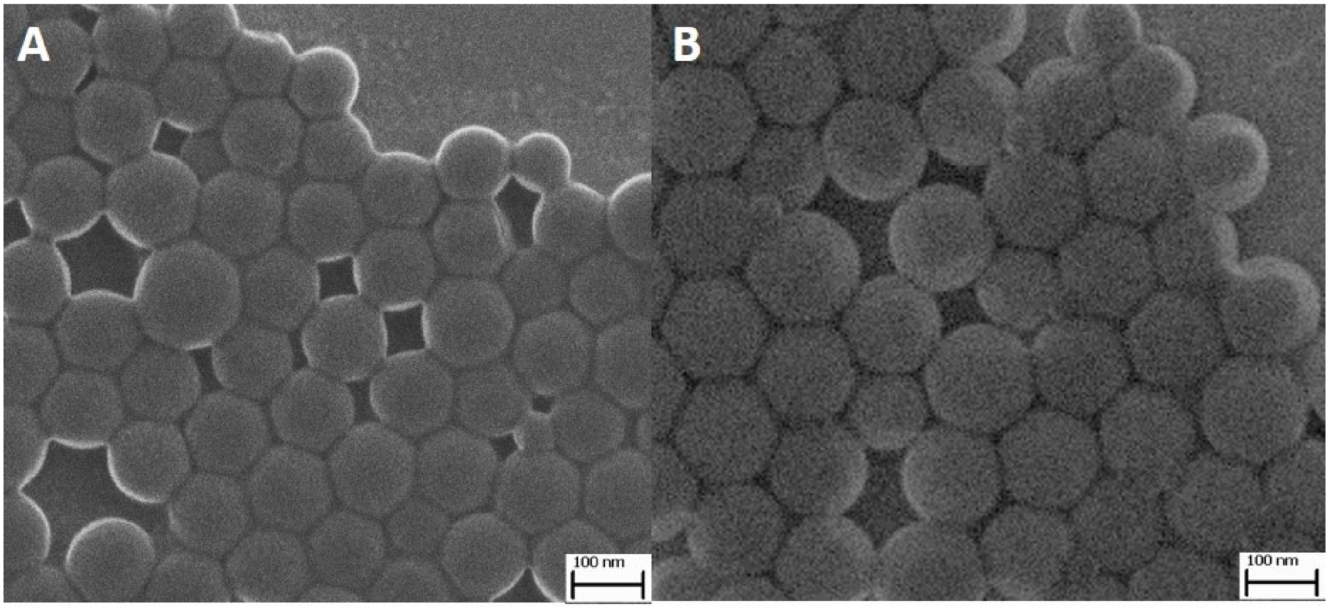

Fig.1 SEM pictures of metal-oxo polymer nanobeads functionalized with acrylic acid (3 wt.-% on Styrene) containing **A.** PyreneMMA , **B.** Fluorescein *O*-methacrylate as fluorophores.

MARM 113

Development of novel substrate inhibitors of bacterial phospholipid biosynthesis as new antibacterial agents

Pooja Saklani, *pooja.saklani15@stjohns.edu, David P. Brown. Chemistry, St. Johns University, Jamaica, New York, United States*

In a statement released by the Infectious Diseases Society of America (IDSA), “infections caused by antibiotic-resistant bacteria, especially the ‘ESKAPE’ pathogens, (***E****nterococcus faecium,* ***S****taphylococcus aureus,* ***K****lebseilla pneumoniae,* ***A****cinetobacter baumannii,****P****seudomonas aeruginosa,* and ***E****nterobacter* species), continue to increase in frequency and cause significant morbidity and mortality. New antimicrobial agents are greatly needed to treat infections caused by Gram-negative bacilli (GNB) resistant to commonly available agents.”

The IDSA has rallied for a leveraging of the intellectual, financial and legislative support of stakeholders to achieve the defined goals of its “10 x ’20 Initiative” – to develop ten (10) new, safe, and effective antibiotics by the year 2020.

Our research team has been exploring a new concept of incorporating bactericidal motifs in the architecture of poly-hydroxylated hydrocarbons and carbohydrate derivatives, Figure 1, yielding novel potential substrate inhibitors of the key bacterial glycerol-phosphate acyltransferase (PlsY). Acyltransferases play pivotal roles in the synthesis of phosphatidic acid (PdtOH), the key intermediate in bacterial phospholipid biosynthesis, rendering them very promising targets for the development of new antibacterial agents. In this presentation we report on our efforts toward the development of new mimics of glycerol-3-phosphate (G3P), a key precursor in the PdtOH synthesis pathway.

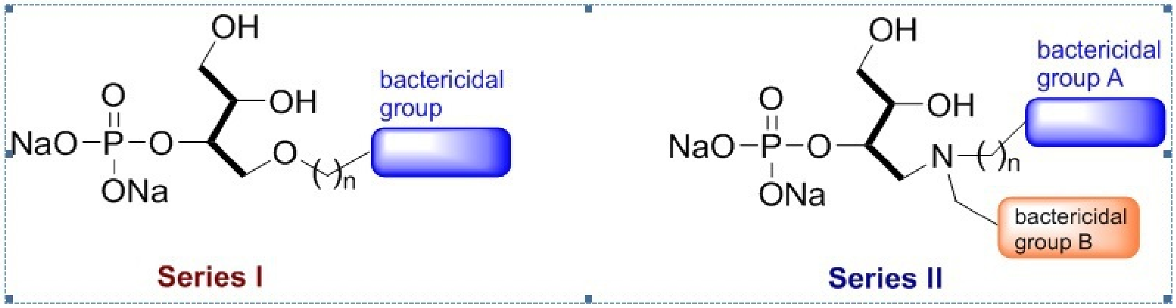

Figure 1: G3P Mimics

MARM 114

Modulation of PEA-15 binding specificity by phosphorylation and possible roles of charge-triad residues in mediating conformational changes

Victor Leon[1], *landmarkvictor@gmail.com*, ***Chanel Wright***[2], *cwright@njcu.edu, Yufeng Wei*[1]. *(1) Chemistry, New Jersey City University, Bayonne, New Jersey, United States (2) Chemistry, New Jersey City University, Jersey City, New Jersey, United States*

Phosphoprotein enriched in astrocytes or PEA-15, is a small, non-catalytic protein that involves in regulation of a variety of remotely related biological pathways. It contains an N-terminal death effector domain (DED) folded into a six-helix bundle and an unstructured C-terminal tail. Also, PEA-15 possesses a characteristic surface feature, termed charge-triad, which is formed among three highly conserved charged residues. PEA-15 can inhibit death receptor-mediated apoptosis (or programmed cell death) by interacting with the adapter protein, Fas-Associated protein with Death Domain (FADD), blocking the recruitment of procaspase-8 to the death-inducing signaling complex (DISC) and preventing caspase-8 activation. The specific binding of PEA-15 to FADD is regulated by phosphorylation of two C-terminal serine residues, S^{104} and S^{116}, which switches PEA-15 from a tumor suppressor to a tumor promoter by inhibiting apoptosis.

We are studying the interaction of $S^{104}D/S^{116}D$ double mutant PEA-15 (PEA-15DD), mimicking the doubly phosphorylated state, with FADD using NMR spectroscopy. We have found that PEA-15 DED may adopt additional conformations in the DED with rearranged relative helical orientations among the six helices in $S^{104}D$ and $S^{116}D$ mutant. The interactions between the FADD DED and PEA-15DD DED are mostly electrostatic, and the binding site of PEA-15 on FADD seems to coincide with the binding site of procaspase-8, and thereby blocking the recruitment and activation of procaspase-8 at the DISC. Future studies will include investigation of PEA-15 and protein-protein interactions using differential scanning calorimetry and fluorometric assays.

MARM 115

The counterion's role in supramolecular self-assembly

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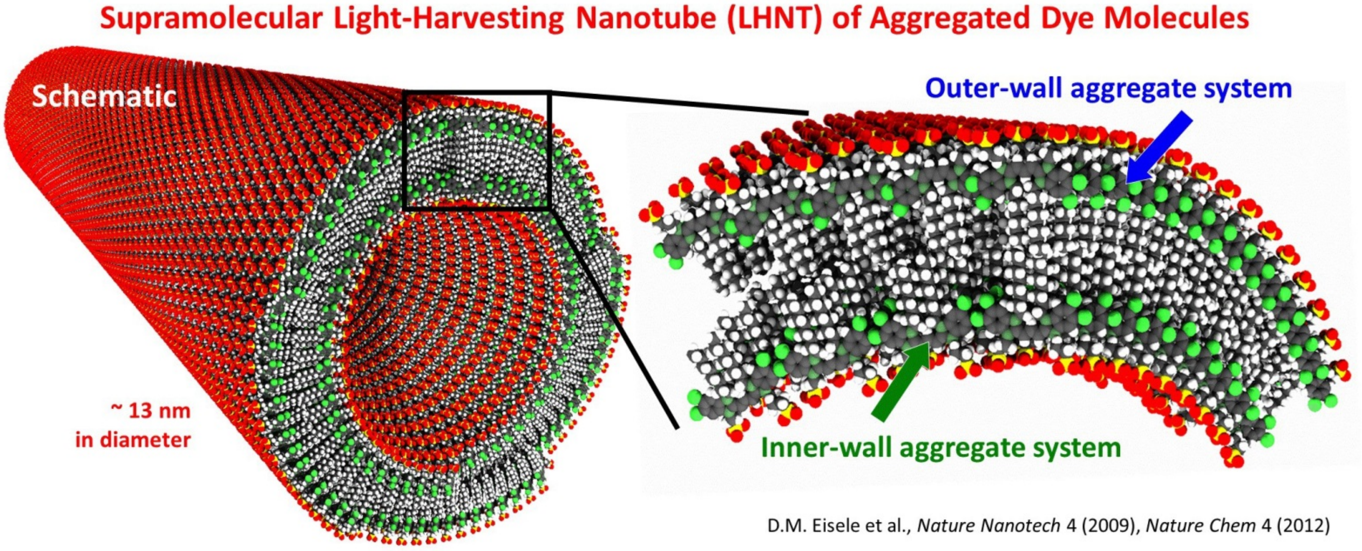
Supramolecular aggregates consist of molecular sub-units (i.e. monomers) that self-assemble under thermodynamic equilibrium conditions into close-packed (i.e. aggregated) molecules via weak (i.e. non-covalent) interactions. Though the forces behind self-assembly (e.g. hydrophobicity) are known, the specific mechanism by which monomers form the supramolecular aggregates still remains an open question. A crucial step towards formulating a complete mechanism is understanding the role of the monomer's counter ion in the self-assembly process. Here this question is addressed by means of a well-defined artificial model system: supramolecular light-harvesting nanotubes (LHNTs) self-assembled from cyanine-dye molecules (figure). Even though this system has been intensively studied [1,2,3,4], the details of the self-assembly process are still not understood. Currently, LHNTs are known to form two different morphologies, individual double-walled nanotubes and bundles of single-walled nanotubes [4]. In this study, counterions with varying properties (e.g. polarizability) were employed to determine their role in the LHNT's self-assembling process. It was found that the rate of formation of bundles of LHNTs is directly correlated with the counterion concentration, and a much lower free ion concentration than electrolyte concentration produces a similar rate effect.

[1] D.M.Eisele et al., **Nature Chem.** 2012; [2] D.M.Eisele et al., **JACS** 2010; [3] D.M.Eisele et al., **Nature Nanotech.** 2009; [4] D.M.Eisele et al., **PNAS** 2014


Supramolecular Light-Harvesting Nanotube (LHNT) of Aggregated Dye Molecules

D.M. Eisele et al., *Nature Nanotech* 4 (2009), *Nature Chem* 4 (2012)

MARM 116

The structure and function of porphyrins in energy transduction: Electrochemical, optical, and quantum mechanical studies of the electronic structure of magnesium porphyrins

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Porphyrins are essential charge-transfer cofactors in life-sustaining biological processes, such as, photosynthesis and respiration. The diverse potentials of porphyrins, leading to important functional differences, are tuned by smart matrix effects from the surrounding protein environment. The fundamental design principles underlying the function of porphyrins in natural systems can be utilized to construct highly efficient bio-inspired artificial systems for the photochemical production of fuels from sunlight. Typically, the components of artificial photosynthetic systems include antennas, reaction centers, catalysts for fuel production and units for photoprotection which incorporate porphyrins as building blocks. In the present study, we are investigating a series of magnesium porphyrin models using cyclic and differential pulse voltammetry to determine the relative redox potentials. In parallel, we are conducting optical spectroscopy and density functional theory to directly determine the electronic properties of each porphyrin in different environments. We correlate the shifts in the redox potential of the porphyrins with the electronic properties of the porphyrin. This study provides direct support for the tuning and control of porphyrin cofactors in biological energy transduction and its application towards the construction of highly-efficient artificial photosynthetic devices.

*This research is supported by the Office of Basic Energy Sciences, U. S. Department of Energy under the contract DE-FG02-07ER15903.

MARM 117

Streamlining the chemical synthesis of novel quorum sensing inhibitors and studies of their biological activity

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Bacteria can synchronize gene expression based on their population density via a type of chemical communication known as quorum sensing (QS). From a simplified viewpoint, QS involves three steps, namely; the bacterial synthesis of small-molecule chemical signal(s), the release of these chemical cues into the surrounding environment and the ultimate integration of the chemical signaling event into changes in gene expression through recognition of the signal by bacterial receptor protein(s). Here we will describe our extensive SAR studies of a novel series of QS modulating compounds active against the LasR QS receptor in *Pseudomonas aeruginosa.* During the course of these investigations we have developed a novel unified strategy for the synthesis of carboxylic acid derivatives which we anticipate to be of broad synthetic utility. Going forward, we aim to establish LasR as a viable target to inhibit *P. aeruginosa* virulence and potentially provide a framework for the inhibition of QS in other pathogens.

MARM 118

Copper-promoted aromatic acyloxylation: Formation of aryl esters from aryl halides using copper(II) complexes

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Previous research has shown that complexes of Cu(I) can successfully promote the cross-coupling reactions of aryl halides to form aryl esters. Since complexes of Cu(II) are often cheaper and more stable, formation of Cu(I) species in situ by comproportionation of Cu(II) salts was explored. It was shown that Cu(II) acetate does, in fact, drive the copper-promoted aromatic acetoxylation of phenyl iodide. Product yields, as measured by gas chromatography, reached up to 90%. Furthermore, the change in color of the copper species as they transition between oxidation states allowed for an in-depth analysis by UV/Vis spectroscopy of the reaction rates. Additionally, Cu(II) sulfate, an even cheaper alternative, can promote the reaction in the presence of acetate salts, though with lower yields. Phase transfer agents, such as ammonium salts of tetraflouroborate and hexaflourophosphate, increased the yield of the Cu(II) sulfate reactions. Ultimately, it was shown that the comproportionation of Cu(II) in the presence of Cu(0) is a viable alternative to using Cu(I) complexes to promote cross-coupling reactions.

MARM 119

Scanning probe forces by rings of charge in electrolytes

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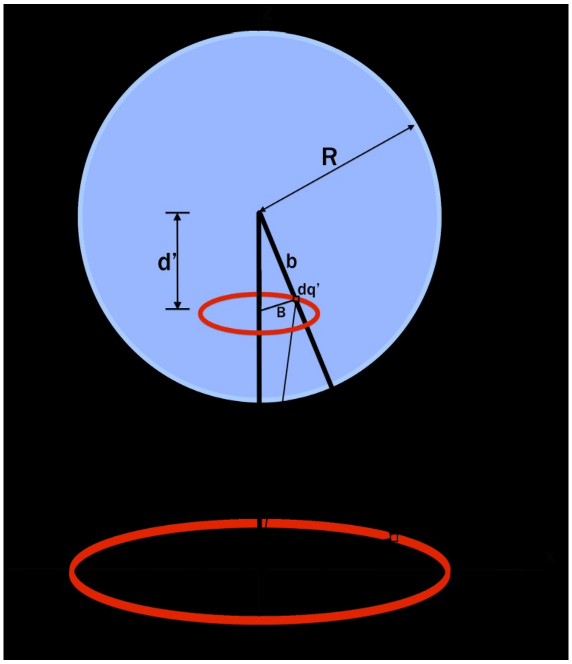
Pi stacking of aromatic rings is driven by elemental electrostatic interactions that control the nucleobase structure within DNA and RNA molecules, protein folding, template-directed synthesis and molecular recognition. Since its origin is not fully understood, we consider the use to of Scanning Probe Microscopy (SPM), which can address nanometric distances and nN forces. Thus we consider a ring of charge laying on an insulating substrate. The SPM tip is brought into close proximity to the ring. We first show how appropriate measurements of forces along the force-separation curve provides values for the charge density and ring size. More importantly, we show the qualitative change in forces as the ring is brought into higher-concentration electrolytes. While forces are always attractive in the low-concentration case, forces can be both attractive or repulsive at high concentrations. We will also present an algorithm to establish the fraction of stacking interaction that has an electrostatic origin.
Acknowledgement. Funding for this project from the National Science Foundation, Chemistry Division, grant #CHE-1508085



MARM 120

The harbor survey program of New York City's Division of Environmental Protection: A case study

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The Harbor Survey Program of New York City's Division of Environmental Agency (NYC-DEP) has evolved to monitor and protect the ecology and vitality of the city waterways. The annual New York Harbor Quality Report is presented in four different divisions and monitors four water quality parameters: fecal coliform, bacteria, dissolved oxygen, chlorophyll "a" and Secchi transparency. Fecal coliform, a collection of bacteria mainly found in human and animal intestines are linked with sewage waste. Chlorophyll 'a' found in phytoplankton is used as an indicator of primary productivity of the food chain. Dissolved Oxygen (DO) levels in water are critical for the respiration of aquatic life forms. The Secci disk estimates the clarity of the surface water via its transparency measurement. A detailed description and case studies will be presented.

MARM 121

New York City's waste water and sewage treatment by the Environmental Protection Agency

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One of the tasks that the Department of Environmental Protection in New York City (NYC-DEP) is responsible for is to treat the waste water collected from rain and snow that flows from the streets into storm lines and is directly discharged into the river. The sewage water from buildings is also collected and taken into waste water treatment plants through sanitary sewers. The procedure involves preliminary, primary, secondary, disinfection, and sludge treatment processes. The preliminary and primary steps involve mechanical process, removal of non-biodegradable waste which is sent to landfills and for sludge treatment respectively. The more complicated secondary process removes 90 percent of organic matter using bacterial decomposition. All disease-causing organisms that remain in the water after the secondary process are removed by sodium hypochlorite. The description and findings of all processes will be described extensively.

MARM 122

Synthesis and characterization of $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ ($0 \leq x \leq 1$) lithium-ion conductors

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Garnet-like oxides with the formula $Li_{7-x}La_3Zr_{2-x}Ta_xO_{12}$ ($0 \leq x \leq 1$) have been synthesized using conventional solid-state reaction methods at temperatures ranging from 1120 °C – 1230 °C. Preliminary characterization has begun with $Li_{6.4}La_3Zr_{1.4}Ta_{0.6}O_{12}$, which has been previously reported to have the largest room-temperature lithium ion conductivity ($\sigma_{Li} \approx 1.0 \times 10^{-3}$ Scm^{-1}) by Goodenough and coworkers. Variable temperature solid state ^7Li nuclear magnetic resonance spectroscopy was used to investigate the local structure and dynamics of the lithium ions. The signal is found in the shift range characteristic of diamagnetic lithium and is composed of a narrow resonance overlapping a broad component. Motional narrowing of the line shape is observed between room temperature and 473 K. ^7Li spin-lattice relaxation (T_1) measurements taken in the temperature range are consistent with the onset of lithium ion motion.

MARM 123

Oxidative ionization under helium-plasma ionization (HePI) mass spectrometric conditions

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The helium-plasma ionization (HePI) technique is a well-established ambient-ionization method to generate gaseous ions for mass spectrometric analysis, by direct insertion of a solid, liquid or gas sample into the ion source, or by performing in situ reactions which yield volatile products. We report that certain analytes, such as hydroquinone and certain quinonoid compounds, undergo “oxidative ionization” under negative-ion HePI-MS conditions. We explore the mechanisms of this ionization pathway and discuss the critical role of the superoxide radical-anion, generated by the HePI plasma, in oxidative ionization. Interesting results have been obtained from the three isomeric dihydroxybenzenes catechol, resorcinol, and hydroquinone; because each of these isomers either prefers to deprotonate or undergo "oxidative ionization" the spectrum produced from each isomer is distinct from the others. Hydrogen-deuterium exchange experiments proved that the hydroxyl protons of the dihydroxybenzenes are involved in the "oxidative" ionization mechanism. In addition, quantum-mechanical calculations also support our proposed mechanism. It was also found that under collision induced dissociation (CID) conditions analytes that prefer to undergo "oxidative ionization" also prefer to lose elements of hydrogen peroxide when their superoxide radical-anion adducts are isolated and fragmented. Dinitriles, which also form

superoxide radical-anion adducts, also prefer to lose elements of hydrogen peroxide under CID conditions.
Furthermore, we found that the balance between oxidative ionization and deprotonation of hydroquinone is critically dependent on the plasma character of the ionization source: at low spray-capillary voltages deprotonation was favored while at high capillary voltages (APCI-like conditions) oxidative ionization predominated. We therefore propose that hydroquinone can be used as a "plasmometer" compound to gauge the relative level of plasma conditions in the ion source.

MARM 124

Role of nucleation mechanism on the size dependent morphology of organic aerosol

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Aerosol particles composed of mixtures of organic and inorganic compounds can undergo liquid-liquid phase separation to form an aqueous two-phase system. In the submicron size regime, the morphology of particles is dependent on size, where for some systems, small particles are homogeneous and large particles are phase separated. In this work, the origins of the size dependence are explored by probing the morphology of aqueous poly(ethylene glycol) 400 (PEG-400)/ammonium sulfate mixtures for many different particle compositions. Surprisingly, we observe a size dependence at some organic/inorganic ratios, but not at others. Our results suggest that phase separation occurs by different mechanisms for the different ratios. At organic/inorganic mass ratios near the critical point where the activation barrier for phase separation is reduced, phase separation is seen at all particle sizes studied. Away from the critical point, the activation barrier leads to a size dependent morphology. Our results suggest that the size dependence occurs due to activated processes. This may have important consequences for the growth of new particles and the activation of cloud condensation nuclei, which impact Earth's radiation budget.

MARM 125

Application of multidimensional time model for probability cumulative function to Brownian motion on fractals in chemical reactions

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Multidimensional Time Model for Probability Cumulative Function can be reduced to finite-dimensional time model with two ordinal numbers 4 for the summation and multiplication over events and their probabilities and ordinal number 17 for the fractal-dimensional time arising from alike supersymmetrical properties of probability. The new method is based on properties of Brownian motion.This can lead to various applications for parameter evaluation so, as the original one-demetional Kramer's model for application of Brownian motion to chemical reactions, which is still in use, can be extended to multidemensional consideration. 2 images are only small parts of the abstract.

Hilbert some 120 years ago, though did not use Cauchy's inequality, but used rather some complicated methods to prove that $\sum\sum\frac{a_m b_n}{m+n} \le C(\sum a_m^2)^{1/2}(\sum b_n^2)^{1/2}$, with C= 2π, where the summations run from 1 to +∞, which was later reduced by I. Schur to C= π.There were some improvements to constant C in Hilbert's inequality such, as by H. Frazer, who showed that it can be reduced to (n+1) sin $\frac{\pi}{(n+1)}$,

and N. G. de Bruijn and H. S. Wilf showed that the best possible constant for the discrite case of summations running from 1 to N in $\sum\sum\frac{a_m a_n}{m+n} \le C(\sum a_n^2)^{1/2}$ can be replaced by C_N= π - $\frac{1}{2}\pi^5$ $(\log N)^{-2}+O(\log\log(\log N)^{-3})$, N→+∞ .
The later remarkable result is very important in light of the Bruijn-Wilf type best constant for nth finite section of Carleman's inequality $\sum_{k=1}^{n}(a_1 a_2 \cdots a_k)^{1/k} < C_n \sum_{k=1}^{n} a_k$. C_n=e-2 π^2 e1/ln(n)^2+O(1/ln(n)^3)C_2=1/2(1+sqrt(2)) C_3=4/3 And for the Hardy's inequality C_n=4-16 π^2 / ln(n)^2+ O(lnlnn/ln(n)^3) ,The extensions of Widder with the remark of Hardy are the following inequalities:

$\sum\sum\frac{\log(m/n)}{m-n}a_m b_n \le \pi(\sum\sum\frac{a_m a_n}{m+n})^{1/2}(\sum\sum\frac{b_m b_n}{m+n})^{1/2}$

$\sum\sum\frac{|\log(m/n)|}{\max(m,n)}a_m b_n \le 2(\sum\sum\frac{a_m a_n}{\max(m,n)})^{1/2}(\sum\sum\frac{b_m b_n}{\max(m,n)})^{1/2}$ where the summations run from 0 to +∞ , and the coefficient on the left-hand side is interpreted as 1/n when *m* = n;

In this form it is very much resembling the famuos Landau-Kolmogorov inequality, which was inroduced by E. Landau 2 years after I. Schur's improvement.that for $\|f\|$ to be the supremum of $|f(x)|$, a real-valued function f defined on $(0,\infty)$. and for a usually defined norm of real-valued function f defined on $(0,\infty)$ as $\|f\|=\sqrt{\int_0^\infty |f(x)|^2 dx}$, there are different constants $C(n,k)$ in inequality $\|f^{(k)}\| \le C(n,k)\|f\|^{1-k/n}\|f^{(n)}\|^{k/n}$.

Similar notions can arise in the discrete inequalities of Ky Fan, Taussky, and Todd that date 50 to 60 years ago: $\sum_{i=0}^{n}(x_i -2 x_{i+1} + x_{i+2})^2 \ge 16\sin^4\frac{\pi}{2(n+1)}\sum_{i=1}^{n}x_i^2$;for the sequence of real numbers x_0=0, x_1,....x_n, x_0=x_{n+1}=0, with equality holding if and only if x_i=csin $\frac{i\pi}{n+1}$, i=1,...,n, where c is a real constant and for the sequence of real numbers x_1=0, x_1,....x_n : $\sum_{i=0}^{n}(x_i - x_{i+1})^2 \ge 4\sin^2\frac{\pi}{2(2n+1)}\sum_{i=1}^{n}x_i^2$.

99 years passed before V. Milman established reverse form of the Brunn–Minkowski inequality that was proposed by Hermann Brunn 1 year before Hilbert's inequality.

PROPOSITION. Therefore, the use of supremum of a function over an interval, or maximum, or minimum instead of sum of the numbers completely loses the notion of multidimensionality and reduces it possibly to 1 dimension instead of *double-number* dimensional.

It is very certain, that this effect is given not only in mathematical formulae, but it has some psychological and methodological outcomes, that affect ability to recognize multidimensionality in the problem or mathematical model, as a way to solve it.

Consequently it is applicable to $m_p/m_e \cong \frac{\pi}{4}\times 432 \cong \frac{\pi}{4}\times 2 \times \zeta_3 \cong 6\pi^5$ and to many other investigations involving Brownian motion.

MARM 126

Biochemical characterization of hemorrhagic shock after transfusion of red blood cells

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Hemorrhagic shock (HS) remains a major cause of early death after trauma, accounting for up to 40% of trauma-related deaths. The optimal HS resuscitation strategy still needs to be determined, but it is recognized that it may include the avoidance of cardiac standstill, prevention of progression to untreatable shock and rescue of protracted HS. HS patients are exposed to pathophysiologic processes and therapeutic interventions, mainly blood transfusion, that predispose to hyperkalemia (hyperK), one of the deadliest electrolyte abnormalities.

Concentrates of red blood cells storage at low temperatures have a significant decrease of metabolites that are important for the viability and functionality of erythrocytes. The development of blood preservation solutions is a big interest for medical services. Normally the bags for storage blood is CPDA-1 and CPD/SAGM for more 21 days. Among the parameters to measure the quality and viability of the use of red cell bags are K+, Na+, Cl-, lactate, HCO3-, ammonia, glucose and pH. On various parameters (K+, Cl-, HCO3-, glucose and lactate) solution of CPD/SAGM kept the energy metabolism of red blood cells more stable.

Several reports describing packed red blood cells (PRBC) related hyperkalemic cardiac arrest have been published. PRBC K concentration is related to processes occurring during processing and storage steps, and is directly proportional to storage time, easily reaching levels higher than 60 mEq/L after 21 days. Is a potential marker of acute ischemic insult, hyperK may indicate that the body's ability to manipulate serum K is exhausted. This K homeostasis exhaustion hypothesis may be a critical factor in post-transfusional hyperK genesis and related complications.

MARM 127

A synthetic analogue of a metallo-β-lactamase and structural characterization of a β-lactam adduct

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Metallo-β-lactamases (MBLs) are a cause of growing concern for global health because of their role in resistance to antibiotics. For example, zinc-containing MBLs catalyze the hydrolysis of the β-lactam core present in most antibiotics. Therefore, we describe here a synthetic analogue of a zinc MBL that is derived from tris(isopropylbenzimidazolylthio)methane ($[\mathrm{Titm}^{\mathrm{Pr^iBenz}}]\mathrm{H}$). Specifically, the ionic species, $\{[\mathrm{Titm}^{\mathrm{Pr^iBenz}}]\mathrm{Zn}\}\mathrm{X}$ (X = $[\mathrm{BPh_4}]$ or $[\mathrm{MeB(C_6F_5)_3}]$), may be obtained by cleavage of the Zn–Me bond of $[\mathrm{Titm}^{\mathrm{Pr^iBenz}}]\mathrm{ZnMe}$ by treatment with $[\mathrm{PhNMe_2H}][\mathrm{BPh_4}]$ or $\mathrm{B(C_6F_5)_3}$, respectively. The non-coordinating nature of $[\mathrm{BPh_4}]^-$ and $[\mathrm{MeB(C_6F_5)_3}]^-$ allows for coordination of the β-lactam, 4-phenyl-2-azetidinone, to the zinc center, such that the molecular structure of $\{[\mathrm{Titm}^{\mathrm{Pr^iBenz}}]\mathrm{Zn(4\text{-}phenyl\text{-}2\text{-}azetidinone)}\}[\mathrm{BPh_4}]$ has been determined by X-ray diffraction. Furthermore, NMR spectroscopic studies have been employed to measure the magnitude of the binding interaction of 4-phenyl-2-azetidinone and other compounds that have potential use as inhibitors for MBLs.

MARM 128

Lanthanide complexes with fluorinated selenolate ligands: Synthesis, structure, and NIR emission

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Luminescent lanthanide (Ln) ions can realize emissions from visible to near-infrared (NIR) regions, and the three most promising candidates for efficient NIR emission are Nd^{3+}, Er^{3+} and Tm^{3+} . Based on the experience from our previous studies, we recently develop three monometallic lanthanide fluorinated selenolate complexes $(DME)_2Ln(SeC_6F_5)_3$ (DME=Dimethoxyethane, Ln=Nd, Er, Tm). Crystallographic data proves that all three complexes are isostructural. The Ln (III) ions are surrounded by three SeC_6F_5 ligands and four oxygen donors from two DME molecules. There is also a dative interaction between fluorine atom of one of the coordinating SeC_6F_5 and Ln (III) in all three compounds (See **Figure.1**). Spectroscopic studies indicate that these compounds show intense NIR emission with characteristic band positions. This can be attributed to the low Ln-Se phonon energies and a reduced number of C-H bonds in the compounds, as C-H functional groups vibrationally quench emissions and shorten excited-state lifetimes. The longer Ln-Se bond also increases the separation between the excited state Ln ion and the aryl group relative to previously studied OC_6F_5 and SC_6F_5 analogs, and this also helps to improve the quantum efficiencies.

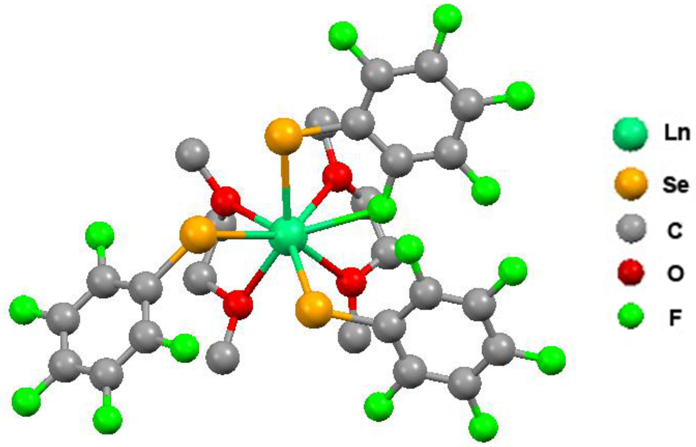

Figure.1 Structure of $(DME)_2Ln(SeC_6F_5)_3$

MARM 129

Fundamental understanding of binuclear alkyl hydrides of chromium and their reaction with hydrocarbons

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We have previously encountered binuclear chromium alkyl/aryl hydrides supported by β-diketiminate ligand (Nn), which resist reductive elimination even upon heating.[1] We have established a general route for the synthesis of such complexes (where alkyl = trimethylsilylmethyl, phenyl, benzyl and neopentyl) by hydrogenolysis of Cr(II) alkyls of the type NnCrR(THF). Notably, we find that the chromium neopentyl hydride readily reacts with various hydrocarbon substrates, such as benzene, toluene and tetramethylsilane to afford the corresponding alkyl hydride complexes. This is an apparent C-H activation. A mechanistic study of the transformation has been carried out, and our suggested mechanism involves a dissociation and σ-bond metathesis pathway. The synthesis, structures and exploration of the reactivities of the chromium alkyl hydrides will be discussed.

[1] (a) MacAdams, L. A.; Buffone, G. P.; Incarvito, C. D.; Golen, J. A.; Rheingold, A. L.; Theopold, K. H. A stable alkyl hydride of a first row transition metal. Chem. Commun. 2003, 1164-1165, (b) Monillas, W.; Yap, G. P. A.; Theopold, K. A Tale of Two Isomers: A Stable Phenyl Hydride and a High-Spin (S=3) Benzene Complex of Chromium. Angewandte Chemie International Edition 2007, 46, 6692-6694.

MARM 130

Ligand-substituted Mn_{12} single-molecule magnet derivatives: Characterization and surface organization

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Single molecule magnets (SMMs) have long been of great interest for their potential ability to store information on the nanometer and sub-nanometer length scale. Organization of surface attached clusters, as well as magnetic characterization, has been investigated with the hope of utilizing these molecules in nanodevices. The most well-known example is the molecule studied here, $Mn_{12}(O_2CCH_3)_{16}$, or simply Mn_{12}. The goal is to design ligands to
confer self-organization to Mn_{12} SMMs, and study the effects of ligand substitution on the 2D and 3D self-assembly.
Structural information, such as maintenance of an intact core and surface crystal packing, as well as magnetic ordering were investigated on both bulk material and thin films to establish whether SMM behavior is maintained.

MARM 131

Reactivity of alkyl/aryl hydride chromium complexes supported by redox non-innocent α-diimine ligand

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Due to unusual electronic and geometric structures as well as unprecedented reactivity, low valent chromium complexes supported by α-diimine ligands have drawn great interest from inorganic chemists.

Previously, our group synthesized a series of chromium alkyl/aryl hydride complexes supported by β-diketiminate ligands, while the alkyl/aryl hydride complexes bearing α-diimine ligands (which are notoriously 'redox-ambiguous') were unexplored. This presentation will focus on the synthesis of a number of alkyl/aryl hydride CrIII-CrIII dinuclear complexes featuring α-diimine ligands, showcasing their unexpected structures, their curious stability, and their reactivity. These studies expand the chemistry of alkyl hydrides of first row transition metals and have the potential to provide a novel approach to the activation and functionalization of hydrocarbons.

MARM 132

New frontiers for synthetic metalloenzymes: Imprinted nanogels with phosphatase-like activity

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Phosphate esters are remarkably stable linkages and are found in the molecules of life DNA and RNA, as well as in toxic compounds, such as nerve agents, pesticides and herbicides.[1,2] The development of artificial metal-based catalytic systems for phosphate ester hydrolysis is currently an active field and is the central focus of this work.[3] Polymerisable Co-cyclen complexes with phosphonate and carbonate templates were used to obtain nanogels that show higher activity and turnover with low catalytic load, compared to the free complex, in the hydrolysis of 4-nitrophenyl phosphate, a nerve agent simulant. This work demonstrates that the chemical structure of the template impacts the coordination geometry and oxidation state of the metal centre in the polylmerisable complex resulting in very significant changes in the catalytic properties of the polymeric matrix.[4] A range of cyclen-based ligands has also been prepared. The hydrolytic activity of the corresponding structurally similar *N*-functionalised 'free' Co(III)-tetraamine complexes **1-6** has been investigated and been shown to be extremely sensitive to modest changes in ligand structure that do not affect the coordination chemistry.

1. Chem. Commun., **48**, 2012, 5545. 2. *Angew. Chem. Int. Ed*., **55**, 2016, 42. *3. Chem. Rev*., **115**, 2015, PR1. 4. *Chem. Eur. J*., **22**, 2016, 3764

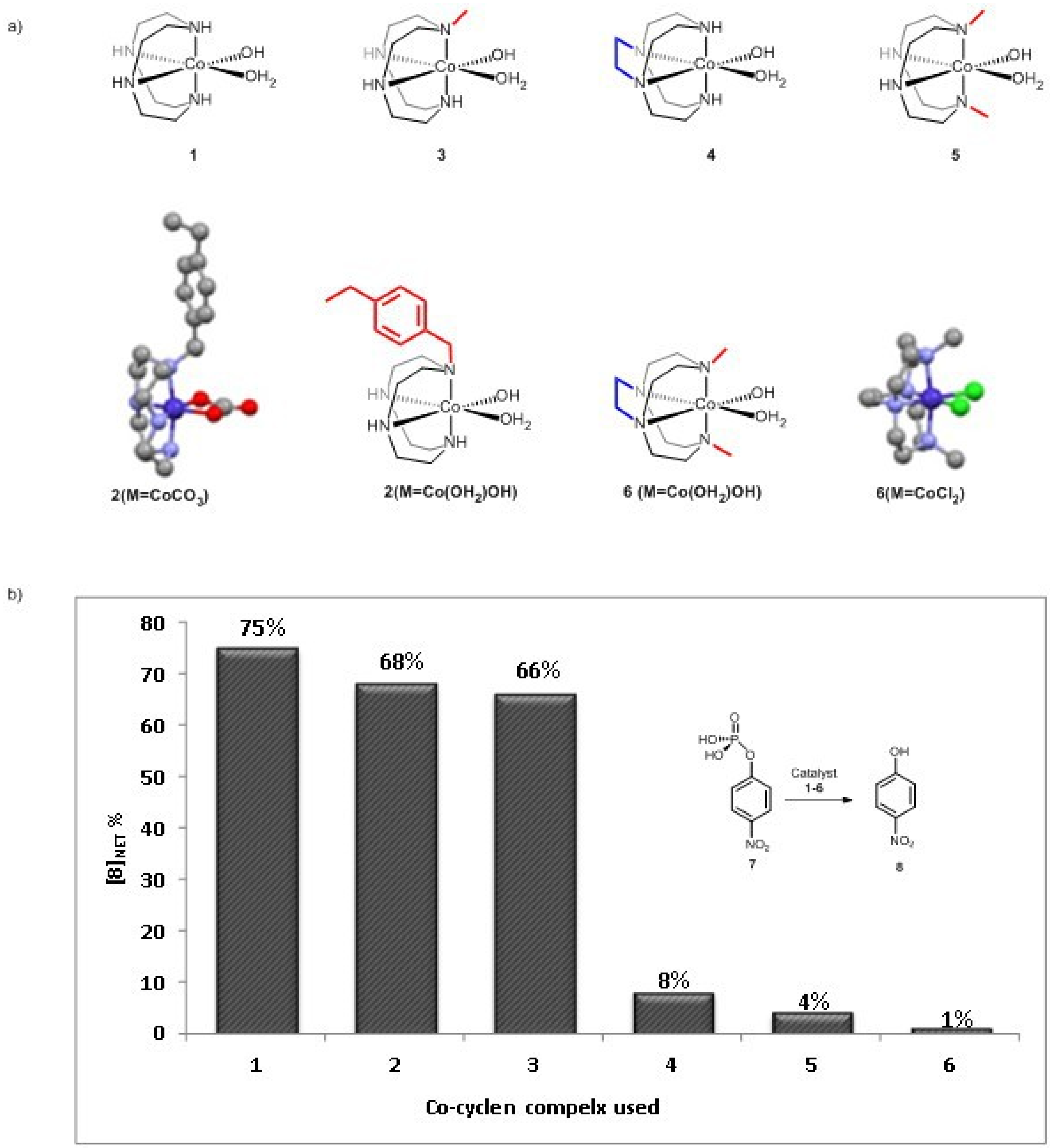

Figure 1. a) *N*-functionalised Co(III)-cyclen complexes used for phosphates ester hydrolysis; crystal structures of **2** (M=CoCO$_3$) and **6** (M=CoCl$_2$); b) yield of **8** after hydrolysis of phosphate ester **7** using complexes **1-6**

MARM 133

Magnetic and electronic studies on magnetic semiconductor solid solutions

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Magnetic semiconductors are of great interest because of their coupled magnetic, electronic, and optical properties. Due to this coupling, europium chalcogenides exhibit spin filtering effects, giant magnetoresistance, large magneto-optical Kerr rotations, and giant magnetocaloric effects at the ferromagnetic ordering temperature. These properties are highly desirable for many applications like memory devices, where magnetic, optical and electrical signals can be interconverted.

Europium selenide is a particularly interesting magnetic semiconductor because it is metamagnetic, meaning it is antiferromagnetic at low- and ferromagnetic at high-magnetic fields. We have prepared bulk powders of $EuS_{(1-x)}Se_{(x)}$ solid solutions by solid-state reactions. Varying the composition at the anion site was used to control the band gap (E_g). ICP-MS and pXRD were used to confirm composition and structure of the alloys. SQUID measurements were then used to study the relationship between the composition (and therefore E_g) and the magnetic ordering temperature.

Another system we are interested in is the $Eu_{(1-x)}Sm_{(x)}Se$ solid solution. By changing the composition at the cation site we can study the how the metal environment can be tuned to control the lanthanide valence. Measurements using pXRD show that the cell constant follows a non-linear trend with the increase in x, which can be explained by the change in the oxidation state of Sm as it is doped into EuSe. Doping Sm^{3+} at low doping levels results to a decrease in cell constant, and as the doping level increases the cell constant also increases approaching that of SmSe. Pending XAS and XMCD experiments will allow us to confirm the oxidation states of both metals in the material. ICP-MS and SQUID measurements also give us a fuller understanding of composition and magnetic properties of the solid solutions.

MARM 134

Impact of the diversity of single molecule junction structure on conductance and link bonds

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The break-junction technique for simultaneous measurement of junction conductance and sustained force in single molecule junctions bridging metal electrodes naturally probes a large ensemble of junctions for each choice of molecule and link group. Analysis of the most probable value of target measured values from histograms has supported fruitful studies of the relationship between molecular structure and junction conductance characteristics as well as the mechanical characteristics of the molecule-metal link bond. However, the ensembles behind the histograms represent an inherently diverse sampling of distinct junction structures. Each structure has a corresponding set of data mapping junction conductance and sustained force as a function of junction elongation. This rich data set offers a much larger scope for understanding structure-function relationships, for example with respect to the characteristics of the metal-link molecule bonds [1]. In this talk I will describe progress towards physical interpretation of the data across histograms, including physical models for both conductance characteristics and force-extension curves. I will also discuss results based on Density Functional Theory calculations, particularly directed to the impact of tip structure on link bond energy and force extension characteristics.

[1] M. S. Hybertsen and L. Venkataraman, Acc. Chem. Res. **49**, 452, 2016.

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MARM 135

Charge transport through single molecules

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Charge transport through and between molecules is central to many important processes in nature. In particular, studying the conductivity of single molecules can contribute to a better understanding of charge transport through molecules, and also help develop better molecular wires and other building blocks of molecular electronics, light harvesting devices, etc. We will discuss the results of different experiments designed to understand these processes at the single molecule level. We measure the conductivity of molecules using the Scanning Tunneling Microscope break-junction (STM-BJ) method that utilizes repeatedly formed circuits where one or a few molecules are trapped between two electrodes, at least one of which has nanoscale dimensions. The statistical analysis of thousands of measurements yields the conductance of single molecules.

One particular interest has been the role of the molecule-electrode contact in charge transport. In the simplest analysis this contact can present a substantial barrier to charge injection, which can have important consequences in devices such as dye sensitized semiconductor nanoparticle solar cells. We have demonstrated that carbodithioate termination of molecules can enhance conductivity by an order of magnitude. We have also shown how the sensitivity of the electrical conductivity of single molecules to external perturbations can allow for switching and sensing, as well as the use of single molecule conductance for the discovery of novel materials.

MARM 136

Junction conductance of fluorene molecular wires

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A novel series of fluorene oligomer molecular wires have been synthesized and their charge transport properties have been measured in molecular junctions using the scanning tunneling microscopy-based break junction (STM-BJ) method. The junction conductance of a series of oligofluorenes containing one through three fluorene subunits has been investigated. In addition, fluorene monomers with different constituents at the bridge carbon (dimethyl, dihexyl, and didodecyl) have been studied. In both series, dimethyl sulfide (–SMe) end groups are used to contact the gold electrodes for molecular junction formation. Charge transport in the Au-oligofluorene-Au junctions occurs via tunneling. The results are benchmarked to STM-BJ conductance measurements of 1,4-diaminofluorene to investigate the role contact chemistry (–NH_2 versus –SMe) has on junction formation and conductance.

MARM 137

Bandgap engineering through controlled oxidation of polythiophene

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The use of Rozen's reagent (HOF CH_3CN) to convert polythiophenes to polymers containing thiophene-1,1-dioxide (TDO) is described. The oxidation of polythiophenes can be controlled with this potent, yet orthogonal reagent under mild conditions. The oxidation of poly(3-alkylthiophenes) proceeds at room temperature in a matter of minutes, introducing up to sixty percent TDO moieties in the polymer backbone. The resulting polymers have a markedly low-lying lowest unoccupied molecular orbital (LUMO), consequently exhibiting a small bandgap. This approach demonstrates that modulating the backbone electronic structure of well-defined polymers, rather than varying the monomers, is an efficient means of tuning the electronic properties of conjugated polymers.

Reference:

Wei, S.; Xia, J.; Dell, E. J.; Jiang, Y.; Song, R.; Lee, H.; Rodenbough, P.; Briseno, A. L.; Campos, L. M. "Bandgap Engineering through Efficient Oxidation of Polythiophenes." *Angewandte Chemie International Edition*, **2014**, 53, 1832-1836.

MARM 138

Effect of intercalator substituent and nucleotide sequence on the stability of DNA- and RNA-naphthalimide complexes

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DNA intercalators are commonly used as anti-cancer and anti-tumor agents. As a result, it is imperative to understand how changes in intercalator structure affect binding affinity to DNA. Amonafide and mitonafide, two naphthalimide derivatives that are active against HeLa and KB cells *in vitro*, were previously shown to intercalate into DNA. Here, a systematic study was undertaken to change the substituent on the aromatic intercalator 1,8-naphthalimide to determine how different functional groups with a variety of physical and electronic properties affect binding of the naphthalimide to DNA and RNA duplexes of different sequence compositions and lengths. Wavelength scans, NMR titrations, and circular dichroism were used to investigate the binding mode of 1,8-naphthalimide derivatives to short synthetic DNA. Optical melting experiments were used to measure the change in melting temperature of the DNA and RNA duplexes due to intercalation. Thermal stabilities were affected by changing the substituent, and several patterns and idiosyncrasies were identified. By systematically varying the substituent, the binding strength of the same derivative to various DNA and RNA duplexes was compared. The binding strength of different derivatives to the same DNA and RNA sequences was also compared. The results of these comparisons shed light on the complexities of site specificity and binding strength in DNA-intercalator complexes.

MARM 139

Structural and functional diversity of RNA induced by 2'-5' backbone linkages

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RNA plays dual roles as a carrier of genetic information and as a catalyst of specific reactions, and it may have been the first biopolymer to have emerged on the early earth. The non-enzymatic replication of RNA was likely a key step in the evolution of simple cellular life from prebiotic chemistry. In the current model of template-directed polymerization of activated monomers, the chemical copying of RNA always generates a mixture of 3'-5' and 2'-5' backbone linkages due to the similar nucleophilicity and orientation of the 2' and 3' hydroxyl groups on the ribose. This lack of regiospecificity has been regarded as a central problem for the evolution of functional RNAs, since the resulting backbone heterogeneity was expected to disrupt their folding, molecular recognition and catalytic properties of functional RNAs such as ribozymes.

However, a recent study has demonstrated that RNAs with a certain percentage of 2'-5' linkages can still retain RNA functions. More interestingly, it has been known for a long time that 2'-5' linkages can reduce the melting temperature of RNA duplexes, making it easier to separate the strands. Considering that strand separation is another unsolved big problem for non-enzymatic RNA replication, this feature may actually afford a selective advantage to duplexes exhibiting backbone heterogeneity. In addition, previous studies have revealed that 2'-5' linkages in a RNA duplex are more easily hydrolyzed compared to normal 3'-5' linkages. Thus, there is a selective advantage for the evolution of homogeneous RNA systems with more accurate replication. Altogether, the coexistence of 2'-5' and 3'-5' linkages may be a critical feature that allowed RNA to play a central role in the original stage of life. In this work, we will present a series of crystal structures of RNA duplexes and aptamer that contain 2'-5' linkages. These structures will provide detailed insights into how RNAs adjust their structures to accommodate backbone heterogeneity and diversify their functions.

MARM 140

Finding the environmental footprints on our genetic materials

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Systematic evaluation of how environmental changes impact our ecosystems requires new technologies that can accurately detect and monitor their footprint on organisms at the molecular level. I will present our latest progress on technological development to answer questions on how genetic materials, such as DNA or RNA, change/modify chemically in response to environmental changes such as changes in food, energy, and water. The resulting data will provide policy makers and the communities working on environmental changes with scientific evidence to better understand and manage the evironmental impact on our ecosystems.

MARM 141

Conformational consequences and structural details of the self-assembly of hIAPP$_{22\text{-}29}$ and hIAPP$_{20\text{-}29}$

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The octapeptide NFGAILSS (hIAPP$_{22\text{-}29}$), derived from human islet amyloid polypeptide, has been extensively used as a model system to study amyloid formation. However, despite being the target of numerous investigations, information describing specific molecular interactions and conformational details are still lacking in regard to aggregates formed by this peptide. We synthesized peptide analogs of hIAPP$_{22\text{-}29}$ and hIAPP$_{20\text{-}29}$ and employed turbidity measurements in conjunction with FTIR, Raman and fluorescence spectroscopy along with computer modeling to investigate and probe the structure of aggregates formed by the NFGAILSS sequence. We provide detailed structural description of the pi-stacking interactions using Raman, IR and fluorescence data. Investigation of amyloid fibrils formed by hIAPP$_{20\text{-}29}$ and hIAPP$_{22\text{-}29}$ showed different orientations of the beta-sheets formed under similar conditions. We also have found correlation between the protonation state of the N or C termini of hIAPP$_{22\text{-}29}$ and the orientation of beta-sheets formed. We believe that pi-stacking interactions serve to enhance peptide-peptide interactions and likely provide the directional and organizational component of the self-assembly process.

MARM 142

Correlation between membrane binding and disruption by the antimicrobial peptide Maximin 3

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Antimicrobial peptides (AMPs) are a promising class of naturally-derived antibiotics that may help counteract the spread of antibiotic-resistant infections. Many AMPs act by binding to and disrupting the membranes of their bacterial targets, thereby allowing leakage across the membrane that leads to cell death. We used fluorescence anisotropy and dye leakage assays to investigate the correlation between membrane binding and disruption of the AMP Maximin 3 from *Bombina maxima*. The cationic Maximin 3 binds more strongly to more negatively charged lipid vesicles and exhibits a corresponding increase in vesicle leakage. By quantifying these effects we have gained insight into the mechanism of membrane disruption and raised questions regarding correlations when other lipid parameters are varied.

MARM 143

The effect of N-terminal and indole amine protonation state on aromaticity and tryptophan quantum yield

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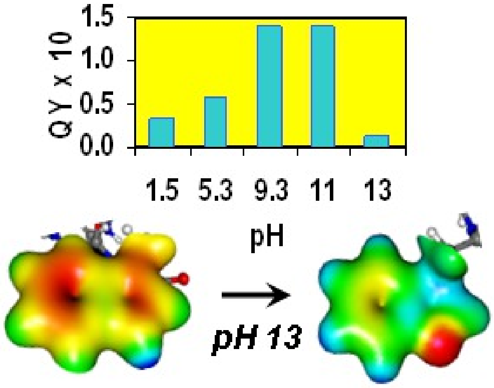
The quest for factors controlling the partition of excitation energy between fluorescence and nonradiative processes in tryptophan is of perennial interest to spectroscopists because its fluorescence has distinct intensity, color and environmental sensitivity. Solving the relationship between specifics of molecular environment and characteristics of tryptophan fluorescence would provide the key for emission spectra interpretation. For fluorescence, quantum mechanical (QM) calculations have shown that the highest occupied molecular orbital (HOMO) for ^1L_a, the primary indole fluorescent transition dipole moment, is the ground state for the fluorescing transition. Our QM calculations and molecular modeling reveal substantial differences in ground state isosurface charge distribution on the indole ring for Lys-Trp, Trp-Lys and Trp-Glu dipeptides when backbone and residue charge is varied. These isosurfaces represent the superposition of all ground state molecular orbital contributions to charge distribution. Comparison of Trp dipeptide species isosurfaces with experimentally derived quantum yields and fluorescence lifetimes reveals a correlation of high, uniform π-electron density on the indole with high quantum yield and long average lifetime. These conditions are met when the N-terminal amine is deprotonated. The isosurfaces for these states resemble the charge distribution of the HOMO for ^1L_a. Low quantum yield and short average lifetime correlate with low, uneven π-electron density over the indole ring and electron density on the exoring methylene carbon. These conditions are met when the N-terminal amine is protonated (low pH) and the indole amine is deprotonated (high pH). Where x-ray crystal structures have shown proteinaceous tryptophans to be hydrogen bonded at the indole amine, and low quantum yields are observed, isosurfaces where π-electron density is concentrated at the indole amine is anticipated for these proteins. These π-electron density losses and redistributions can be identified as a loss of aromaticity.



MARM 144

Phosphorylation study of HIV regulatory proteins using mass spectrometry

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Introduction:
This investigation aims to comprehensively identify and characterize possible phosphorylation sites of HIV- regulatory proteins using bioinformatics prediction strategy followed by MALDI mass spectrometric characterization *in vivo* as well as *in vitro*.
Method:
Amino acid sequences of HIV- regulatory proteins from 13 different strains are aligned using CLUSTALW to assess conservation- as conservation strongly suggests biological function in rapidly mutating HIV sequences. Bioinformatics tools such as NetPhosK, GPS and KinasePhos are used to predict potential phosphorylation sites of HIV- regulatory proteins at conserved sites. Initially synthetic HIV-peptide corresponding to bioinformatics predictions are incubated with specific kinases and ATP and

analyzed to detect phosphorylation. Preliminary hits are further investigated at protein level using SDS-PAGE gel electrophoresis followed by in-gel proteolysis and mass spectrometric analysis. Site-specific antibodies and HIV proteins mutant will be generated to probe as well as to study biochemical relevance of potential phosphorylation sites.

Preliminary Data:

We have determined more than 25 potential phosphorylation sites from HIV-proteins including Nef, Rev, Tat, Vif, Vpr and Vpu using phosphorylation prediction algorithms such as NetPhosK, GPS and KinasePhos. Based on high score from prediction algorithms we have incorporated 14 different kinases in this study. *In-vitro* kinase assay of Rev peptides show potential phosphorylation at 3 predicted sites including Ser5, Ser8 and, Ser54 by using Casein kinase II and Protein Kinase A. Likewise *in-vitro* kinase assay of Nef peptides resulted in phosphorylation at 4 predicted sites- Ser6, Thr15, Thr128 and Ser163 using Protein Kinase C (alpha, beta and theta), MAPK and Casein Kinase I. Currently the research project is further extended to evaluate phosphorylation at protein level as of some interesting results have been observed with Rev and Nef-peptides.

Novel Aspect:

This study can provide detail understanding of host-kinase/phosphorylation sites interaction, and represents the first attempt at a comprehensive host-kinase/HIV substrate proteomics study.

MARM 145

^{13}C, ^{2}H NMR studies of structural and dynamical alterations of glucose-exposed porcine aortic elastin

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Elastin, the principal component of the elastic fiber of the extracellular matrix, imparts vertebrate tissues with remarkable resilience and longevity. This talk will highlight solid state NMR spectroscopy and relaxation measurements used to elucidate dynamical and structural modifications of porcine aortic elastin exposed to glucose. Results from macroscopic stress-strain tests will also be presented showing that glucose treated elastin is mechanically stiffer than the same tissue without glucose treatment. These measurements showed a large hysteresis in the stress-strain behavior of glucose treated elastin --- a well known signature of viscoelasticity. Two dimensional relaxation NMR methods were also used to investigate the correlation time, distribution, and population of water in these samples. Differences are observed between the relative populations of water, while the measured correlation times of tumbling motion of water across the samples were similar. ^{13}C magic angle spinning NMR methods were applied to investigate structural and dynamical modifications following glucose treatment. While some overall structure is preserved, the process of glucose exposure results in more heterogeneous structures and slower mobility. The correlation times of tumbling motion of the ^{13}C-^{1}H internuclear vectors in the glucose treated sample are larger than in untreated samples pointing to a more rigid structure. The ^{13}C cross polarization spectra reveal a notable increased α-helical character in the alanine motifs following glucose exposure. Results from molecular dynamics simulations are provided adding further insight into dynamical and structural changes of a short repeat $[VGPVG]_5$, an alanine pentamer, desmosine, and isodesmosine sites with and without glucose. The simulations point to changes in the entropic and energetic contributions in the retractive forces of VPGVG and AAAAA motifs. Most notably, the energetic contribution in the retractive force due to peptide-glucose interactions of the motif VPGVG increases and apears to be an important contribution to the observed stiffening in glucose treated elastin

MARM 146

You can have a rewarding career as an adjunct professor with the help of online media

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The media has highlighted the problems concerning the "Adjunct Professor”. The disease of “Adjunctavitis” is seen as a growing problem for our higher education system. Because of the availablity of media and online communication it is made much easier to navigate. Another positive aspect is that it can often lead to collaborations and other unforeseen opportunities. In addition, if one is simultaneously teaching at multiple institutions it can aid in the planning of more effective courses, as one observes both good and bad pedagogy. These topics will be presented from the “Itinerants” Adjunct and full time professors' perspectives. `

MARM 147

Creative design of the textbook for today’s students

Jason S. Overby*, overbyj@cofc.edu. Chemistry and Biochemistry, College of Charleston, Charleston, South Carolina, United States*

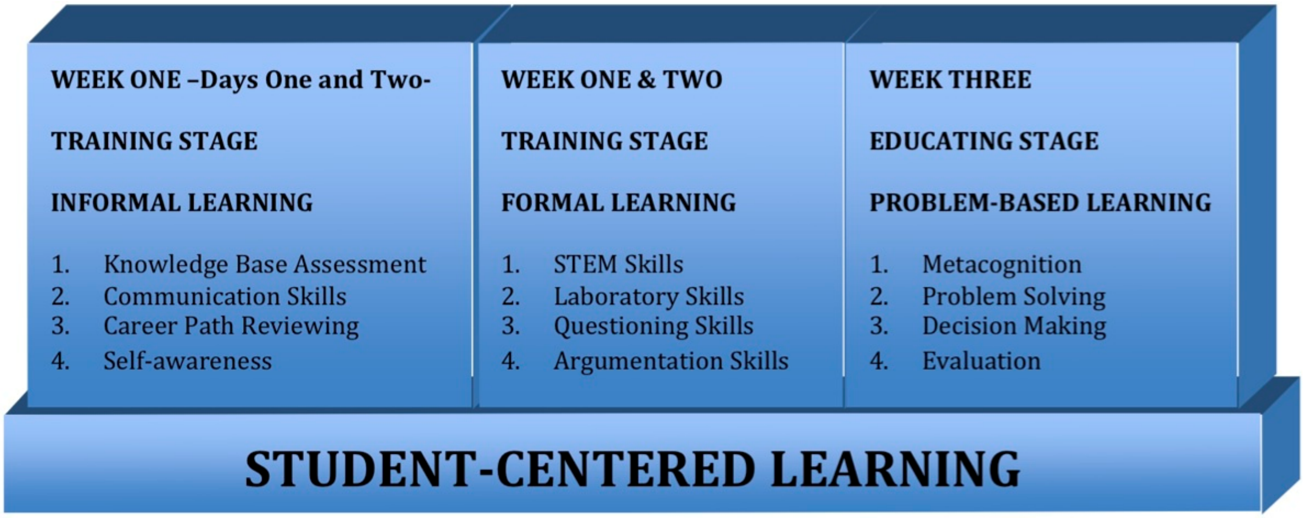
The model of textbook creation has traditionally focused on instructor input to craft the presentation of content. Textbook authors heavily rely on instructors providing insight to student behaviors and learning difficulties. But how much do instructors actually know about their students’ learning? While virtually all chemistry instructors know the major topics that students struggle with, it is not always clear where serious misconceptions exist with students. Now with adaptive learning tools, we have probes of deep insight into what students know, what they don’t know, what they think they know, and what they don’t know that they don’t know. With this valuable information, truly student-centered textbooks are a reality. This talk will investigate the role of using adaptive learning tools to create textbooks for today’s students by address their true stumbling blocks in learning chemistry.

MARM 148

A student-centered approach to materials science and nanotechnology for high school students

Luis A. Avila*, laa4@columbia.edu. Chemistry, Columbia University, New York, New York, United States*

A three-week student-centered summer program designed to expose junior and senior high school students to materials science and nanotechnology is described. The activities are grouped into two learning stages: the training-learning stage, which makes use of verification-structured experiments, and the educating-learning stage, in which the students solve a problem. The two-week training-learning stage integrates a wide range of teaching strategies, including informal and formal learning. The one-week educating-learning stage uses Problem-Based Learning (PBL) strategies in the form of independent projects. At the end of the program the students present the solution to the problem in a public poster session. The effectiveness of the program has been evaluated qualitatively and quantitatively using Student Assessment of their Learning Gains (SALG) surveys



MARM 149

Assessing the teaching and learning experience between hybrid and traditional coursework

__Keith A. Baessler__, 30737224@acs.org. Chemistry, Suffolk County Community College, Brentwood, New York, United States

How do we know if our chemistry students are “getting it”; that is, achieving the goals and objectives (student learning outcomes) of the course? This presentation details an assessment method used to determine success in achieving student-learning outcomes. Assessments like these identify strengths and weaknesses, which lead to improved instructional strategies and student learning outcomes.

MARM 150

New chemistry experiment: Implementation of a partially online chemistry course for allied health majors at Queensborough Community College

__Kevin Kolack__, kevin@professorKshow.com. Chemistry, Queensborough Community College - CUNY, Woodside, New York, United States

Introduction to General Chemistry (CH127) is the first semester of a traditional, 2-semester Introduction to General, Organic, and Biochemistry (GOB) course offered in approximately two dozen sections of 30 students each semester at Queensborough Community College - City University of New York (QCC). To date, the chemistry department at QCC has offered no online courses. The author developed this partially online course offering students online lectures, online homework and discussion boards, and in-person problem sessions and quizzes. (Students register for the in-person laboratory component separately.) Student outcomes are assessed in comparison to the traditional face-to-face course.

MARM 151

Teaching chemistry to undergraduates at the community college level: Preparing the student for the transferring process and beyond

***Paris D. Svoronos**, psvoronos@qcc.cuny.edu. Chemistry, QCC of CUNY, Bayside, New York, United States*

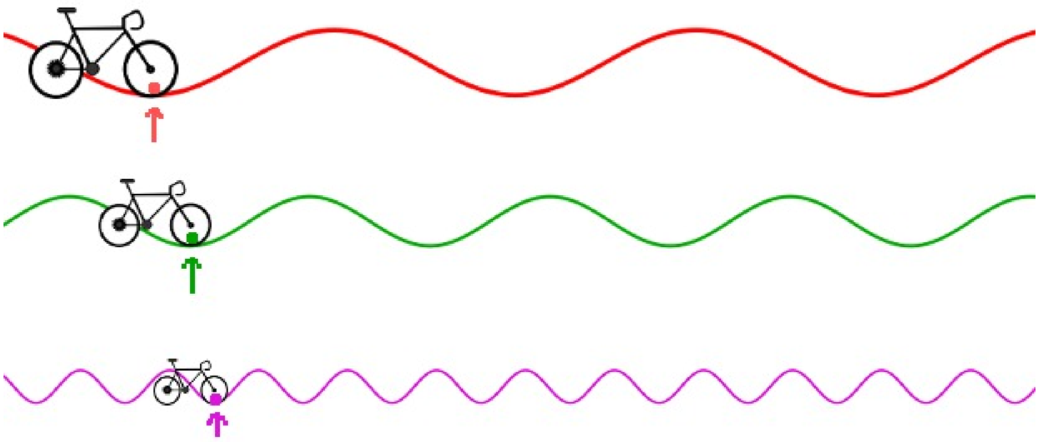
Queensborough Community College of the City University of New York has had a surge of science majors in the last 15 years. This has been achieved via continuous personal advising, mentoring, group tutoring, frequent testing and efforts to create a cohort. The results have led to several students pursuing and achieving graduate degrees in well-reputed programs. The strategies and results of this effort will be presented.

MARM 152

Bridging low- and high-stakes in writing: Intensive chemistry and the arts

***Derek A. Bruzewicz**, dbruzewicz@qcc.cuny.edu. Chemistry, Queensborough Community College, Bayside, New York, United States*

Chemistry and the Arts links physical and chemical topics such as the structure of light, the theory of color, and hands-on laboratory activities in inorganic synthesis to some of their applications in the arts, in design, and in digital media. Because the course requires no prerequisites in science or mathematics, beginning students in Chemistry and the Arts must master a great deal of new vocabulary and the format of laboratory reports in addition to the usual topics in general chemistry, such as chemical nomenclature and use of the periodic table. Non-native speakers of English and first-year students particularly struggle with the new language required by the course. The current work updates the design and implementation of Writing-Intensive (WI) Chemistry and the Arts for non-science majors at an urban community college by emphasizing student writing in a variety of contexts: laboratory reports, essays and research papers, and low-stakes reflections on contemporary news articles. Preliminary surveys show that the emphasis on reading and vocabulary enhance students' understanding of concepts in both chemistry and in the arts. Reflective writing in a science course also provides frequent opportunities for bi-directional feedback regarding students' interests and mastery of the material. Other low-stakes writing assignments, such as group work in editing and revision, serve as scaffolds for formal papers or oral presentations. Preliminary assessment data suggests that participants in the WI version of Chemistry and the Arts complete the course feeling more invested in their program of study and better equipped to communicate through writing.



Bicycles of difference sizes moving at constant speed to illustrate varying wavelength and frequency in visible light.

MARM 153

Liquid scintillator physics

Minfang Yeh, *yeh@bnl.gov. Chemistry, Brookhaven National Laboratory, Upton, New York, United States*

The BNL Neutrino and Nuclear Chemistry group is well-known for its world-leading expertise in metal-doped and water-based liquid scintillator and has the state-of-art scintillator development facility that is capable of formulating various scintillator detectors for different nuclear and particle physics experiments. Different chemical elements doped in various organic scintillators (metal-loaded liquid scintillator) have a variety of applications in neutrino detection. In addition, water-based liquid scintillator (WbLS) is a newly developed, cost-effective detection medium for future massive detectors with the unique capability of exploring physics below the Cherenkov threshold and has the ability of loading any (hydrophilic) metallic ions of interest for neutron tagging or other physics enhancements. The same water-based detector could also serve as the near detector for long baseline neutrino beam monitoring or be used for detection of diffuse neutrino flux from distant past supernovae. In this presentation, the applications of liquid scintillator to a variety of future experiments including double-beta decay, dark matter search, reactor neutrino and beam physics, will be discussed.

MARM 154

Neutrino detection utilizing novel metal-loaded organic and highly purified scintillators

Steven D. Rountree, *rountree@vt.edu. Physics, Virginia Tech, Shawsville, Virginia, United States*

Multi-ton-scale organic liquid scintillator detectors have been essential to an array of fundamental and groundbreaking measurements in neutrino physics. It begins with the discovery measurement of neutrinos [1], measurement of the antineutrino oscillation parameter Δm^2_{21} in KamLAND [2], direct real-time measurement in Borexino of the ^{7}Be and pp solar neutrinos [3,4], and the Daya Bay measurement of the θ_{13} mixing angle [5]. This presentation will discuss the neutrino detection methods in liquid scintillator, the state of the art in organic liquid scintillator and metal-loaded organic liquid scintillator that led to Borexino's and Daya Bay's success, and the future of neutrino detection using organic scintillators, including searches for sterile neutrinos, $0n\beta\beta$ decay, and investigations into the neutrino mass hierarchy.

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MARM 155

Cherenkov scintillation separation in liquid scintillator

Zhe Wang, *wangzhe-hep@mail.tsinghua.edu.cn. Tsinghua University, Beijing, China*

Water-based liquid scintillator or oil-like liquid scintillator is proposed as the detection material of the Jinping Neutrino Experiment, which will have a good sensitivity for neutrino physics, solar physics, geoscience, and supernova relic neutrino researches. We studied the light yield and the time profile of scintillation light emission of linear alkylbenzene (LAB) with 2,5-diphenyloxazole (PPO) as the fluor. We found that without PPO or with a small concentration of PPO, the emission of scintillation light is slow enough, and it allows Cherenkov light to be distinguished using the detected time spectrum with photomultiplier tubes. With the separation of Cherenkov and scintillation light, this slow scintillator inherits both the feature of water Cherenkov detectors and traditional liquid scintillator detectors, and gain a new property for particle identification. In this talk, the measurements of the time profile and light yield of LAB with PPO will be reported and its physics application will also be discussed.

MARM 156

A sterile neutrino search in Japan using 50 tons of liquid scintillator

Joshua Spitz, *spitzj@umich.edu. Physics, University of Michigan, Ann Arbor, Michigan, United States*

A set of possible observations of neutrino oscillations at short distances may be indicative of a new neutrino. The resolution of these anomalies with explanation has been identified by the neutrino community as one of its most important near/mid-term goals. The J-PARC Sterile Neutrino Search at the J-PARC Spallation Neutron Source (JSNS^2) experiment will directly address these anomalies and will also be able to make precision measurements of monoenergetic muon neutrinos from charged kaon decay-at-rest for the first time. The experiment, which will employ 50 tons of liquid scintillator, will also provide much needed research and development relevant for a number of next generation projects. This talk will introduce the JSNS^2 experiment, present its status, and discuss the related current and planned liquid scintillator development.

MARM 157

Water-based liquid scintillator performance

Lindsey J. Bignell[2], *lbignell@bnl.gov, Sunej Hans*[1], *David Jaffe*[2], *Richard Rosero*[3], *Elizabeth Worcester*[2], *Minfang Yeh*[3], *Chao Zhang*[2]. *(1) Chemistry and Chemical Technology, Bronx Community College, Bronx, New York, United States (2) Physics, Brookhaven National Laboratory, Upton, New York, United States (3) Chemistry, Brookhaven National Laboratory, Upton, New York, United States*

Water-based Liquid Scintillator (WbLS) is a novel scintillating material developed at Brookhaven National Laboratory with applications envisaged in particle physics and medical physics. By combining the best qualities of two established particle physics technologies -- water Cherenkov and liquid scintillation -- WbLS will enable development of next-generation detectors with outstanding sensitivity to important problems in particle physics. The near water-equivalence of WbLS also gives it an advantage over other detection media for quantitative real-time dose measurements for radiotherapy. Understanding the basic properties of this material is critical for assessing and optimizing its performance in these application areas. We will present results of the performance of WbLS in small test geometries, and discuss results from a 1 tonne WbLS experiment currently underway at Brookhaven National Laboratory.

MARM 158

ICP MS measurements of low-level radioactivity in solid materials to be used in neutrino experiments

***Maria Laura di Vacri**, divacrim@lngs.infn.it, Stefano Nisi. INFN-LNGS, L'Aquila, Italy*

Experimental searches for rare events, such as neutrinoless double beta decay, require an extremely low radioactive background. Common sources of background include cosmic rays, environmental radioactivity surrounding the detector and radioactive contaminations naturally present in the materials used to build the detector itself. Underground laboratories and suitable shielding around the detector are used in order to suppress the cosmic ray flux and the environmental radioactivity. A strict selection of ultra-pure materials is a fundamental aspect in the design and construction of the experiment. Due to the extremely low radioactive background required by the experiments, very sensitive analytical techniques are used for the measurement of radioactive contamination, such as alpha and gamma spectroscopy, neutron activation analysis (NAA) or inductively coupled plasma mass spectrometry (ICP MS). In this work, mass spectrometric measurements of the long-lived radionuclides Th and U at ultra-trace levels in a solid material is presented. A sample treatment procedure, involving cleaning and chemical separation through chromatographic extraction techniques, has been applied in order to reach excellent detection limits (10^{-13} g/g).

MARM 159

Gadolinium-doped scintillator for reactor neutrino and dark matter search

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Neutrino is leading into a fascinating research. Gadolinium is one of the metals with large neutron cross-section area that makes it an excellent target to capture neutrino. Gd-doped liquid scintillator was selected for Daya Bay antineutrino reactor experiment for precision measurement of mixing angle theta-13. The LZ dark matter experiment is also proposing to use similar Gd-doped liquid scintillator as a veto liquid for its central Xe counter. To dope the Gd metal in scintillator, a Gd-trimethylhexanoic acid complex need to be formed and dissolved in the scintillator. All the reagents are purified to obtain the highest purity and optimum optical properties, as it is one of the requirements for the successful experiments. To detect the resulting photons released from the interaction of incoming neutrino and scintillator in the detector, wavelength shifters are used to match the sensible range of photomultiplier tubes. Quality control of the raw material and synthesized product is important for the success of metal-doped scintillator experiments.

MARM 160

Lithium-doped liquid scintillator for shore baseline antineutrino experiments

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PROSPECT is a Shore Baseline experiment located at HFIR at ORNL focusing on precise measurements of the reactor flux and energy spectrum from nuclear reactor antineutrinos. The main experiment goals are to search for the oscillation signature of sterile neutrinos and to resolve the reactor anomaly by understanding the emission spectrum and flux of antineutrinos from the fission products in a nuclear reactor. Although the theory of sterile neutrinos is getting more acceptance in the scientific community, there still no clear evidence of the existence of sterile neutrinos compelling to new developments in neutrino detectors and liquid scintillators. Lithium-doped liquid scintillator has been optimized for capture of neutron and gamma separation, high light yield performance, and long term stability. The development of metal-doped Liquid Scintillators could further serve as an on-line monitoring tool for nuclear nonproliferation.

MARM 161

Gadolinium-doped water-based liquid scintillator

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The detection of neutrinos that are being bombarded every second to the earth from the universe is one of the biggest challenges that scientists from all over the globe are facing. These neutrinos can be detected by the interaction with detection matter and its signals can be enhanced by different metallic ions which have to be loaded into the detection liquid (i.e. scintillator) that later will be used in the underground detector. However, the loading of inorganic salts into an organic solvent is non-trivial. The purpose of our research is to find the most effective way to load those metals in an environmental friendly and stable organic solution in application for a large scale detector. There are several known methods for the loading of the metals with specific properties for the detection of subatomic particles, nevertheless our goal is to create a new and innovating metal loading water-based liquid scintillator that will help to optimize the detection of neutrinos.

MARM 162

Tellurium-doped liquid scintillator for double beta decay experiments

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Among several known double beta decay isotopes, Tellurium ^{130} has been targeted for a successful loading in liquid scintillator in the search for neutrinoless double beta decay. The high natural abundance and good optical transparency promise tellurium isotope as a potential candidate for the SNO+ experiment in the search of double beta decay. To this end, 0.3% and 3% tellurium loadings are prepared in organic liquid scintillator for such search. However, several parameters need to be considered in order to achieve a successful loading, for example, light transmission and chemical stability of the metal-organic complex.

MARM 163

Engaging students with chemistry and art hands-on activities in a large enrollment course for non-science majors

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Non-science majors are traditionally placed as entering freshmen in a science course that fulfills their science or general education core requirement. The lack of motivation and preparedness can make teaching this type of courses quite challenging, especially when the enrollment is large. Using relevant topics, like the chemistry of art, is one way to engage the interest of students and increase motivation. However, that alone might not be enough. In this paper we will discuss how chemistry and art hands-on activities have been used to enhance the quality of the teaching and greatly improve student participation and engagement. Results from this three-year long study sponsored by an NSF-TUES grant will shed some light on what works and what can be sustained with little or no resources.

MARM 164

Inquiry at the intersection of chemistry and art

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Inspired in part by Chemistry Collaborations, Workshops, and Community of Scholars (cCWCS) workshops, the "Chemistry and Art" course offered at Ithaca College is team-taught by a chemist and an art historian, underscoring the complementary nature of the two disciplines. Populated primarily by non-science majors, our class highlights the importance of using both historical knowledge and empirical measurements to address particular questions about a work of art. The "Chemistry and Art" course at Ithaca College will be discussed, and two very different research projects inspired by intersections in these fields will be summarized. First, a collaborative student research project in which students must select a non-accessioned art object, generate a series of questions about the object, and subsequently use available scientific tools to attempt to address these questions will be discussed. Undergraduates are exposed to a variety of techniques used in the analysis of art objects, including visible and Infrared (IR) spectroscopy, gas chromatography and mass spectrometry (GC/MS), x-ray fluorescence spectroscopy, and microscopy. Second,a recently reported porous polymer designed for the removal of organic micropollutants[1] will be demonstrated using organic dyes as a simulated pollutant. This project was developed as a hands-on teaching tool to illustrate organic synthesis, polymer chemistry, Beer's Law, color chemistry, and intermolecular forces.

[1] Alsbaiee, A.; Smith, B. J.; Xiao, L.; Ling, Y.; Helbling, D. E.; Dichtel, W. R. *Nature*, **2016**, *529*, 190.

MARM 165

Using different computational and experimental spectroscopies to demonstrate phosphate and metal interaction at different pHs

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Phosphate groups are unquestionably one of the most important components of living organisms, such as DNA, RNA, and $NADP^+$. The negative charge of the phosphate interacts with protein (such as histones) and metal (such as K+, Mg2+, and Fe3+) in the biological systems. It is important to stabilize the structure of nucleic acid such as RNA and DNA and also plays important role in protein function and regulation. Given its importance in stabilizing the fundamental units of life, it is important to understand

and monitor how phosphate groups interact with essential metals of the body.
This project was established in order to observe the interactions between the metal and the nucleic acid. Two types of interactions are mainly discussed, pH effect and electron density substitution and how the concentration of the metal affect the change in interaction. Probing these interactions has been proven to be difficult to put in use in nucleic acids. Therefore, simpler system was employed to mimic the interaction of phosphodiester bonds with metals ions. This project focus was to build a model for this interaction by using both computational and experimental Raman and Infrared Spectroscopy. These experimental results combined with theoretical analysis, yield meaningful information about the interaction of phosphates with key metals. In both pH 4 and 8, the shifts in phosphate modes were monitored as the concentration of metal was increased. The results also showed that metal phosphate interactions are stronger for higher charged to smaller size ratio metal such as Mg^{2+}. This result directly correlates between both the computations and the experimental results and the concentration of metal is directly proportional to the peak shifts.

MARM 166

Non-destructive analysis of pigments on cultural heritage objects

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A variety of spectroscopic techniques and imaging methods can be used for the identification of pigments found on works of art. These powerful tools can aid in the dating, authentication, conservation, and restoration of cultural heritage objects. Raman microscopy, X-ray fluorescence spectroscopy, ultraviolet photography, infrared reflectography, and X-radiography are non-destructive techniques that allow for in situ analysis of artworks. This presentation will describe how these methods were used to analyze pigments on a variety of objects including Romanesque wall paintings from a church in the central Pyrenees, medieval and Renaissance Italian manuscript cuttings, works by the so-called “Spanish Forger”, and English portrait miniatures. The London-based artist William Wood produced over 1,200 portrait miniatures over a 15 years period in the late 18th and early 19th centuries. Wood wrote detailed ledger entries for each piece that included not only the name of the sitter, the date completed and the purchase price but also the identity of the pigments he used, often recorded in a numerical code. The goal of an ongoing project at the Victoria and Albert Museum in London is to crack this code through a combination of spectroscopic pigment identification on known Wood miniatures and detailed analysis of the information found in the ledgers. Lastly, the Juniata College Special Collections have some interesting treasures that have been studied using a multi-disciplinary approach, such as an illuminated manuscript copy of the *Bhagavad Gita*, several examples of Pennsylvania fraktur, and a 17th century book from the well-known Abraham H. Cassel collection that was reputed to be bound in human skin.

MARM 167

Characterization of the binding medium used in Roman encaustic paintings on wall and wood

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The characterization by means of Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy and Gas Chromatography-Mass Spectrometry of the binding medium present in eight samples of Roman wall paintings coming from three archaeological sites in Spain and a sample of a Roman-Egyptian mummy portrait on wood showed strong evidence that the medium in all the studied samples was composed of beeswax and soap. These results suggest for the first time that Roman artists used in wall and easel paintings a water soluble encaustic paint of beeswax and soap. Experimental studies with a wax-and-soap technique showed that this painting technique allows reproduction of the physical characteristics of many Roman-Egyptian encaustic mummy portraits with greater accuracy than the hot wax encaustic paint and the alkali-treated encaustic paint often considered to be the painting techniques used in these portraits. Wax-and-soap encaustic also showed greater accuracy in reproducing the physical characteristics of Roman wall paintings than the fresco painting technique, generally thought to be the technique used to execute such paintings. This study suggests that wax-and-soap encaustic could be a common painting technique among Roman artists, and its composition could correspond to a lost ancient encaustic formulation searched for the last five centuries by many artists and researchers dissatisfied with the former reconstructions of the ancient encaustic painting technique.

MARM 168

Synthesis of historical organic pigments: The challenge and opportunity of the nearly forgotten

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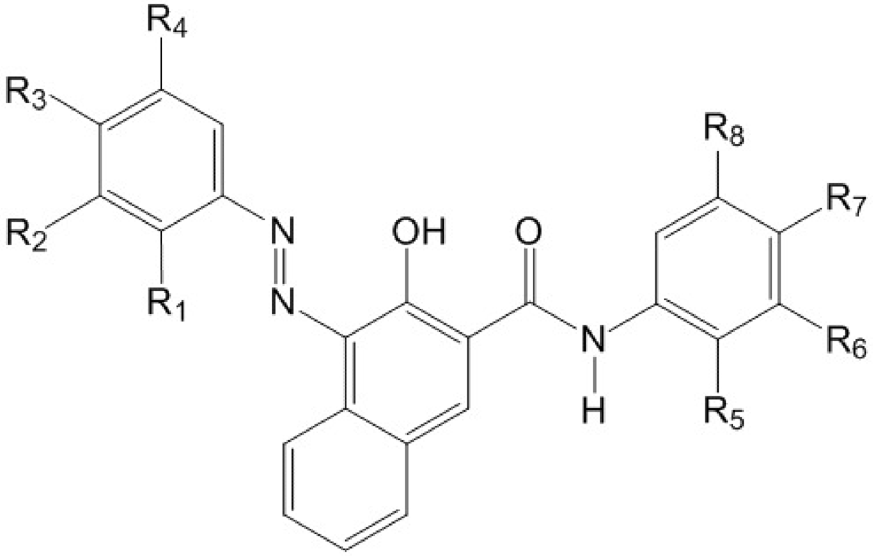
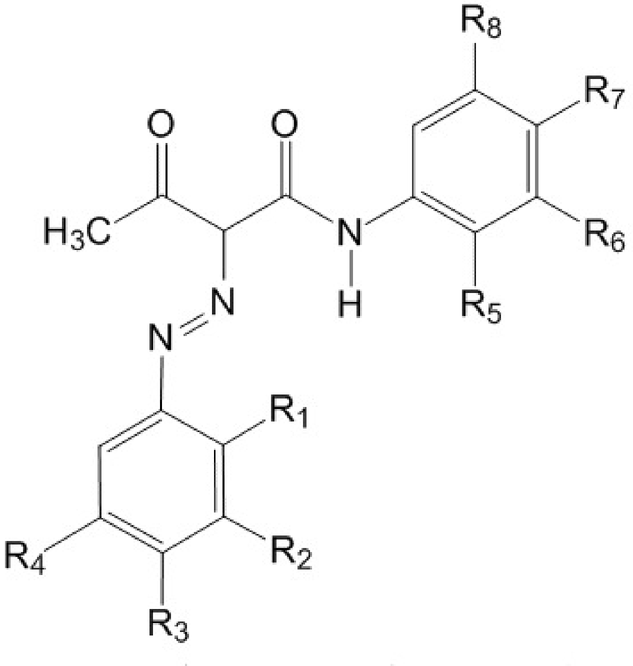
Historical organic pigments are ones that have been synthesized, manufactured and subsequently removed from manufacture. Though manyorganic pigments are still commercially manufactured, certain of these are not available and have no modern analytical data. Thus if they are found, for example in artwork, it would be difficult if not impossible to identify them. Without their identity, the art history of the object would be less comprehensive and deep, and display and conservation decisions would be less informed. With their identity, a specific time range of pigment use can be inferred. We have investigated the literature and have targeted a series of historical Napthol AS (Fig. 1 including PR7, PR10, PR11, PR18, PR19) pigments and Hansa Yellow (Fig. 2 including PY49, PY98, PY203) pigments. Synthesis from commercially available chemicals will be described. Analysis of the product pigments by FT-IR, Raman, mass spectrometry (GC/MS, MALDI) and NMR will be presented as appropriate. The utility of this method to assist in art conservation and provide opportunities in undergraduate research will be highlighted.



PR7: R_1=Me, R_3=Cl, R_5=Me, R_7=Cl and R_2,R_4, R_6,R_8=H
PR10: R_1=Cl, R_4=Cl, R_7=Me and R_2,R_3,R_5,R_6,R_8=H
PR11: R_1=Me, R_4=Cl, R_5=Me, R_8=Cl and R_2,R_3,R_6,R_7=H
PR18: R_1=NO_2, R_3=Me,R_6=NO_2 and R_2,R_4,R_5,R_7,R_8=H
PR19: R_1=OMe, R_3=NO_2, R_5=Me and R_2,R_4,R_6,R_7,R_8=H



PY49: R_1=Me, R_3=Cl, R_5=OMe, R_7=Cl, R_8=OMe, and R_2,R_4,R_6=H
PY98: R_1=NO_2, R_4=Cl, R_5=OMe, R_7=Cl, R_8=OMe and R_2,R_4,R_6=H
PY203: R_1=NO_2, R_4=Me, R_5=OMe and R_2,R_3,R_6,R_7,R_8=H

MARM 169

Pigments in antiquity: A window on a long-lost world

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Our ancient forebears certainly made use of colors to color virtually everything they used or had: bodies, caves, pottery, sculpture, stone structures, clothing and other textiles. This paper will document their evolution with an emphasis on mineral pigments and how a gradually increasing understanding of the nature of these colorants eventually led to other surprising advances in civilization.

MARM 170

Configuration interaction energy between lowest pair of excited states in the circular ring model of porphyrin: Experimentally determined in metmyoglobin

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J. R. Platt, H. C. Longuet-Higgins and M. Gouterman explained many basic features of light absorption by porphyrin-related molecules by means of an appoximate electronic structural model with 18 electrons delocalized in a π-bonded circular ring of four p_z orbitals. The top level of the ground state has $m_{az}=\pm4$ and excited states $m_{az}=\pm5$, $m_z=\pm6$, etc. The ±5 and ±6 configurations interact to produce levels which give rise to π-π transitions in the Soret ("B") and visible ("Q"). The configuration interaction energy is given by $(E_B-E_Q)/2$. In the absence of perfect circular symmetry the B and Q transitions are split into x and y transitions. Center energies are obtained from band analysis of absorption spectra. Identification of the B and Q among them is enabled by $E_{Bx}-E_{Qx} \approx E_{By}-E_{Qy} \approx 6.7$kK and $E_{Bx}+E_{Qx} \approx E_{By}+E_{Qy}$. Also, the configuration interaction energy should be essentially independent of temperature. For the aquo, fluoride, azide and cyanide complexes of horse metmyoglobin at 25.0°C the configuration energy is in the range 3.2 to 3.4kK. The configuration energy for the aquo complex is 3.29kK at both 9.7° and 25.0°C.

MARM 171

A revolutionary idea in context of x-ray quantum crystallography (QCr) and the kernel energy method (KEM)

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Here is a revolutionary suggestion, at once obvious and also of overwhelming importance. The Kernel Energy Method (KEM) we suggest, if applied to Quantum Crystallography (QCr), implies a new field of study. The possibility of such study is much to be desired, because for truly huge molecular systems it would allow the illumination of important biological problems by using the power of true abinitio quantum mechanical explanation.

Crystallographic data is the basis for calculation of the complete Quantum Mechanics (QM) of crystallized biological molecules of any size. “Any size” envisions molecules of up to many hundreds of thousands of atoms in a biological complex. And, KEM has made this doable with any chemical model of any chosen accuracy. That is the revolution within crystallography to which reference is made. What we must recognize now is that KEM is capable of providing the entire quantum mechanics of crystallographic biological molecular systems because, given the X-ray structure the KEM formula delivers the energy E, and density matrices ρ_2, ρ_1, and the electron density ρ. The KEM formula approximations to E, ρ_2, ρ_1, ρ, *and the X-ray structure factors* F(K) are expressed in equations below. On the right side of all the equations the first sums are over double kernel quantities and the second sums are over single kernel quantities. The energy and the 3 density matrices, of proven accuracy, are sufficient for the complete ground state quantum mechanics of any molecular system, including the X-ray structure factors. The complete quantum algorithm here suggested, is as follows: Recognize that the KEM formula delivers E , ρ_2, ρ_1, ρ *and* F(K); Given any crystal structure cut it into kernels; Calculate the kernels in the chemical model most appropriate to the accuracy needed; Calculate the full molecule energy E and the density matrices ρ_2, ρ_1, and ρ using the KEM formulas; From the density matrices calculate any Quantum Mechanical property of interest for the whole molecule, including*the –X-ray structure factors* F(K). Note Well: No one has suggested extraction of the complete QM from crystallography as have we here.

$$E_n^{total} = \sum_{1\le i<j\le n} E_{ij} - (n-2)\sum_{1\le i\le n} E_i \tag{1}$$

$$\rho_2 = \sum_{1\le i<j\le n}^{n} \rho_{2_{ij}} - (n-2)\sum_{i=1}^{n} \rho_{2_i} \tag{2}$$

$$\rho_1 = \sum_{1\le i<j\le n}^{n} \rho_{1_{ij}} - (n-2)\sum_{i=1}^{n} \rho_{1_i} \tag{3}$$

$$\rho = \sum_{1\le i<j\le n}^{n} \rho_{ij} - (n-2)\sum_{i=1}^{n} \rho_{i} \tag{4}$$

$$F(K) = \int e^{iK.r}\{ \sum_{1\le i<j\le n}^{n} \rho_{ij} - (n-2)\sum_{i=1}^{n} \rho_{i} \}\, d^3r \tag{5}$$

MARM 172

Mechanisms of the lignin monomers pyrolysis: Cinnamyl alcohol

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Lignin is one of the major biomass components. Its pyrolysis is an alternative way to obtain liquid fuels, hydrogen and chemicals. The elementary reaction mechanisms mainly remain unknown due to the complex structure of the lignin, which is a cross-linked amorphous copolymer, synthesized from random polymerization of three primary phenylpropane monomers: coumaryl, coniferyl, and sinapyl alcohols. Cinnamyl alcohol ($C_6H_5CH{=}CHCH_2OH$, CnA), in turn, is the simplest backbone model of these key monomers. Thus, the exploration of the decomposition pathways of CnA can shed a light on the reactivity

and pyrolysis mechanisms of lignin.

The low temperature matrix isolation-EPR experiments revealed formation of the intermediate radical mixtures described by high g-values dependent on pyrolysis temperature. The formation of major products is also varied by temperature.

In this report, we present a mechanistic analysis of the CnA pyrolysis based on the DFT- evaluated bond dissociation patterns and unimolecular decomposition pathways involving dehydrogenation, dehydration, 1,3-sigmatropic H-migration, 1,2-hydrogen shift, C-O and C-C bond cleavage and other intermediary processes.

Unimolecular decomposition channels (Fig.1) are shown to be operative only at high temperatures, whereas accompanied radical processes can occur at much lower energy costs. Comparison of the experimental data with theoretically evaluated isotropic g-values for model radicals and the model reaction energetics suggested the dominant formation of the intermediate oxygen-linked conjugated radicals, thus providing evidence on the fundamental role of radicals in the thermal degradation of lignin.

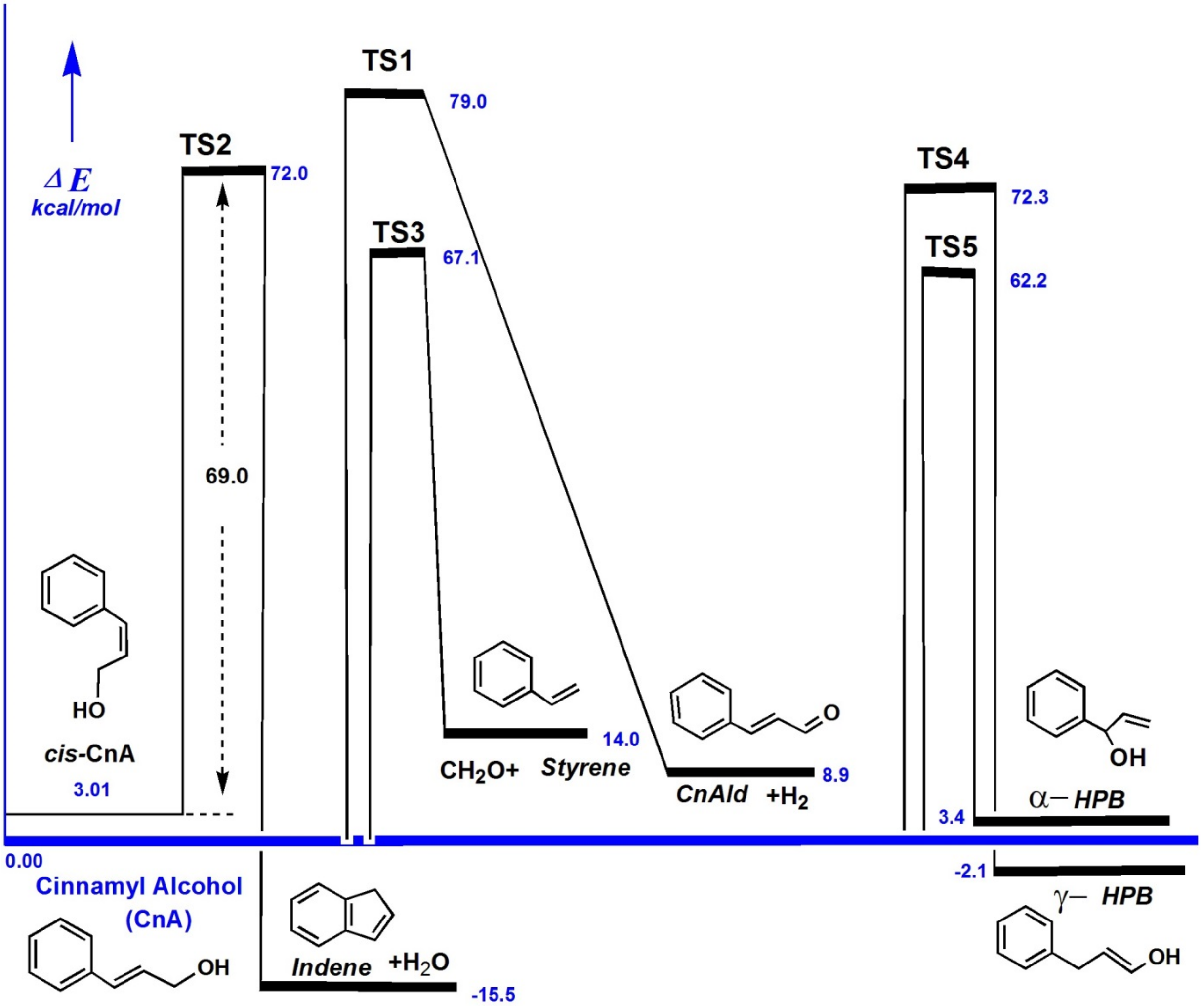

Fig.1. Calculated at B3PW91/6-31+G(2d,p) level unimolecular decomposition pathways for CnA.

MARM 173

Multiconfigurational quantum chemistry on graphical processing units

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There is a surprising lack of electronic structure methods that are both accurate and efficient in treating electronic excited states. Accurate methods for excited states, such as multireference perturbation theory, multireference configuration interaction, or equation-of-motion coupled-cluster, are far too computationally demanding to be generally applicable. More approximate methods, such as configuration interaction singles or time-dependent density functional theory, are scalable to larger systems, but suffer from a variety of errors that severely limit their applicability. As a result, methods that belong to the complete active space configuration interaction (CASCI) family are widely used in theoretical studies of photochemical processes. Despite their popularity in this context, modern algorithms for performing CASCI computations have lagged far behind those for single reference methods, such as Hartree-Fock or Kohn-Sham density functional theory. Recently, we have developed new algorithms for performing CASCI computations that exploit sparsity in the atomic orbital basis that allows these methods to be applied to systems with more than 1000 atoms. The new algorithms have been extended to include the evaluation of the gradient and nonadiabatic coupling vectors for CASCI-type methods. Our new algorithms have been implemented to exploit the parallelism intrinsic to graphical processing units. The combination of our new algorithms and modern computer hardware makes excited-state molecular dynamics simulations and conical intersection optimization routinely possible for molecular systems with roughly 500 atoms.

MARM 174

Chitin-based sorbents for mining metals from oceans: A sustainable alternative to terrestrial mining

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The increased pressure from society for more sustainable practices is leading to the promotion of less material- and energy-intensive activities, together with the diminishing or even elimination of waste generated during the processes. In particular, it has been proposed that mining the oceans has lower environmental impacts than terrestrial mining and represents an alternative to reduce the generation of waste during the extraction processes. Among the possible materials that can be used for ocean mining, chitin-based sorbents have been developed by our group as biodegradable extractants for harvesting metals from seawater. Native chitin (poly(N-acetylglucosamine)) can be extracted from biomass by dissolution in ionic liquids (IL) such as 1-ethyl-3-methylimidazolium acetate and shaped into usable materials such as fibers or nanomats. The final sorbents are insoluble in most other solvents and can be exposed to solutions of reactive chemicals to selectively functionalize only the exposed surfaces. The surface-specific functionalization of chitin results in a measurable change in metal affinity without compromising bulk physical properties such as strength. Additionally, the nucleophilic amine in chitin can be easily tied to almost any functional group with almost any linker, giving chitin-based materials potential for fine tuning. Here we present the preparation and characterization of these materials, together with examples of their affinity for specific metal ions.

MARM 175

Global freshwater systems at risk: Challenges and remediation

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Global freshwater systems are increasingly strained by demands of expanding populations and forces of climate change. The average temperature of the earth's atmosphere has risen by more than 0.74 C in the past 100 years primarily due to a rapid upsurge of CO_2. The resulting consequences, presented herein, have dire impact on production of food and clean energy. A warmer atmosphere holds more water vapor, releases more energy during precipitation, intensifies floods and storms which bring environmental and economic devastation, and reduces the amount of freshwater that can be harvested. Warmer oceans are less dense, contributing to sea level rise, to salinization of river basin deltas and coastal aquifers, and the destruction of natural wetlands ecology. Melting of mountain glaciers threatens agriculture dependent on seasonal crop growth. Melting of ice caps around the poles decreases the total reflectivity of snow and ice to irradiate incoming solar radiation back to space. As more sunlight strikes the surface of lakes, temperatures rise, evaporation is enhanced, waters become more stratified, and lake ecosystems are disrupted. Prolonged droughts caused by rising temperatures cause crop failures (US southwest) and, when severe, lead to malnutrition and disease (central Africa). By 2030, 47% of the world's population will be living in areas of high water stress, which will promote aquifer pumping to further deplete groundwater tables. While increasing the supply of freshwater via technologies such as wastewater recycling and desalination are vital, more economically viable conservation methods can mitigate risks to freshwater systems. This talk addresses the latter. Key among them is drip irrigation, a drop-to-crop irrigation system that minimizes waste and evaporation and avoids spreading fertilizers over an entire farm. A conservation measure to replenish groundwater is stormwater catchment. Hydropower is a clean energy source from river waters especially applicable in the developing world where burning biomass for fuel is still common. However, massive dam constructions have created disruptions of migratory species that serve as food supply for local populations. Dams across smaller tributaries may avoid major upheavals. Finally, proper river management requires strict adherence to established protocols.

MARM 176

Tailoring the surface of solid wastes for their application as adsorbents of antibiotics

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The prevalence of antibiotics has become a major concern in environmental remediation. Their negative impacts reside on the development of bacterial resistance. Bioremediation has emerged as a tentative solution for this problem by the use of biological wastes and mechanisms that remove pollutants from aqueous systems. Our research group has studied the elimination of heavy metals and dyes by using raw solid wastes and marine algae as biosorbents. From this prior data, carboxyl and amino groups report a higher affinity towards these pollutants. Therefore, this study was driven by the hypothesis: enrichment of adsorbent's surface with active centers will increase the adsorption properties of these biomaterials. Carboxylated (C), sulfonated (S) and thiolated (T) spent tea leaves of chamomile (CM), green tea (GT) and peppermint (PM) were prepared in aqueous phase. Instrumental analysis indicates that chemical modification occurred. Moreover, addition of these groups slightly changed the morphological and thermal properties of these materials. Batch adsorption tests were conducted at room temperature. Results

are shown in Fig.1, displaying that adsorption of Penicillin G is pH-dependent and that adsorption percentage increases by 61% when compared to the raw adsorbent. pH played an important role on the adsorption, observing a maximum antibiotic uptake at pH 4. Adsorption percentages followed the trend: TPM≥SPM>CPM>>PM. More tests are being conducted to obtain all equilibrium parameters to optimize the removal of Penicillin G.

Acknowledgements: Innovate Peru and Grant 169-PNICP-ECIP-2015 by FINCyT/CONCYTEC (Perú)

MARM 177

Environmental remediation with polymer-supported reagents: Application to the complexing of uranium from acid mine drainage and wet process phosphoric acid

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The immobilization of ion-selective ligands onto polymer beads and fibers yields polymer-supported reagents that can be applied to environmental remediation. Uranium is important to the nuclear fuel cycle and is the subject of terrestrrial mining as well as seawater recovery. However, it is also present as a contaminant in various industrial processes and its recovery would be an example of valorization: turning waste into a resource. The application of polymers to the removal of uranium from acid mine drainage and wet process phosphoric acid will be detailed. Aminomethylphosphonate has been identified as a critical ligand to its recovery.

MARM 178

A simple extraction method for detecting the fecal indicative bacteria in urban soil

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Anthropogenic activities cause an increase of organic materials and nutrients and this poses a serious threat in urban environments. The densities of fecal indicator bacteria (FIBs) in the urban area exhibit a clear land-use dependency in the natural water and are often linked with nutrient inputs. This research was conducted to investigate the relationship of microbes found in water and soil. The study has been carried out on occurrence of Fecal Indicative Bacteria in two parks of Queens county: Flushing Meadow Park and Kissena Park with intense and less recreational activities respectively. EPA approved IDEXX method was used to detect the Fecal Indicative Bacteria (FIBs) including total coliforms, E. coli and enterococcus in water. We hypothesized that there would be more microbes found in water after raining due to movement of microbes from soil to water as runoff. A simple extraction procedure was optimized to mobilize the indigenous fecal indicative bacteria in the soil and to detect them reliably using EPA approved IDEXX method. This new approach provided the opportunity to identify the sources for FIBs in adjacent water bodies. FIBs concentration in soil is critical to understand the microbial variation in lakes and ponds both spatially and temporally. l Variation in FIBs occurrence were investigated by capturing different weather conditions, activity level, soil type and water content of soil. Data from preliminary investigation indicated elevated FIBs in soil and water of a NYC lake with intense recreational activities. Very few studies on mobilization of FIBs in natural water from surrounding soils were reported in NYC area. In an attempt to study temporal and spatial bio-geochemical dynamics of both fresh and brackish water lake environments, the study was done in two NYC lakes that vary in terms of recreational activities and different environmental settings. This study focused on environmental research to improve understanding of FIBs transport processes in the environmental system which is a critical aspect of decision-making in risk assessment, and remediation strategies. Preliminary results were found to exceed the EPA permissible limit for total Coliform, E. coli and Enterococci respectively.

MARM 179

Black sand as mineral-based photocatalyst for hydrogen production under UV-Vis irradiation

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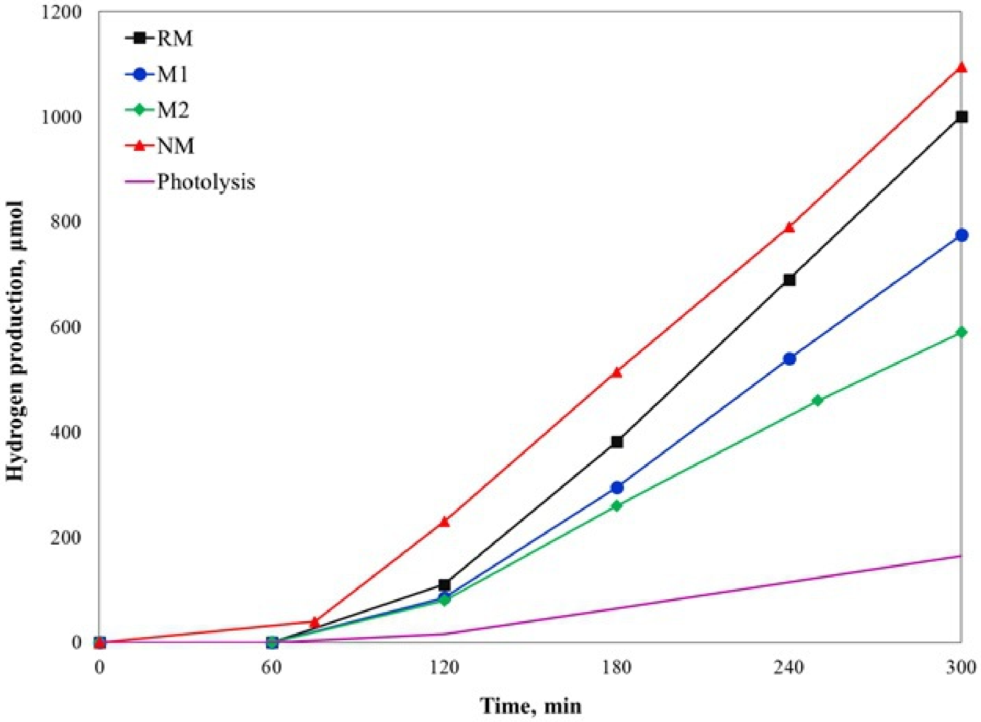
Currently the low applicability of photocatalytic hydrogen generation it's due to that the efficiencies obtained in these processes are still not satisfactory. This has motivated the development of techniques which involve the electrochemical cell configuration (photoanode) and development of suspended semiconductor with narrow band gap which can use more than 4% of the solar spectrum. In present study, black sand as raw material and its fractions magnetically separated (Mag. 1, Mag. 2, Non mag.) corresponding to 0.016 and 0.3 T, respectively, were tested through a number of batch experiments under same conditions. The fractions were identified chemical and physically by SEM, FTIR, UV-Vis, XRF and TGA techniques. Mineral-based photocatalyst has been found to be effective for hydrogen production using EDTA solution as sacrificial agent. Results reveal that the reactivity of the system for photocatalytic hydrogen production was different for all fractions after 5.0 hours of treatment. Raw material and Mag. 1 fraction showed similar behavior, while non magnetic fraction was highest. The mineral was found to greatly enhance the photocatalytic activity toward hydrogen production from aqueous EDTA solution.



Time course of photocatalytic H_2 evolution from black sand photocatalysts: (a) Raw material (b) M1 (c) M2 (d) NM (e) Photolysis

MARM 180

Dissecting electrostatic contributions to folding and self-assembly using designed multicomponent peptide systems

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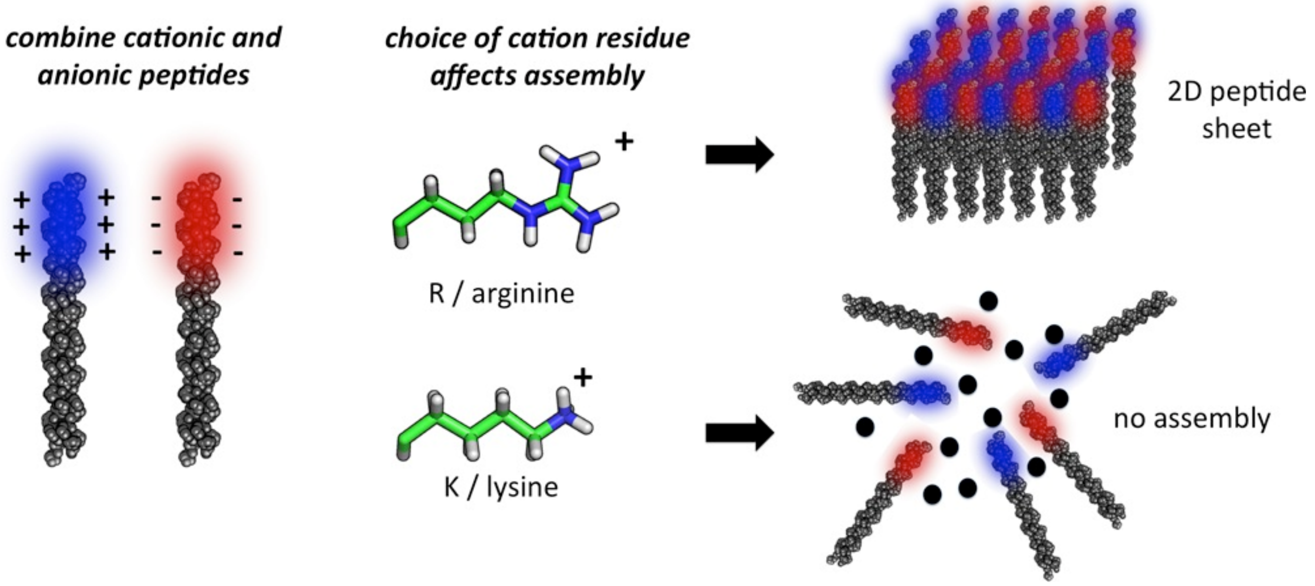
We investigate formation of micron-scale peptide fibers and sheets where assembly requires association of two distinct collagen mimetic peptides (CMPs). The multicomponent nature of these designs allows us to decouple amino acid contributions to peptide folding versus higher-order assembly. While both arginine and lysine containing CMP sequences can favor triple-helix folding, only arginine promotes rapid supramolecular assembly in each of the three two-component systems examined. Unlike lysine, the polyvalent guanidyl group of arginine is capable of both intra and intermolecular contacts, promoting assembly. A model is developed for describing the supramolecular diversity of CMP morphologies observed throughout the literature. It also connects CMP self-assembly with a broad range of biomolecular interaction phenomena, providing general principles for modeling and design.



MARM 181

Supramolecular block copolymers

***Marcus Weck**, marcus.weck@nyu.edu, Elizabeth Elacqua, Anna Croom, Kylie Manning. Chemistry, New York University, New York, New York, United States*

Owing to the mastery exhibited by Nature in integrating both covalent and noncovalent interactions in a highly efficient manner, the quest to construct polymeric systems that rival not only the precision and fidelity, but also the structure of natural systems has remained a daunting challenge. The ability to reliably control polymer self-assembly is essential to generate ‘smart’ materials and has the potential to tailor polymer properties through fine-tuning the noncovalent interactions that comprise the polymer architecture. The presentation will describe engineering principles being developed and pursued by our group that exploit the orthogonal nature of noncovalent interactions, such as hydrogen bonding, metal coordination, and Coulombic interactions, to direct the self-assembly of functionalized macromolecules, resulting in the formation of supramolecular block copolymers. In particular, we will describe the synthesis of heterotelechelic polymers that self-assemble into complex ABC supramolecular triblock polymers and have the potential to fold into 3D architectures.

MARM 182

Nanoscale building blocks in solid-state chemistry

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The overall goal of our research is the development of novel solid state materials through the controlled assembly of functional nanoscale building blocks. The emergence of collective properties in a family of metal chalcogenide molecular clusters, which we call "superatoms", allows us create novel materials in which the building blocks are not only tunable but also uniquely defined at the atomic level. In this work, we describe a new class of superatomic solids formed from the binary assembly of independently prepared, electronically and structurally complementary superatoms. Our results demonstrate that the constituent clusters are able to exchange charge and interact electronically to produce long-range cooperative properties that are distinct from those of the independent subunits, akin to atoms in traditional solid state compounds. For example, electrical conductivity and bulk ferromagnetism are present in many binary superatomic crystals, including [Co6Te8(PEt3)6][C60]2 and [Ni6Te6(PEt3)8][C60], but absent in the constituent clusters. These materials are defined at the atomic scale and we use this atomic precision to dictate the superstructure of the solids, to control the interactions between the building blocks, and to manipulate the resulting physical properties. I will discuss the assembly, characterization and uses of superatomic solids with two-dimensional structures, as well as our efforts in making a new family of thermoelectric materials from molecular cluster building blocks.

MARM 183

Pattern formation of confined periodically sequenced polypeptides

***Raymond S. Tu**, tu@ccny.cuny.edu. Steinman Hall, Chemical Engineering, The City College of New York, New York, New York, United States*

Periodically sequenced peptides can be confined to interfaces and assembled into patterns that present chemical functionalities with exceptional spatial precision. These rationally designed peptides and polypeptides are rapidly becoming useful components in nanostructured materials for applications ranging from drug delivery to energy storage. This presentation will examine several fundamental aspects of self-assembly and pattern formation of well-defined sheet forming peptides confined at interfaces. Our

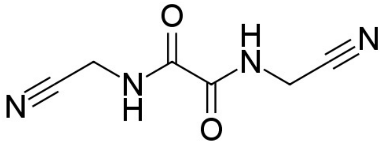
approach involves three steps. (1) We design and synthesize simple periodic peptide sequences, yielding surface-active β-strands that self-organize into aggregates to form patterns as a function of the peptide sequence. Rational peptide design allows us to systematically explore the role of hydrophobicity, electrostatics and molecular size on materials properties. (2) We use a set of interfacial characterization tools to examine in intermolecular assembly and supramolecular mechanics of the self-assembled structures. (3) We apply two-dimensional equations of state that define both the phase behavior and the critical surface concentrations of nascent aggregates at the interface. Subsequently, we can apply these parameters to predict the dimensions of pattern formation and to determine the potential of the peptide assemblies as biomimetic materials.

MARM 184

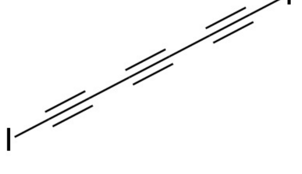
Synthesis and characterization of poly(iodoethynyliododiacetylene) (PIEDA)

Matthew Freitag[2], *Renantiomer@gmail.com, Racquel DeCicco*[2]*, Gary P. Halada*[2]*, Christopher Young*[3]*, Nancy S. Goroff*[1]*. (1) SUNY Stony Brook, Stony Brook, New York, United States (2) Stony Brook University, Massapequa Park, New York, United States (3) Stony Brook University, Stony Brook, New York, United States*

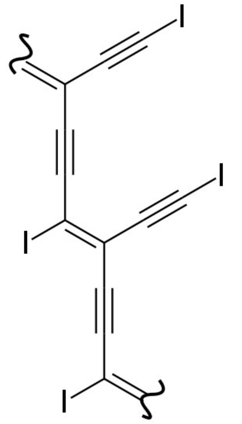
We report here the preparation and characterization of co-crystals of the monomer diiodohexatriyne with a bis(alkyl nitrile) oxalamide host, in which halogen bonding between host and guest aligns the monomers for 1,4-topochemical polymerization. Mild heating (40 C/ 2 weeks) is then used to induce ordered polymerization, leading to a deep change in color from blue-green to purple and then deep brown. Raman spectroscopy and solid-state ^{13}C MAS-NMR demonstrate the formation of a single highly ordered polydiacetylene, poly(iodoethynyliododiacetylene) (PIEDA). This work represents the first successful ordered 1,4-polymerization of a triyne using the host-guest method.



bis(heptanenitrile) oxalamide
Host



diiodohexatriyne
Guest



PIEDA

MARM 185

Green chemistry outreach: Spreading science education to the national level

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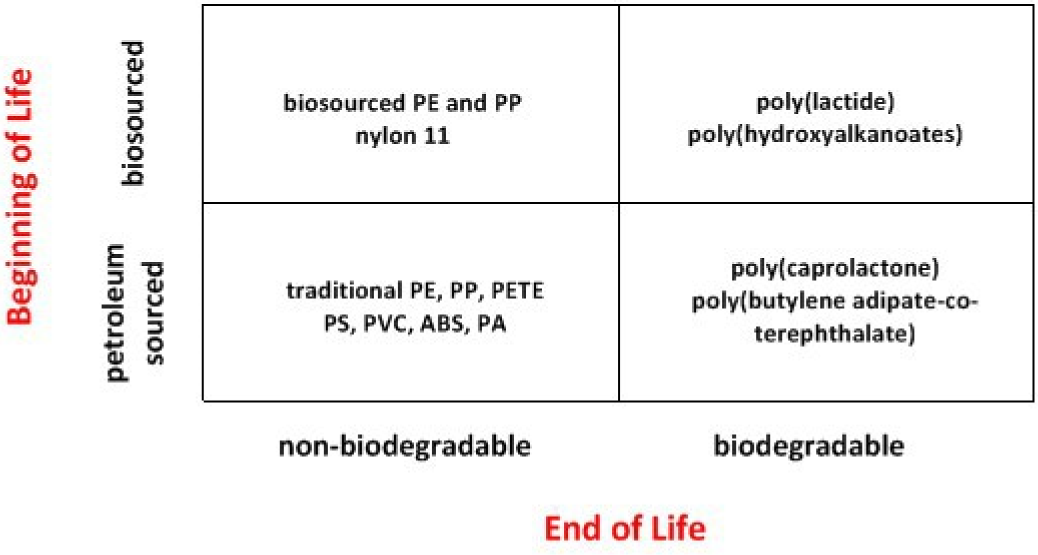
The ACS has longsponsored NCW / CCED activities. We worked with the ACS Green Chemistry Institute to offer a similar type of program. The participants work on requirements similar to the NCW / CCED fun patch requirements to earn fun patches related to Green Chemistry, Green Engineering, and Sustainability. Our program in the Lehigh Valley LS is a template for what other local sections and student groups can do for teaching sustainabiility concepts. We held activities at Davinci Science Center.

MARM 186

An overview of biosourced and biodegradable polymeric materials: Current commercial uses and challenges for more widespread adoption

Katherine Aubrecht, *kaubrecht@notes.cc.sunysb.edu. SUNY Stony Brook, Stony Brook, New York, United States*

The sustainability of a polymeric material is largely determined by its feedstock (petroleum or biosourced) and what is done with it at the end of its use (landfill, mechanical recycling, chemical recycling, incineration, biodegradation). Polymeric materials can be classified into one of four categories: (1) biosourced and biodegradable (ex. polylactide and polyhydroxyalkanoates), (2) biosourced and non-biodegradable (ex. biosourced polyethylene), (3) petroleum sourced and biodegradable (ex. polycaprolactone), and (4) petroleum sourced and non-biodegradable (traditional polyethylene and polypropylene, polystyrene).This presentation will give an overview of: commercialized biosourced and/or biodegradable polymers, current research foci and research needs, drivers and challenges for the more widespread use of biodegradable and/or biosourced polymers, and considerations and metrics for evaluating the sustainability of a material.



		non-biodegradable	biodegradable
Beginning of Life	biosourced	biosourced PE and PP nylon 11	poly(lactide) poly(hydroxyalkanoates)
	petroleum sourced	traditional PE, PP, PETE PS, PVC, ABS, PA	poly(caprolactone) poly(butylene adipate-co-terephthalate)

MARM 187

Novel liquid-like nanoparticle organic hybrid materials with tunable chemical and structural properties for combined CO_2 capture and conversion

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Fossil fuels, which contribute significantly to anthropogenic CO_2 emissions, are likely to remain the main source of energy in the foreseeable future. Therefore, the development of efficient carbon capture and storage (CCS) technologies is one of the great challenges faced by humanity. A new advancement in the area of CCS includes the utilization of captured CO_2 as a chemical feedstock, resulting in new approaches to carbon capture, utilization and storage (CCUS). While a wide range of materials ranging from aqueous amine solvents to solid sorbents, a reactive system that can effectively host both CO_2 capture and conversion do not exist. Thus, a new class of nano-scale materials called Nanoparticle Organic Hybrid Materials (NOHMs) has been developed as an alternative CO_2 capture media. NOHMs consist of inorganic cores with a grafted polymeric canopy providing negligible vapor pressure, great thermal stability, and interesting chemical and physical tunability. Both entropic and enthalpic interactions among polar fluid units, solid surfaces and gaseous molecules are investigated, while correlating the molecular level understanding macroscale properties such as the sorption and diffusion behaviors and reactivity of CO_2 molecules in NOHMs. During this study, it has been found that NOHMs not only have interesting CO_2 capture properties but can also serve as an electrolyte for subsequent reduction of CO_2. Thus, NOHMs' electrolytic properties in the presence of various secondary fluids and salts are evaluated to design them as a dual-purpose reactive media for combined CO_2 capture and conversion. This CCUS scheme would capture and convert CO_2 in an integrated pathway, and therefore, has a great potential to minimize the parasitic energy consumption.

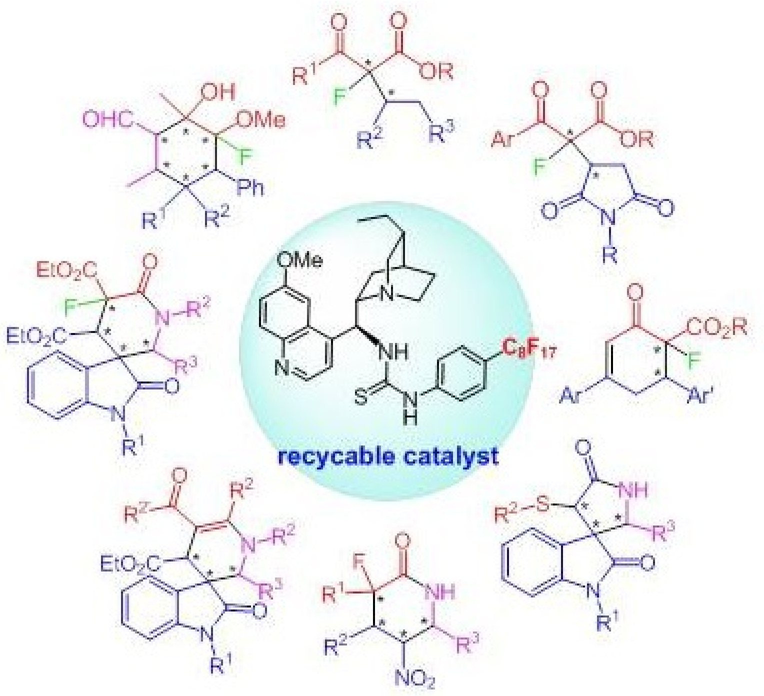
MARM 188

Sustainable organocatalysis for one-pot asymmetric synthesis

***Wei Zhang**, wei2.zhang@umb.edu. University of MA Boston, Dorchester, Massachusetts, United States*

Toxic heavy metal-free organocatalysis is a powerful tool for asymmetric synthesis and a topic of current interrest. Organocatalysis requires high catalyst loading (up to 20 mol%) and the separation of organocatalysts is not an easy task. The development of recycable fluorous organocatalysis provides an efficient way to address seaeration issue. In addition to phase tag separation, the stereoelectronic effect of the fluorous chain can be used to modify the reactivity and selectivity of the catalysts. This presentation highlights our recent effort on the development of recyclable organocatalyst-promoted fluorination, Michael addition, Robinson annulation, and one-pot addition/cyclization for asymmetric synthesis of biologically interested molecules.

- Huang, X.; Pham, K.; Yi, W.; Zhang, X.; Clamens C.; Hyatt, J. P.; Jasinsk, J. P.; Tayvah, U.; Zhang, W. *Adv. Synth. Catal.* **2015**, *357*, 3820.
- Huang, X.; Pham, K.; Zhang, X.; Yi, W.-B.; Hyatt, J. P.; Tran, A. P.; Jasinski, J. P.; Zhang, W. *RSC Advances* **2015**, *5*, 71071.



One-pot synthesis of molecules with multiple chiral centers

MARM 189

A mild Cu-catalyzed oxidative aromatization of indolines to indoles

***Feng Peng**, feng.peng@merck.com. Process Chemistry, Merck, Rahway, New Jersey, United States*

A novel method for the oxidation of indolines using a benign organic oxidant and Cu catalyst will be discussed. The method was successfully applied to Elbasvir (a novel hepatitis C therapy) synthesis reducing PMI 73%.

MARM 190

Design and development of a greener manufacturing route for NNRTI doravirine

***Yang Cao**, yang.cao@merck.com, Donald R. Gauthier, Benjamin Sherry. Process Chemistry, Merck, Rahway, New Jersey, United States*

Abstract: Non-nucleoside reverse-transcriptase inhibitors (NNRTIs) are important components of Highly Active Anti-Retroviral Therapies (HAART), which are the standard of care for the treatment of human immunodeficiency virus (HIV) infection. Doravirine is being developed at Merck as a next-generation NNRTI for the treatment of HIV. The presentation will focus on the development of a highly efficient chemical synthesis of Doravirine suitable for commercial supply. The newly designed route features *de novo* construction of the highly functionalized pyridone core under continuous-flow conditions and direct installation of the *N*-methyltriazolinone heterocycle. Ultimately the target structure was prepared via the

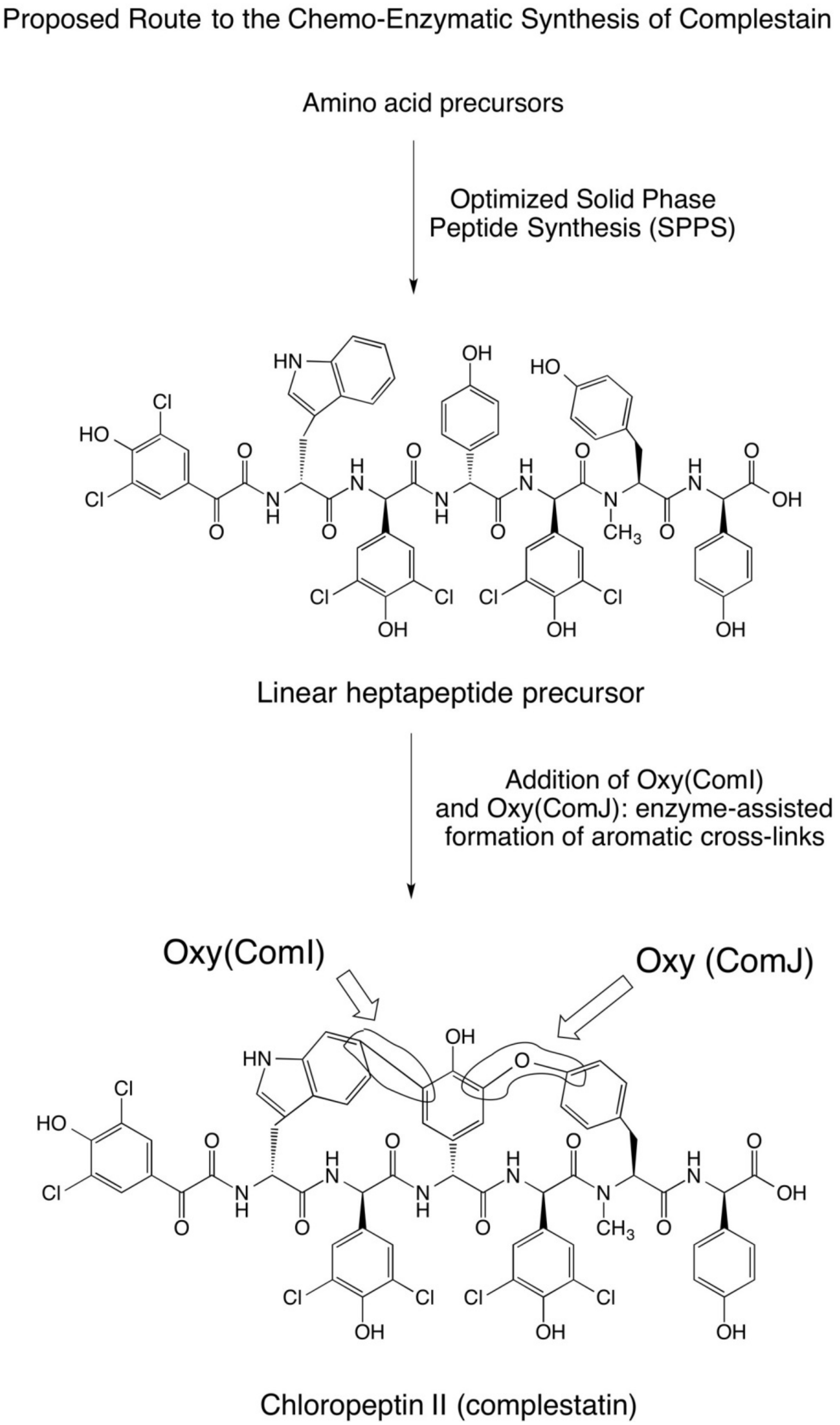
chlorination/alkylation through-process with excellent control of chemical purity, and the goals of cost reduction, process efficiency, and lower environmental burden had been demonstrated

MARM 191

Towards a chemo-enzymatic synthesis of the heptapeptide antibiotic complestatin: Investigating the role of the P450 oxygenases ComI and ComJ in aryl linkage formation

Aurelio Mollo, *amollo@haverford.edu. Chemistry, Haverford College, Haverford, Pennsylvania, United States*

Complestatin is a heptapeptide antibiotic discovered in the early 1980's. Although the total synthesis of the molecule has been achieved, two critical cross-links between its aromatic side chains are such that current synthetic methods require numerous steps and rely heavily on transition-metal-based catalysis. This inevitably leads to both low overall yields and an environmentally unsustainable approach, effectively prohibiting large-scale synthesis of the molecule. To overcome this limitation, we are developing a chemo-enzymatic synthetic strategy: we will first synthesize the linear heptapeptide precursor using solid phase peptide synthesis (SPPS) and then enzymatically cross-link the aromatic side-chains using the P450 oxygenase enzymes ComI and ComJ. The presence of base-labile 4-hydroxyphenylglycine residues required us to develop an SPPS protocol void of harsh reaction conditions. Here we present our synthetic route to relevant peptide substrates for cyclization studies and our approach to evaluating the ability of the P450 oxygenases to install the two critical aromatic cross-links for the complete chemo-enzymatic synthesis of complestatin.



Proposed Route to the Chemo-Enzymatic Synthesis of Complestain

MARM 192

3Rs in green chemistry: Resources, recycling, and responsibility

***Ann E. Shinnar**, ann.shinnar@touro.edu. Chemistry, Lander College for Men/Touro College, Kew Gardens Hills, New York, United States*

In order to familiarize students with principles of green chemistry, we have introduced an annual lecture and laboratory session into our general chemistry curriculum. Our lecture is scheduled in the spring semester close to Earth Day and focuses on 3Rs: resources, recycling and responsibility. Key topics focus on materials widely used in our daily lives: aluminum, glass, plastic polymers, and batteries. Lecture content also reviews classic chemical principles such as redox chemistry in Hall-Heroult process for manufacturing aluminum. Coverage of polymers includes an overview of step-growth versus chain-growth polymers, plastic recycling symbols 1-7, and their identification via signature IR spectra. Following lecture, students enter the lab where they categorize household items including a variety of plastic food containers, reusable plastic bags, metal cans, and batteries. We also test testing packing peanuts of Styrofoam versus starch by contrasting their solubility with acetone versus water. The combined lecture and laboratory sessions provide an opportunity to incorporate green chemistry themes into our college curriculum. Students show overall enthusiasm for our 3Rs integrated experience.

MARM 193

Synthesis and characterization of polyampholyte ionomer networks

***Kevin A. Cavicchi**, kac58@uakron.edu, Guodong Deng. Polymer Engineering, University of Akron, Akron, Ohio, United States*

In polymer materials, dynamic bonding is a useful approach to generate structurally dynamic polymer architectures leading to stimuli-responsive materials, such as self-healing and shape memory polymers, and/or polymers with enhanced mechanical properties through energy dissipative bond re-arrangement. This talk will present the synthesis and characterization polyampholyte ionomer networks through the free radical copolymerization of an alkyl acrylate and an ion-pair comonomer. Ion pair comonomers were synthesized the through metathesis ion-exchange of an anionic (e.g. sodium styrene sulfonate) and a cationic monomer (e.g. vinyl benzyl tri-*n*-octylammonium chloride). It will be shown that these ion-pairs where both anion and cation are bound to the polymer chain are able to act as dynamic crosslinks giving rise to complex viscoelastic behavior that is tunable through the choice of ion-pair and the overall polymer formulation. These results will also be compared to other classes of dynamically bonded polymers, such as hydrogen bonded systems.

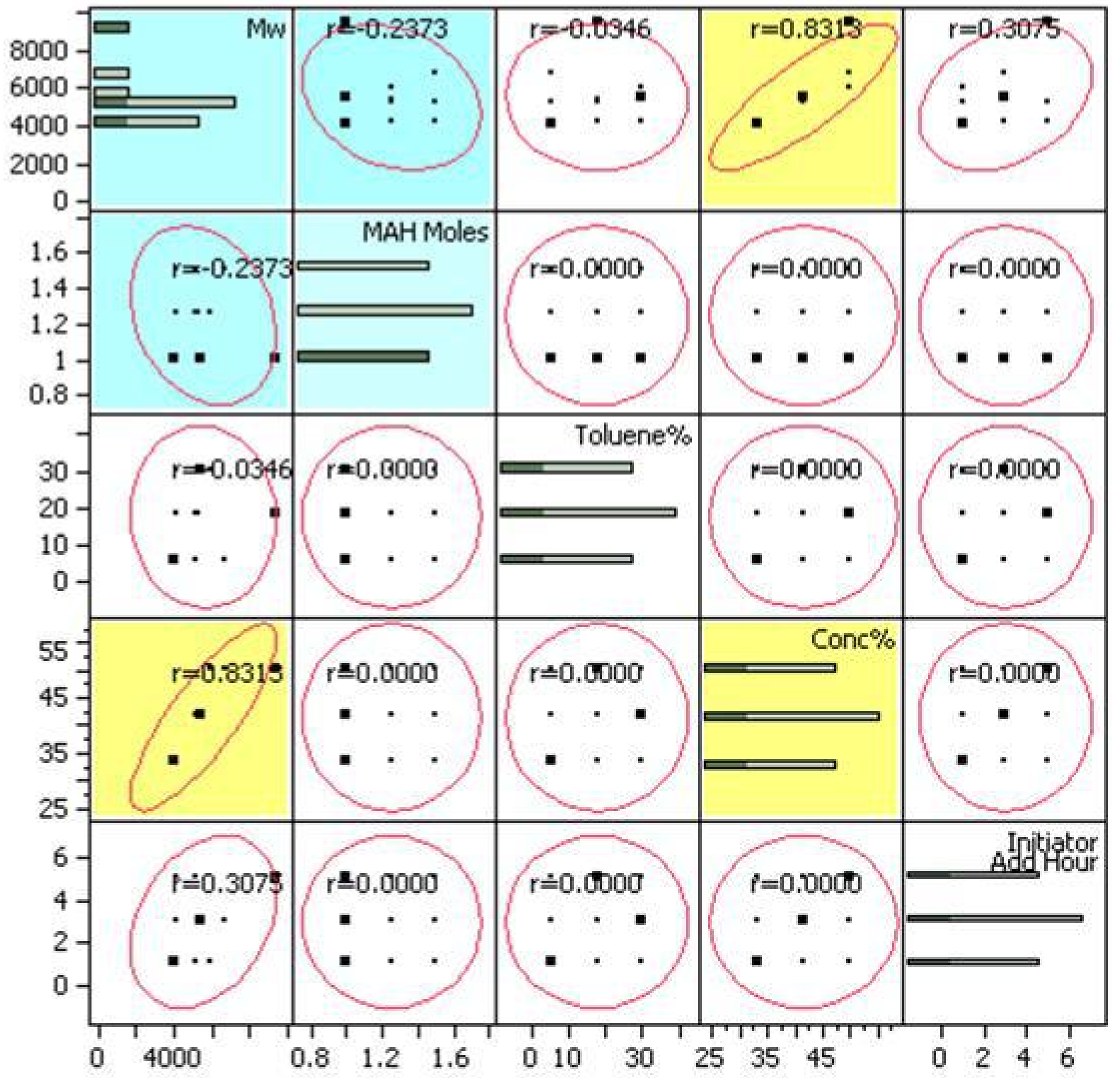
MARM 194

Factors affecting the copolymerization of α-olefin and maleic anhydride in dual solvent system

*Colleen Tabasko[1], Judy Arroyave[2], Ramesh Sharma[2], **Hoon Kim**[1], hoon.kim@chemetall.com. (1) Technical/Innovation, Chemetall, New Providence, New Jersey, United States (2) Molecular Analysis Group, Albemarle, Baton Rouge, Louisiana, United States*

Olefin-maleic anhydride copolymers have long been of great interest due to their unique amphiphilic nature, which can be modulated by simple general organic reactions such as carboxylic acid salt

formation, esterification, amidation and imidation, etc. Accordingly, through the various modification methods, olefin-maleic anhydride copolymer derivatives can play multifunctional roles in diverse industrial applications serving as a component in lubricants, cosmetic compositions, wax dispersants, oil sorbents, pour point depressants and diverse surface modifiers. α-Olefin-maleic anhydride copolymers have been known for many years. Although α-olefins as well as maleic anhydrides are considered as the representative monomers with low activity in radical homo-polymerization, both monomers easily copolymerize together forming unique alternating copolymer structure. So far, much effort has been devoted to achieving high conversion in both polymerization and further modifications, and most researches have focused on diverse properties and applications of the final polymers. But there is little information available about the formation mechanisms and kinetics. Here in this paper we report our latest research results on polymerization kinetics and the effect of monomer concentration and solvent system on the copolymerization especially in dual solvent system.



MARM 195

Morphology of carbon nanofilled polymers

Raul E. Rivas-Sanz[1], *raulrivas.gompers@gmail.com, Charles Seaks*[2], *Vicki Flaris*[1]. *(1) Bronx Community College, Bronx, New York, United States (2) Fordham University, Bronx, New York, United States*

In this paper, composites of polypropylene (PP) with four different carbon based fillers are compared. These are single-walled carbon nanotubes (SWCNTs), multi-walled carbon nanotubes (MWCNTs), nanodiamonds (ND) and nanohorns (CNH). The geometry and properties of these filler and the effects on composites' properties such as conductivity and morphology are correlated. Initial conductivity was measured by electrometer, then secondarily by atomic force microscope (AFM) in the conductivity mode. Morphology studies were performed using the AFM as well using the topography mode. Furthermore, scanning electron microscope images were taken to view the distribution of carbon based nanofillers at the surface of the composite polymer samples.

MARM 196

Preparation and characterization of coatings with tung-oil-based reactive diluents and linseed oil alkyd

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Two kind of reactive diluents were prepared from tung oil via a Diels-Alder reaction with two different dienophiles: methacryloxypyropyl trimethoxysilane (MAS) and triallylether acrylate (TAEA). Triallyl-functionalized tung oil has been prepared by two-step reactions. In the first step, trieallyl ether acrylate was prepared by esterifcation of pentaerithriol ally ether with acrylic acid. In the second step, the triallyl ether acrylate was reacted with tung oil via a Diels-Alder reaction. Linseed oil alkyd resin was prepared by the monoglyceride process. The modified alkyds and diluents were characterized by ^{1}H NMR, ^{13}C NMR and MALDI-TOF MS. The reactive diluents were mixed with linseed oil alkyd, a metal drier package and a wetting agent and then cured. Formulations were prepared as a function of reactive diluents. Tensile, thermomechanical and coating properties were evaluated after curing the films. The addition of two reactive diluents, MASTO and TAEATO, improved the tensile stress and tensile modulus of the alkyd. The addition of the diluents, however, did not significantly change the extension at break. Also, the addition of MASTO firstly increased crosslinking density and storage modulus of the alkyd up to 20wt% and after that decreased with the amount of MASTO. On the contrary, the addition of TAEATO firstly decreased crosslinking density and storage modulus of the alkyd up to 20wt% and after that decreased with the amount of TAEATO. Basic film properties including hardness, impact resistance, adhesion and gloss were not adversely affected by the introduction of any of the tung oil based diluents.

MARM 197

Ring-opening polymerization of ε-thionocaprolactone

Partha Datta, *partha_datta@my.uri.edu. Chemistry, University of Rhode Island, Jamaica, New York, United States*

Organocatalytic ring-opening polymerization (ROP) is an effective method for the synthesis of increasingly well-defined poly(lactones). The mild conditions typical of organocatalytic ROP provide a route to the controlled synthesis of polymers with altered backbones (vs lactones), which have been largely unexplored. Indeed, the altered reactivity of thionoesters renders the synthesis of homo-poly(thionolactones) impossible with traditional transesterification catalysts. One thionolactone, ε-thionocaprolactone (ε-tnCL), is synthesized from readily-available starting materials. The application of H-bond mediated organocatalysts results in ROP, effecting for the first time ever the controlled production of homo-poly(thionocaprolactone). The ROP exhibits the characteristics of a 'living' polymerization. Copolymers of ε-tnCL and δ-valerolactone were synthesized and are the only known copolymers of thiono- and traditional ester monomers.

MARM 198

Protein structure analysis of gonococcal cell surface protein antibody binding domains using a molecular model approach

Yu S. Ting, *yting@jstar-research.com. Zeus Scientific, Somerville, New Jersey, United States*

Pilin is the major surface protein of bacteria *N. gonorrhoeae* which is responsible for the STI gonorrhea. In the 1980s, after the pilin protein from a variant of strain MS11 was isolated, clinical laboratories sought to identify the best peptide sequence antigen to produce antibodies with high specificity and less cross-activity. Three synthetic peptide sequences (69-84, 48-60 and 135-151) were found to produce antibodies with high titer levels. The first two sequences are from the protein's common region while the third (135-151) is from variable region.

Recently in 2006, the structure model of the pilin protein was determined using electron microscopy and x-ray protein crystallography. In this presentation, protein structure analysis using the RCSB protein database (code: 2HI2 and 1IGY) and Swiss PDB viewer molecular model software was conducted for the analysis of three pilin epitopes (69-84, 48-60 and 135-151) binding domain against the immunoglobulin. The molecular level analysis provides structural rationale on why the epitopes exhibits high antibody affinity properties found in previous immunoassay techniques.

The pilin epitope loop bends due to the position of proline and provides a "key and lock" fitting to the IgG Fab clam shell size binding pocket. The pilin epitope at residue 48-60 shows the best fit into the hole between hyper variable loops from both IgG heavy chains and light chains, which attach to a beta-sheet of immunoglobulin domain. Additionally, the pilin protein structure model elucidated its multiple function site behavior such as glycosylation site, assembly/disassembly interaction, and protein aggregate related to new immuno-diagnostic reagent and biopharmaceutical vaccine development for gonorrhea disease will be discussed

MARM 199

Detergent mediated unfolding of proteins in the presence of ionic liquids

*Louisa Abiuso, Eric Kohn, Timothy D. Vaden, **Gregory A. Caputo**, caputo@rowan.edu. Chemistry and Biochemistry, Rowan University, Glassboro, New Jersey, United States*

The recent expanded interest in applications of ionic liquids has developed into variety of investigations on the interactions between ionic liquids and biomolecules. Previous work has shown that ionic liquids, depending on their chemical composition, can affect protein stability. However, little is understood regarding the molecular mechanisms of stabilization or destabilization. We investigated the effects of aqueous solutions of sevral ionic liquids including $BMIBF_4$, EMIAc, and $PyrBF_4$ on the denaturation profile of myoglobin by the anionic detergent sodium dodecyl sulfate (SDS) and the zwitterionic detergent N,N-Dimethyl-N-dodecylglycine betaine (Empigen BB). Detergents traditionally unfold proteins through the disruption of hydrophobic contacts at the interior of the folded structure. The hypothesis was IF ionic liquids, or some component of the ionic liquids, were acting through a similar mechanism, the detergent mediated unfolding would be enhanced. A combination of absorbance, FRET, and circular dichroism spectroscopy were used to monitor unfolding. In all cases examined, the protein denaturation profile remained a traditional, cooperative process. In the case of SDS, we found that some ILs destabilize the protein structure, but the $BMIBF_4$ had the greatest effect. Interestingly, the zwitterionic detergent N,N-Dimethyl-N-dodecylglycine betaine showed a more complex profile. In some cases, such as BMIBF4, ionic liquids that destabilized protein structure to unfolding by SDS became more resistant to unfolding by N,N-Dimethyl-N-dodecylglycine betaine.

MARM 200

A retrospective and prospective view of iron-sulfur protein design

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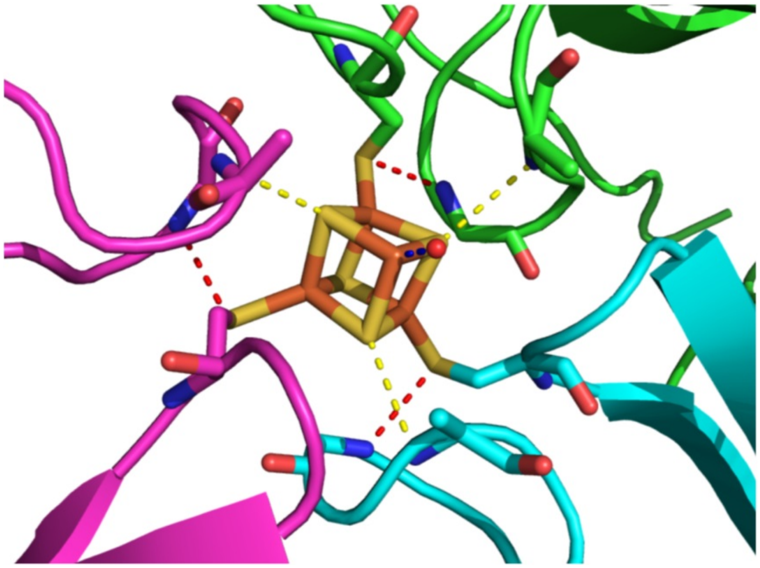
Natural biochemistry uses cofactors and prosthetic groups to supplement protein structure and function. Our approach to the study of metalloproteins is to engineer and fabricate peptide and protein structures containing metal cofactors toward the goal of generating molecular *maquettes*, protein-based synthetic analogues. Twenty years ago, we developed the first iron-sulfur protein designs that faithfully reproduced the spectroscopic signatures and electrochemical behavior of natural ferredoxins in aqueous buffers. Using a simple 16 amino acid ferredoxin maquette, we have explored the engineering requirements for [4Fe-4S] incorporation and stabilization within biological system. These results were consistent with th results of data mining of the protein data bank. In addition, we have used the simple [4Fe-4S] ferredoxin maquette as a module to incorporate [4Fe-4S] centers into four-helix bundle scaffolds. This led to the construction of the first designed multi-cofactor metalloproteins. Our [4Fe-4S] designs led us into a fruitful exploration of the role of zinc(II) binding in zinc finger transcription factors where we showed that the cost of protein folding was minimal (0-5 kcal/mol) relative to the contribution of zinc(II) coordination (about 15 kcals/mol). As we explored Zn(II) binding, several novel [4Fe-4S] proteins have appeared in the literature with properties similar to our original design. Most recently, we have collaborated to incorporate a [4Fe-4S] cluster into a pore of a bacterial microcompartment, as shown in the Figure, in our on going efforts to design functional iron-sulfur proteins from scratch.



MARM 201

Assemblies of macrocyclic peptides as functional catalysts

***Zsofia Lengyel**, zlengyel@syr.edu, Ivan Korendovych. Chemistry, Syracuse University, Syracuse, New York, United States*

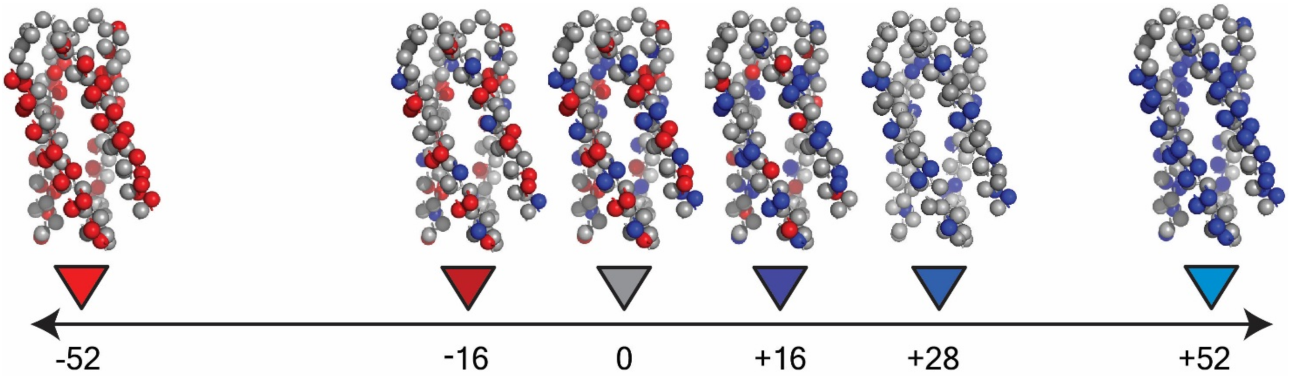
Recently we have demonstrated that amyloid-forming peptides not only are capable of promoting their own self-assembly, but they can catalyze chemical reactions (1). Short de novo designed sequences self-assembled in the presence of zinc ions to form catalytic amyloids that are capable of hydrolyzing p-nitrophenyl esters with efficiencies that are on par with those shown by natural enzymes by weight. To better understand the structure-activity relationship in catalytic amyloids, we developed macrocyclic peptides that constrain functional groups in various distinct arrangements. Our results support parallel orientation of peptide strands and determine the origins of synergistic relationship observed by mixing different peptides.
(1) Rufo *et al. Nature Chem.* **2014**, *6*, 303-309

MARM 202

Adventures in supercharging

*Joseph Brisendine, Peter Schnatz, **Ronald L. Koder**, koder@sci.ccny.cuny.edu. Physics, The City College of New York, New York, New York, United States*

In 2007 the Liu group demonstrated that mutating the surface-exposed residues in Green Fluorescent Protein to dramatically increase its net charge makes it resistant to aggregation, even in the unfolded state. We have implemented this surface 'supercharging' into our Inside-Out protein design algorithm and increased our functional design success rate to over 50%. We demonstrate that at moderate solution ionic strengths these supercharged proteins exhibit the ligand-induced folding property inherent to natural intrinsically disordered protein function. Furthermore, we demonstrate that the introduction of surface supercharging can be used to infix positive cooperativity into proteins that bind more than one substrate or cofactor.



MARM 203

Neutral model of subcellular pH constraints on proteome-wide isoelectric point distributions

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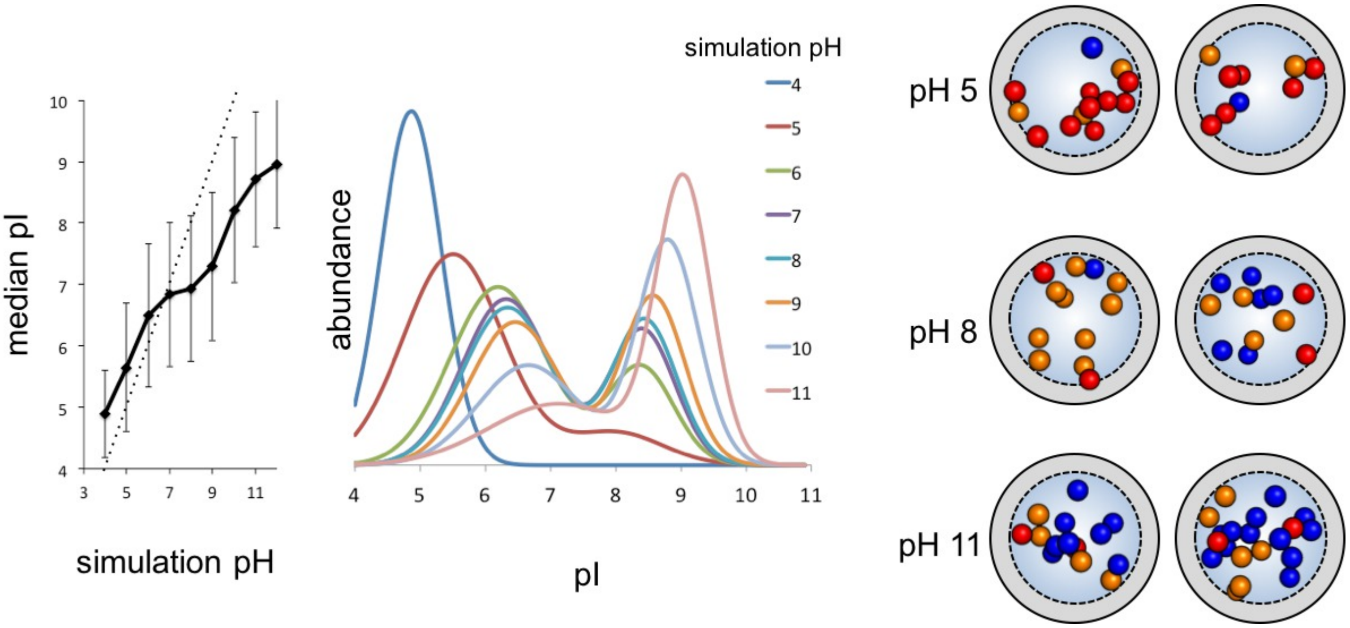
Genomic studies of extremophiles reveal how physiochemical properties of proteomes compensate for unusual environments. Likewise unique conditions within subcellular compartments of eukaryotes affect the properties of associated proteins. Proteins within the lysosome – a highly acidic compartment in the cell - have a median isolelctric point (pI) of 6.6, whereas relatively basic mitochondria contain proteins with a median pI of 8.0. There is a positive correlation between subcellular compartment pH and the median pI for the associated proteome. One possible explanation for this correlation is the adaptation of enzyme active site general acid/base residue pK_as to match environmental pH – but such effects would be limited to a few amino acids and to specific proteins, making it unlikely that such adaptations would affect average properties of the proteome. Using an idealized protein model that considers only pairwise electrostatics and residue burial upon folding, we find a robust positive correlation between proteome pI and environmental pH can be adequately described by neutral evolution – no specific functional adaptation is required. In this model, proteins in acidic environments incur a lower energetic penalty for burying acidic residues such as aspartate or glutamate than basic residues such as arginine or lysine, resulting in a net accumulation of acidic residues in the protein core. A similar bias toward basic amino acids in the protein core occurs under alkaline conditions. Thus the distribution of titratable residues in proteins may not be a direct functional adaptation, but a molecular ‘spandrel’ stemming from marginal stability of neutrally evolving proteins.



Evolution of a spherical model protein. Sequence evolution in acidic environments results in a core with a higher number of Asp and Glu. Neutral pH environments result in a number of buried His. Basic environments favor higher counts of basic Lys and Arg residues.

MARM 204

Educational applications of Thermo Fisher Scientific picoSpin instrumentation for NMR spectroscopy

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Nuclear Magnetic Resonance (NMR) Spectroscopy is the preferred analytical technique for identifying crucial changes in chemical structure within organic molecules and understanding the synthesis and mechanisms of chemical reactions. Direct experience with acquiring and processing NMR spectra is extremely valuable, particularly for undergraduate organic chemistry students. Unfortunately, there are a number of challenges involved in using high-field NMR instrumentation in a classroom setting: access to the instruments for student usage, relatively complex instrument operation, funding expensive equipment for teaching purposes, and the lack of NMR applications developed to complement existing lab curricula. The recent development of benchtop NMR by Thermo Fisher Scientific addressed many of these challenges by providing small scale, affordable, easy to use spectrometers with superior resolution. We will discuss benchtop NMR's role in the undergraduate chemistry curriculum using two examples from the Thermo Fisher Scientific lesson plan library, *Micro-scale Friedel-Crafts Acylation of Ferrocene* and *Hydrolysis of Acetic Anhydride with Heavy Water*. These procedures underscore some fundamental organic chemistry concepts with hands-on use of NMR instrumentation.

MARM 205

Implementation of C-13 and 2-D NMR in organic laboratory sequence

***Anthony J. Kiessling**, akiessli@mansfield.edu. Mansfield Univ of Pa, Mansfield, Pennsylvania, United States*

Mansfield University recently obtained an Anasazi Instruments, 90-MHz FT-NMR spectrometer replacing a Hitachi R1200 60-MHz spectrometer. This change allowed the acquisition of C-13 spectra and the usual 2-Dimension NMR experiments. This afforded an opportunity to modify existing synthetic lab experiments to include additional structure verification through the addition of NMR techniques, and to enhance student learning. Two experiments were modified toward this goal: the preparation of nitrophenacetin and the preparation of esters. Comparison of actual spectra with predicted chemical shifts available through Wavefunction, Inc.'s Spartan and ACD/Labs, Inc.'s NMR Predictor allowed for further analysis by students.

MARM 206

Incorporation of benchtop NMR spectroscopy into undergraduate laboratories: an active-learning approach

***Juan Araneda**, james.grebinski@nanalysis.com, **Susanne Riegel** Nanalysis Corp., Calgary, Alberta, Canada*

NMR Spectroscopy is one of the most widely used characterization techniques in chemical research. Despite pedagogical shifts towards active-learning and guided-inquiry approaches, incorporation of NMR spectrometers directly into undergraduate curriculum has remained largely limited due to mitigating factors of size, cost and availability of high-field spectrometers. As a result, students rarely gain hands-on access to this instrumentation, particularly in the beginning stages of their programs. An emergence of a new class of benchtop NMR spectrometers (42 – 60 MHz) that are affordable, portable and do not require weekly upkeep or maintenance can facilitate the introduction of this technique at all stages of chemical education. They also offer sufficient resolution and sensitivity for structure elucidation, reaction monitoring, and basic quantitation.

Herein, we describe methods for unique incorporation of the NMReady benchtop spectrometer into undergraduate laboratory experiments and illustrate how students can learn the proper technique to use an NMR spectrometer, prepare samples, monitor and characterize reaction mixtures.

MARM 207

What we discovered from providing undergraduates with high-field NMR

***Susan M. Schelble**, sschelbl@msudenver.edu. Campus Box 52, Metropolitan State University of Denver, Denver, Colorado, United States*

Through generous funding from NSF, our undergraduate chemistry majors and minors were able to use high-field NMR in their laboratory courses. This talk will look at the impact this instrumentation has made on the curricular and pedagogical aspects of our degree program. We will report successes and challenges for helping students master the instrumentation. We will also discuss what we learned about our teaching and learning strategies.

MARM 208

Determination of active ingredients in analgesic drugs by thin-layer chromatography coupled with compact mass spectrometry (TLC-CMS)

***Changtong Hao**, haoc@advion.com, Nigel Sousou, Simon Prosser, John D. Henion. Advion Biosciences Inc, Ithaca, New York, United States*

Thin layer chromatography (TLC) is a simple, useful technique for the separation and estimation of compounds in complex mixtures. It is routinely used to monitor the progress of synthetic reactions by observing the consumption of starting materials against the appearance of single or multiple products. A frequent organic laboratory experiment for chemistry students in colleges and universities is the TLC analysis of samples containing analgesic drugs. Traditionally, the visual comparison of an unknown spot with an analytical standard under UV light has been sufficient to provide the confirmation of a compound's identification.

In this application, a direct TLC-CMS analysis is used to determine the active ingredient in analgesic drug samples. The benefit of TLC-CMS analysis is to analyze the sample directly from the TLC plate without further sample preparation after the TLC separation is completed. The active components can be selectively identified by detecting the mass-to-charge ratio (*m/z*) using mass spectrometry. Chemistry students can benefit from this TLC-CMS experiment by gaining TLC experience as well as compound analysis by mass spectrometry which is typically not available for undergraduate students.

MARM 209

Resveratrol and piceid production and storage by Japanese knotweed

*Matthew Yatison[2], Jared Luchetta[1], Abiail Mikolon[2], David Pupaza[2], Kenneth Klemow[2], **Donald E. Mencer**[1], donald.mencer@wilkes.edu, William Terzaghi[2]. (1) Chemistry, Wilkes University, Wilkes-Barre, Pennsylvania, United States (2) Biology, Wilkes University, Wilkes-Barre, Pennsylvania, United States*

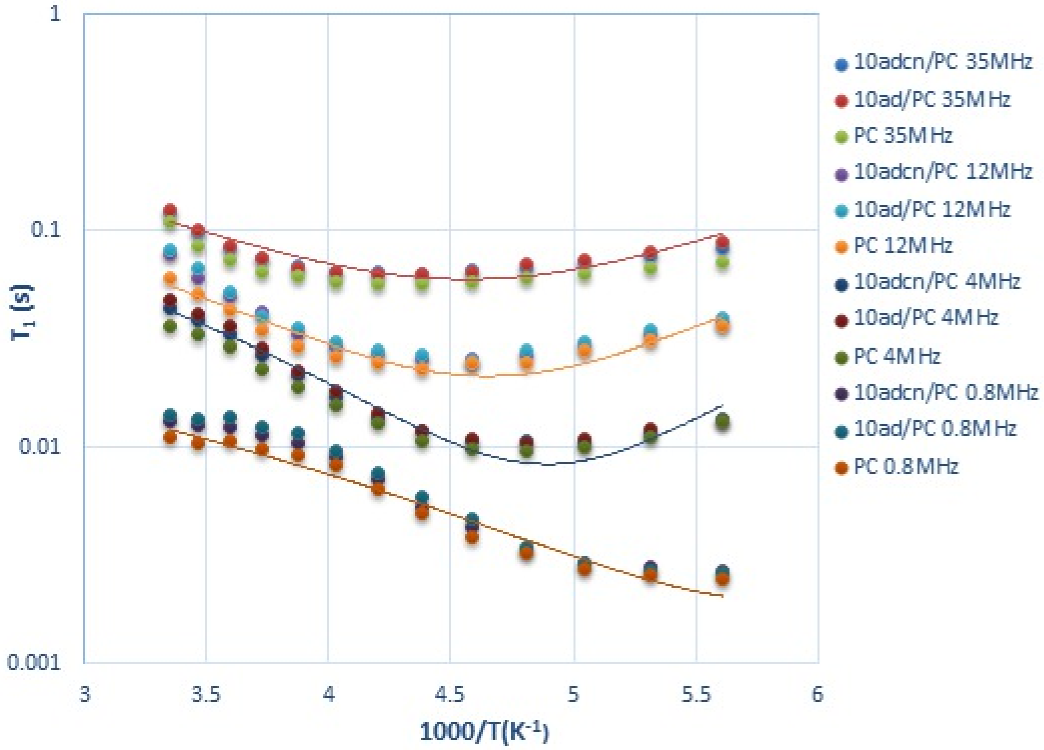
Resveratrol is a natural compound with demonstrated medicinal properties including an ability to extend the lifespan of various organisms. Japanese Knotweed (*Fallopia japonica*) and its close relative Giant Knotweed (*F. sachalinensis*) are known to store large quantities of resveratrol and its glycosylated derivative piceid. The role of genetic variation on the production of resveratrol and piceid by Japanese knotweed is not well studied. In this study, ten samples of knotweed from Luzerne County in northeastern Pennsylvania were collected and analyzed using primers that amplified genomic and plastidic DNA polymorphisms. Four of the primers (KW4, KW6, atpB-1/rbcL-1, trn-T/TRN-L) showed differing patterns between different plant samples (BB10, K2, K3, and DNA1). Rhizomes of these plants were processed and resveratrol and piceid extracted using 80% ethanol. Analysis was completed using reverse-phase HPLC with both UV and MS detection. Piceid levels were consistently higher than resveratrol (3-50 times higher). Sample BB10 had 19-fold higher resveratrol content than sample K2 whereas there was no significant deviation in piceid content, suggesting that BB10 may have less piceid synthesis or a more active glycosylase. Conversely, K2 had 1.5 fold more emodin, another natural product with possible medicinal properties, than BB10. Preliminary findings also suggest that post-harvest storage at room temperature enhanced resveratrol content in many samples but had little effect on piceid content, and that piceid was 3 fold higher in the pith than in the cortex, whereas resveratrol increased moving from the pith to the epidermis. This differential localization might be due to deglycosylation of piceid stored in the pith to the active compound resveratrol as it is transported to its site of action in the epidermis.

MARM 210

Nuclear magnetic resonance studies of polycarbonate films for high power thin film capacitors

Shen Lai[1], *airlaishen@gmail.com, David A. Boyles*[2], *John Fontanella*[3], *Steven Greenbaum*[4]. *(1) City University of New York, New York, New York, United States (2) SD School of Mines and Technology, Rapid City, South Dakota, United States (3) U. S. Naval Academy, Annapolis, Maryland, United States*

The continued development of thin film polymer dielectrics for high power capacitors requires new materials with a reasonably high dielectric constant and high dielectric breakdown strength. Polycarbonates have recently been considered as a replacement for currently used polypropylene. In this collaborative investigation with D. Boyles (South Dakota School of Mines) and J. Fontanella (U.S. Naval Academy), we explore the use of molecular diluents Films of glassy Bisphenol-A polycarbonate (BPAPC) to enhance orientation motion, in particular the dipole moments, thus increasing the dielectric constant. Indeed, the electric constant increases as predicted when the diluents were added into the polycarbonate. High-resolution solid-state ^{1}H and ^{13}C magic angle spinning (MAS NMR) experiments were performed on Polycarbonate containing 2-adamantanone or 1-Adamantanecarbonitrile (ADCN), as diluents to analyze structural and dynamic details of the polycarbonate- diluent systems. Conventional variable temperature (VT) NMR ^{1}H proton spin- lattice relaxation time T_1, relaxation time in rotating frame $T_{1\rho}$ measurements and VT fast field cycling nuclear magnetic resonance relaxometry (FFCNMR) measurements were carried out in order to better understand T_1 relaxation dispersions shed light on polymer dynamics containing diluents compared to pure polycarbonate. Combining conventional NMR relaxation and FFNMR measurements with dielectric relaxation measurements provides a detailed view of the effect of molecular diluents on ring-flip dynamics over a wide range of frequencies.



MARM 211

Fluorinated porphyrinoids as efficient platforms for new photonic materials

*N. V. S. Dinesh K. Bhupathiraju, Waqar Rizvi, James D. Batteas, **Charles M. Drain**, cdrain@hunter.cuny.edu. Chemistry and Biochemistry, Hunter College of the City University of New York, New York, New York, United States*

Porphyrinoids are robust heterocyclic dyes studied extensively for their applications in photonic materials because of their tunable photophysical properties, diverse means of modifying the periphery, and the ability to chelate most transition metals. Commercial applications include phthalocyanine dyes in optical discs, and platinum porphyrins as oxygen sensors. Most applications of these dyes require exocyclic moieties to improve solubility, modulate photophysical properties, or direct the self-organization into architectures with desired photonic properties. The synthesis of the porphyrinoid depends on the desired application, but the de novo synthesis often involves several steps, is time consuming, and results in low isolated yields. Thus, the application of core porphyrinoid platforms that can be rapidly and efficiently modified to evaluate new molecular architectures allows researchers to focus on the design concepts rather than the synthesis methods, and opens porphyrinoid chemistry to a broader scientific community. We have focused on several widely available, commercially viable porphyrinoids as platforms: meso-perfluorophenylporphyrin, perfluorophthalocyanine, and meso-perfluorophenylcorrole. The perfluorophenylporphyrin is readily converted to the chlorin, bacteriochlorin, and isobacteriochlorin. Derivatives of all six of these core platforms can be efficiently and controllably made via mild nucleophilic aromatic substitution reactions using primary S, N, and O nucleophiles bearing a wide variety of functional groups. The remaining fluoro groups enhance the photo and oxidative stability of the dyes and can serve as spectroscopic signatures to characterize the compounds e.g. using 19F NMR. This talk provides an overview of the chemistry of fluorinated porphyrinoids that are being used as a platform to create libraries of photo-active compounds for applications in materials.

MARM 212

Light management in thin-film organic optoelectronic devices for energy efficiency and energy harvesting applications

***Deirdre O'Carroll**, ocarroll@rutgers.edu. Rutgers University, Piscataway, New Jersey, United States*

Thin-film organic semiconductor materials are emerging as energy-efficient, versatile alternatives to inorganic semiconductors for display and solid-state lighting applications. Additionally, thin-film organic laser and photovoltaic technologies, while not yet competitive with inorganic semiconductor-based analogues, can exhibit small device embodied energies (due to comparatively low temperature and low energy-use fabrication processes) which is of interest for reducing overall device cost. To improve energy conversion efficiency in thin-film organic optoelectronics, light management using nanophotonic structures is necessary. Here, our recent work on improving light trapping and light extraction in organic semiconductor thin films using plasmonic metasurfaces will be presented [1,2]. Numerous optical phenomena, such as absorption induced scattering, out-of-plane waveguiding and morphology-dependent surface plasmon outcoupling, are identified due to exciton-plasmon coupling between the organic semiconductor and the metasurface. Interactions between localized and propagating surface plasmon polaritons and the excitonic transitions of a variety of organic conjugated polymer materials will be discussed and ways in which these interactions may be optimized for particular optoelectronic applications will be presented.

[1] C. E. Petoukhoff, D. M. O'Carroll, Absorption-Induced Scattering and Surface Plasmon Out-Coupling from Absorber-Coated Plasmonic Metasurfaces. *Nat. Commun.* 6, 7899-1-13 (2015).
[2] Z. Shen, D. M. O'Carroll, Nanoporous Silver Thin Films: Multifunctional Platforms for Influencing Chain Morphology and Optical Properties of Conjugated Polymers. *Adv. Funct. Mater.* 25, 3302-3313 (2015).

MARM 213

Fuels of the future: Using diatoms as a platform for renewable energy

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Despite the fact that there are still abundant natural petroleum reserves (supplies will last for more than a century), significant carbon mitigation cannot be achieved without the development of environmentally sustainable and renewable fuels. Owing to their high productivity-to-biomass ratio, ease of cultivation, and ability to grow in saline water, algae have been considered as a leading biodiesel feedstock. To displace fossil fuels, however, algae must be grown at a scale that yields approximately 10 million barrels of oil per day – which would supply approximately 50% of the total U.S. consumption. For the last few decades, researchers have searched for the "sweet spot" between algae's triacylglycerols (TAG) production and biomass accumulation to obtain a strain with increased lipid production that can be developed as a commercially viable algal feedstock for biofuel production. Diatoms, a unique algal taxon, naturally accumulate TAGs as storage components, which can be readily converted to biodiesel. In fact, lipids derived from fossil diatoms are a major component of the highest quality petroleum. Therefore fast growing, lipid accumulating, diatoms can be an excellent platform for biodiesel production. For many years, studies have been performed to environmentally optimize diatoms' lipid production and biomass accumulation, yet no economically sustainable strain has been reported. In my talk, I will present our unique, genetically modifies, strains generated from the model diatom *Phaeodactylum tricornutum*, that could be used as a test-case for economical sustainable biofuel production. These strains are characterized by high lipid yield, yet keep relatively fast growth rates and are more efficient in using solar energy for lipid production.

MARM 214

Enhanced gas recovery: Density functional theory computation of adsorption of CO_2, CH_4, and H_2O to shale surfaces

Lorena Tribe, *lut1@psu.edu. Penn State Berks, Reading, Pennsylvania, United States*

Supercritical carbon dioxide (sCO_2) can be used to increase the yield from gas reservoirs in a process known as enhanced gas recovery (EGR). High-level *ab initio* electronic structure calculations free of adjustable parameters can provide insight into the structure and dynamics of surface complexes relevant to EGR. We address adsorption/desorption issues in this work using first principles Molecular Orbital/Density Functional Theory to model two clay minerals, Na-montmorillonite and kaolinite, and their interactions with CO_2 and CH_4 molecules. The free energies of adsorption of the clay models, the adsorbates, and the adsorbate-substrate clusters are determined, and the difference used to provide results for ΔG_{ads}. The values obtained are contrasted with data derived from experimental adsorption isotherms. Preliminary calculations with selected input structures indicated that the adsorption of CH_4 to a clay surface is less favored that that of CO_2 and that the presence of water molecules, modeled explicitly, leads to significant differences. The outcomes depend strongly on the clay model, the adsorbate, and the initial adsorbate-substrate cluster. Small differences in the initial geometry did not produce much change in the adsorption of CO_2 on kaolinite, which remained unfavorable, but significantly changed the interaction of this adsorbate with Na-montmorillonite with outcomes as different as physisorption and mineralization. In this work we explore the causes for these different outcomes by implementing a systematic approach to sampling the surface and by determining the activation energy and the rate constant for the adsorption/desorption processes. The influence of the presence of water molecules on the vibrational frequencies of carbon dioxide is calculated and contrasted with experimental and molecular dynamics results from the literature.

MARM 215

Trash to treasure: Biowaste-to-energy as next fuel source

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The seafood industry produces over 100 million pounds of seashell waste every year. With landfill space diminishing quickly, ways to recycle waste materials are becoming more sought for. Herein, we utilized waste mussel, clam and oyster shells as heterogeneous catalysts for the transesterification of various feedstocks into biodiesel. One of the feedstocks, camelina sativa oil, provides a reliable solution for biodiesel production because it has high tolerance of cold weather, drought, low-fertility soils and contains approximately 40% oil content. Another feedstock, waste coffee grounds, is appealing choice for biodiesel production because they contain up to 20 % oil by dry weight.The catalysts from waste seashells were characterized by X-ray powder diffraction and Fourier Transform Infrared spectroscopy. High biodiesel yields were achieved at a 12:1 (alcohol: oil) molar ratio with 1 wt. % waste seashell catalysts in 2 hours at 65 °C. Biodiesel was analyzed by 1H NMR and FT-IR spectroscopy and the fuel properties of the biodiesel were compared with ASTM standards.

MARM 216

Brown grease pyrolysis mechanism

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Brown grease results from fats, oil and grease entering the sewage system. This is a major urban problem. We have shown that brown grease can be converted to a mixture of aliphatic hydrocarbons by heating under relatively mild conditions. This mixture contains primarily n-alkanes and 1-alkenes with between 8 and 30 carbon atoms in the chain. Furthermore, this conversion occurs without or with addition of a catalyst such as iron sulfate. Investigation on pyrolysis of Oleic and Palmitic acid was conducted because those are the main components of Brown grease. Understanding their pyrolysis mechanism will provide great insight about the Brown Grease Pyrolysis. Results from the pyrolysis were obtained using GC-MS.

MARM 217

Value-added products from pyrolysis of sludges from pork production

Lawrence M. Pratt[1], *lpratt@mec.cuny.edu, Michele Vitadello*[1], *Sam Groveman*[1], *Duong Pham*[3], *Van Luong*[2], *Nhi Ngoc*[3], *Phi Phung Kim*[3], *Tuyen Pham*[2]. *(1) Chemistry and Environmental Science, CUNY Medgar Evers College, Brooklyn, New York, United States (2) Environmental Science, Saigon University, HCM City, Viet Nam (3) Chemistry, University of Science, HCM City, Viet Nam*

Treatment of waste products from pork production results in two types of sludge. The first is high-fat sludge from physical treatment and dewatering. That sludge is further treated by a proprietary biological process, resulting in a second type of sludge that generates less odor. Pyrolysis of both sludges results in an oily distillate, an aqueous distillate, and biochar. The oily distillate from the physical treatment consists primarily of aliphatic and aromatic hydrocarbons that are components of diesel fuel, and thus, has commercial potential as a fuel precursor. The oil from the biological treatment is a complex mixture with less commercial potential. The biochar from both types of sludge was evaluated for its potential as a fuel and as a soil amendment.

MARM 218

MK-7655, A broad-spectrum β-lactamase inhibitor for combination with the carbapenem antibiotic Primaxin®: A Merck drug discovery story spanning 30 years

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Merck has a long-standing presence in the antibacterial field, punctuated by the discovery of Primaxin®, a combination of the carbapenem antibiotic imipenem and the renal DHP inhibitor cilastatin. Carbapenems, a subset of β-lactam antibiotics, have been especially important for the treatment of serious nosocomial infections. In response to these antibiotics, some bacteria have developed enzymes known as β-lactamases that enable survival even at high concentrations of the β-lactam antibiotic. A proven strategy to restore antibacterial activity is to combine a β-lactamase inhibitor (BLI) with the antibiotic drug . With the rising emergence of imipenem-resistant strains mediated by β-lactamases, the need for a new generation of β-lactamase inhibitors (BLI's) has become more pronounced. Herein, we report the path that led to the discovery of MK-7655, a Class A/C β-lactamase inhibitor that effectively restores imipenem's activity against imipenem-resistant *Pseudomonas* and *Klebsiella* strains at clinically achievable concentrations. A combination of MK-7655 and Primaxin® is currently in Phase II clinical trials for the treatment of Gram-negative bacterial infections.

MARM 219

Ion-charged polymers' effect on bacterial growth

Robert C. Josman, *rjosman@msn.com. City University of New York, New york, New York, United States*

The exponential increase of antibiotic resistant bacteria has created a heightened need for new polymer material development. This should not only aid in the reduction of medical costs, but also provide better patient outcomes.

In this paper we evaluate the antimicrobial effects of thin-films containing varying concentrations of sodium and potassium ions. The samples are then assessed against two separate genus of bacteria at three concentrations of each of the bacteria. The bacteria is cultivated within wells coated with the polymer films, in the presence of a broth. These samples are compared against a control set of samples without the

presence of ions.

The experimental process used, also allowed for the diffusion of the antimicrobial properties throughout the entire thin-film Plastic Polymers. This helped eliminate the problem of degradation in the antimicrobial properties throughout the polymer, to address the persistent degradation of antimicrobial properties.

MARM 220

Synthesis and antimicrobial activity of fullerenol and fullerenemalonic acid

Alisha Pitchford*, apitchford@maryu.marywood.edu, Deanne D. Garver. Science, Marywood University, Scranton, Pennsylvania, United States*

The absence of water solubility of pristine fullerenes hinders its biological applications and thus addition of polar functional groups can enhance their potential for study. Previous studies against *Escherichia coli* and *Bacillus subtilis* has shown potential for these classes of compounds. It is with this in mind that two compounds were synthesized: a polyhydroxylated fullerene (fullerenol) and a mixture of mono-, bis- and tris- malonate derivatives, fullerenemalonic acid. Synthesis of the fullerenol was accomplished through hydroxylation using hydrogen peroxide, while the fullerenemalonic acid was synthesized by carboxylation from diethyl malonate. Each compound was evaluated for antimicrobial and bactericidal activity against four bacteria comprising the biofilm harvested from the water reservoir of a hydroponic lettuce grower. The isolated bacteria included *Bacillus thuringiensis, Pseudomonas aeruginosa, Bacillus amyloliquefaciens, and Pigmentiphaga daeguensis*. Three concentration ranges were prepared and assessed on Mueller-Hinton agar for its diffusion quality to measure zones of inhibition for antimicrobial and bactericidal activity. Positive controls were also performed using a 1.5% benzalkonium chloride solution. Results of these studies provide evidence for the further study of novel polar fullerene compounds as antimicrobial and bactericidal agents against pathogenic bacteria.

MARM 221

Modeling cell permeation and proteolytic cleavage of peptides

Alexander S. Bayden[2]*, alexander@bayden.net, Joseph Audie*[2,3]*, Jon Swanson*[2,1]*, Mark Jarosinski*[2]*, David J. Diller*[2]*. (1) ChemModeling, LLC, Weldon Spring, Missouri, United States (2) CMDBioscience, Inc., New Haven, Connecticut, United States (3) Chemistry, Sacred Heart University, Fairfield, Connecticut, United States*

Peptides are playing an increasingly important role in medicinal chemistry occupying a niche between therapeutic antibodies and small molecules. Despite their potential advantages, to become relevant therapeutics peptides must overcome critical pharmacokinetic problems including limited cell permeability and rapid proteolytic cleavage. To address these problems, we have implemented 1D and 3D descriptor-based descriptor. In this presentation, we will describe how we have built upon validated cheminformatics descriptors to derive general peptide descriptors that are applicable to amino acids well beyond the standard 20. Further, we show how these descriptors have been applied to the problems of proteolytic stability and passive cell permeability.

MARM 222

Ancient medicines wearing new disguises

Krishnaswami S. Raja, *krishnaswami.raja@csi.cuny.edu. Chemistry, College of Staten Island CUNY, Staten Island, New York, United States*

Many approved drugs are based on natural product sources that have been employed by alternative medical systems to treat the same medical conditions for thousands of years. The historical use of such therapeutics will be explored and the present disguises they wear in the form of isolated single molecule or nanoparticle formulations etc. will be presented. Western Science has explored only ~5% of the approximately 25,000 species of higher plants for drug leads and this has provided over 60-80% of all approved drugs. The alternative medical systems such as Ayurveda/Siddha/Unani/Chinese medical systems have been used for clinically for thousands of years and have examined a much larger spectrum of plants and natural products for the treatment of diseases. A systematic collaborative approach between alternative medical system experts and drug development scientists can potentially result in accelerated drug development and approvals.

The efforts of my lab in exploring this approach using *Curcuma longa* and other herbal sources by employing synthetic chemistry/formulation and bioconjugation will be discussed. The potential advantage of promiscuity in natural product drug candidates (with respect to the number of biochemical pathways they modulate) in the treatment of diseases will be discussed. The relative advantages/disadvantages of using a purified extract composed of multiple chemical entities versus a single molecule drug candidate for therapeutic use will be outlined.

MARM 223

Enabling capabilities in drug discovery

Petr Vachal, *petr_vachal@merck.com. RY800-C300, MerckCo., Rahway, New Jersey, United States*

I will outline the principles of an emerging capability with a potential for being truly transformational in our efforts to improve efficiency and reduce attrition rate in drug discovery and consequently increase the overall drug pipeline fitness. Recent advances in several discrete scientific and technological disciplines enhanced our ability to mine, fuse and analyze large data sets, predict and model relevant drug-like chemical space, and enhance the ability to execute on medicinal chemistry and in vitro pharmacology. Harnessing these aptitudes, we developed and piloted an integrated workflow for drug discovery design. This approach enables rational, data-rich prosecution of entire sets of drug candidates simultaneously instead of the traditionally throughput-limited singleton candidate evaluation, allowing for holistic understanding of trends and multiplex correlations of the structure-activity-relationship (SAR). I will discuss several examples of drug discovery projects already facilitated by our approach.

MARM 224

Assessing ligand-induced GPCR cell signaling with dissipation monitoring of the QCM-D

Jennifer Y. Chen, *jchen249@gmail.com, Lynn S. Penn, Jun Xi. Chemistry, Drexel University, Philadephia, Pennsylvania, United States*

The quartz crystal microbalance with dissipation monitoring (QCM-D) is a highly sensitive, noninvasive, and label-free sensing device capable of measuring changes in frequency (Δf) and changes in dissipation (ΔD) of a layer attached to the quartz crystal surface. We have developed a real time non-invasive technique using the quartz crystal microbalance with dissipation monitoring to quantitatively observe such cellular processes. Previously, we have successfully tracked real time changes in cellular adhesion due to mediated through the EGFR pathway using the QCM-D. Here we will use the QCM-D to monitor and study G protein coupled receptor (GPCR) signaling pathway. GPCRs are a large family of receptors responsible for the signal transduction and more than 50% of the current therapeutics target GPCRs directly or indirectly making this family of receptors one of the largest groups of druggable targets. The QCM-D technique can potentially be a useful application in studying and providing insight on cellular processes such as cell signaling and trafficking and can potentially be a useful in vitro method for drug and biomarker screenings.

MARM 225

Determination of the electrochemical parameters of ferrocene in nanoemulsion

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Nanoemulsion, a kinetically stable system of nanosized oil droplet in water has been used as a medium in biological, medicinal and dermatological process. It has laos found used in most industrial applications. Ferrocene which is liberally soluble in the formulated nanoemusion is foud to undergo a quasi-reversible process in this medium. Advantage of this fact is therefore take to evaluate its electrochemical kinetic parametrs such as the heterogeneous rate constant, k_o, the formal redox potential, E^o, the half wave potential, $E^{1/2}$, the electron tranfer coefficient, alpha, and its diffusion coefficient, D. These important electrochemical parameters including the observed current function has been used to determine the mechanism of EC for the oxidation of ferrocene in the formulated nanoemulsion.

MARM 226

Optimization of a spectrophotometric method to determine ammonia in groundwater

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High concentrations of arsenic in groundwater have been reported from different regions in the world. Serious health effects due to elevated arsenic consumption have been documented in several South Asian countries. However, the link between arsenic and other ions in shallow aquifer waters containing much higher nutrients (TOC, TN, NH_4 and P) remain poorly understood. In the study area of Chittagong, Bangladesh, the northern part of the city is a part of Anticline associated with Tertiary aquifers and the southern part of the city is plain land associated with Quaternary aquifers. Preliminary studies have reported elevated arsenic and manganese (Mn) in those aquifers. However, as to date, no study has been conducted to investigate the relation between arsenic and nutrients to understand the geochemical processes that control the As distribution in groundwater. This study reports the modification of a spectrophotometric inexpensive reliable method to measure the ammonia concentration in a set of several groundwater samples collected from both shallow and deep aquifers in Chittagong area. The preliminary results showed high level of ammonia is associated with elevated level of As and Mn, suggests that reducing condition may control the As and Mn release in groundwater. The results suggest that the role of nutrients on the microbial activity and the mobility of As in both aquifers warrant further investigation.

MARM 227

Particle sizes and singlet oxygen production of silica-porphyrin-liposomes

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We prepared pH-triggered silica-liposome carrier for photodynamic therapy in cancer treatment, in which porphyrin sensitizers can only be efficiently released at acidic tumor pH (5-7) but not at normal physiological pH (~ 7.4). The lipid film hydration method is used to encapsulate the silica attached-Meso-tetra(4-N, N,N-trimethylanilinium) porphine tetrachloride (TTMAPP) into liposomes composed of 1,2-dioleoyl-sn-glyscero-3-phopsho chloride (DOPC) in the presence of Cetyl trimethylammonium bromide (CTAB). The resulting silica-liposomes are extruded for particle size measurements on a Joel 1400 Transmission electron Microscope. A uniform size for porphyrin particles was keep around 100-400 nm. The production of singlet oxygen was determined to be more efficient at pH 5.5 than weak basic solutions. The silica attached TTMAPP in liposomes are stable in a natural pH environment, in a lower pH the liposomes break down and the silica and TTMAPP separate. Over time the liposomes breakdown and the TTMAPP and silica also separate. At lower at lower pH such as in the region of cancer cells this method is meant to be a sight specific treatment method for various types of carcinoma. To allow for limited adverse side effects, that are common with other types of cancer treatments.

MARM 228

Thyroid hormone transport in the cardiac myocyte

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Thyroid hormone has profound effects on the heart and cardiovascular system, in part by regulating the expression of important cardiac genes. We studied the specific transport proteins, the monocarboxylate transporters Mct8 and Mct10, and their potential role in delivering thyroid hormones to the cardiac muscle cell. Our data supports the hypothesis that only the active form of thyroid hormone, triiodothyronine, (T3) enters the cardiac myocyte. Many other cell types are able to transport the prohormone, T4, and convert it to the active form, T3. This has important implications for the treatment of human disease, specifically patients with heart failure and low T3 syndrome. The current paradigm for treatment is prescribing T4 instead of T3. Our goal is to further elucidate the roles of these specific thyroid hormone transporters in the cardiac myocyte.

MARM 229

Neurons of the barrel cortex and their connections: A quantitative morphological analysis

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A ‘bottom-up’ approach to resolving neuronal circuits involves deciphering their building blocks, the individual neurons. Specific morphologies have been correlated with specific circuit functions. We have

been taking a morphological approach to understanding neuronal circuits in the primary somatosensory cortex, more specifically those associated with supragranular neurons in the barrel field (S1BF) of the mouse. After defining groups of neurons that are distinguished from one another based on morphological characteristics, our aim is to determine if specific morphological groups are associated with particular cortical connections. Individual neurons are labeled using Diolistics and reconstructed from confocal images. Morphological measurements are analyzed using principal component analysis followed by cluster analysis, revealing distinct groups of neurons. Cortical connections are shown by in vivo injections of fluorescent beads in synaptic target areas of S1BF. These experiments show the correlation between anatomical classes of neurons and specific roles within the cortical circuit.

MARM 230

Hydra polycystins exhibit specific expression patterns and may regulate *Hydra* behaviors

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The cnidarian *Hydra* is one of the most primitive metazoans with a nervous system, but nevertheless displays complex behaviors including cnidocyte (stinging cell) discharge and a stereotypical set of movements during its feeding response. Chemical, mechanical and photo stimuli have been shown to affect these behaviors, but the molecular mechanisms regulating these activities are not yet fully understood. TRP channels are a diverse superfamily of nonselective cation channels that function as polymodal cell sensors. Most families of TRP genes are found in the hydra genome, including members of the TRP polycystin 2 (PC2) family. Several potential polcystin 1 (PC1) homologs were also identified in the hydra genome. It has been proposed that a PC1 protein responds to a signal (chemical or mechanical) through its extracellular N terminus, and in turn gates its associated PC2 protein. Whole mount *in situ* hybridizations revealed that three polycystin genes exhibit specific patterns of expression in hydra. A PC2 and a PC1 gene are expressed in hydra tentacles and bases, and a second PC2 gene is expressed in cells immediately surrounding the mouth and in discrete patches of cells in the hydra body. These expression patterns suggest potential roles for the polycystins in cnidocyte discharge and in mouth opening. To investigate this possibility, non-specific chemical inhibitors of PC2 channels were used in behavioral assays. The inhibitors reduced prey capture and cnidocyte discharge, and also reduced the mouth opening response to glutathione (a known mouth-opening stimulus in hydra). In addition, the PC2 activator triptolide increased cnidocyte discharge. Examining the role of polycystins in hydra will lead to insights into the regulation of complex behaviors by signal transduction events in single cells. In addition, studying polycystins in hydra can further our understanding of the function of these proteins in more complex organisms.

MARM 231

IL6-STAT3 and sphingosine-1-phosphate signaling in inflammation-induced colorectal tumor progression

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Patients with inflammatory bowel diseases (IBD) often show increase level of serum interleukin-6 (IL-6). The level of IL6 is considered as a prognostic marker for IBD patients who are predisposed for the development of colorectal cancer (CRC). IL-6 signaling in cancer cells involves activated transducer and activator of transcription 3 (STAT3) and persistently activated STAT3 is found in many tumors in addition to CRC. STAT3 in immune cells (macrophages), however, acts as a downstream of anti-inflammatory response such as IL-10. Using a mouse model in which the *stat3* gene is deleted in macrophages (Stat3-IKO mice), we demonstrated that conditional knock out mice developed severe inflammation in the colons which led to spontaneous colon cancer development at a rate similar to human IBD. We recently demonstrated functional STAT3 in colonic epithelial cells regulate the expression of sphingosine kinases (sphK1 and sphK2) leading to the production of sphingosine 1 phosphate (S1P). Conditional knock out of STAT3 in colonic epithelial cells in Stat3-IKO mice showed a decrease in the expression of sphK1 and sphK2, a decrease in the severity of inflammation and a delayed in tumor progression suggesting S1P, the product of sphK1 and sphK2, mediating inflammation induced tumor progression. Our preliminary data further suggest that the IL-6/STAT3/S1P pathway is differentially regulated in different human cell lines (Caucasian vs African American). The crosstalk between IL-6, STAT3 and sphingolipid regulated pathways may play an essential role in tumorigenesis and tumor progression in inflamed intestines.

MARM 232

CRISPR/Cas 9, a novel tool for site-specific gene targeting

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The creation of mutations in model organisms have been essential to elucidating the function of genes. Historically, such techniques have proven time consuming, labor intensive, and of low targeting efficiency when attempting to generate null mutations. In a short time, the CRISPR/Cas9 site-specific mutagenesis strategy has revolutionized how we generate mutants. It has been adopted for highly efficient gene targeting in zebrafish, plants, *Drosophila*, *C. elegans,* and many other model organisms. This workshop will detail how CRISPR/Cas9 works, its applications in model systems like *Drosophila melanogaster*, and speculate on future uses.

MARM 233

Surface water discharges of disinfection byproducts from wastewater treatment plant effluent under wet weather conditions

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Wastewater treatment plants in New York City are combined systems that treat the precipitation and runoff from wet weather events along with municipal wastewater flow. To protect surface water sources, the effluent is disinfected with chlorine before it is discharged into surface water. During disinfection, chlorine reacts with organic matter in the effluent, resulting in the formation of carcinogenic disinfection by-products (DBPs). If DBPs are present in the effluent, the general public can be exposed to these surface water contaminants through recreational use of the receiving waters. In particular, under wet weather conditions, the chlorine doses are increased to meet effluent regulations for bacterial counts, which may result in higher formation of DBPs. The objective of this work was to study the formation of regulated and emerging disinfection by-products in two wastewater treatment plant effluents under wet weather events. Wastewater effluent samples were collected and batch tests were conducted under different chlorination conditions (dose and contact time). Samples were collected at different time intervals from each test and analyzed for DBPs in the following groups: regulated species such as trihalomethanes (THMs) and haloacetic acids (HAAs) as well as species that are not currently regulated

including halogenated acetonitriles (HANs) and chlorinated solvents. Preliminary results from one wastewater treatment plant show that the dominant DBP species that form in disinfected wastewater are HAAs, which show higher concentrations at higher initial chlorine dose. However, HAA concentrations decrease with increasing chlorine contact time (>30 minutes), likely due to a reduction in residual chlorine. HANs and chlorinated solvents were also present and show similar results to HAAs at initial chlorine doses of 4 mg/L and 6 mg/L. However, at an initial chlorine dose of 8 mg/L, certain HAN and chlorinated solvent species increase with increasing chlorine contact time (>30 minutes), likely due to the excess chlorine and longer reaction time. These results as well as the results for other DBP species from a second wastewater treatment plant will be presented.

MARM 234

Validation and verification of model predictions for chemical releases in estuaries

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Predicting the transport, dispersion, and fate of reactive chemical releases in aquatic systems is challenging, especially in estuaries where physiochemical conditions change on fine spatial and temporal scales. These changes influence the partitioning of reactive constituents between the dissolved, colloidal, and particulate phases, determine chemical, physical, and biological degradation rates, and influence the cycling and distribution of reactive constituents between the water column and the sediments. The System for Hazard Assessment of Released Chemicals (SHARC) is an advanced waterborne hazard fate and transport modeling and analysis tool developed by Maritime Planning Associates (MPA). From 2011-2015, a series of SHARC validation and verification (V&V) studies were conducted in the tidal-fresh Potomac River in the vicinity of the Blue Plains Advanced Wastewater Pollution Control Plant (BPWPCP). For each V&V event, SHARC model simulations were run for timed point source inputs of waterborne agents of interest using the location of the BPWPCP effluent outfall. Constituents released into the tidal-fresh Potomac River from BPWPCP effluent were measured in the receiving waters and used as proxies for agents of interest to conduct V&V of SHARC model predictions. Results from these studies demonstrate that SHARC does an adequate job in predicting the chemical plume for semi-conservative constituents and potentially for more reactive constituents in this representative tidal-fresh estuary. Results also highlight areas for SHARC model improvement, such as better integration of high-resolution hydrographic & meteorological model data into SHARC and refinement of SHARC chemical fate algorithms to better quantify how variability in key water column parameters impacts the partitioning and fate of specific reactive constituents. These improvements can be implemented in follow-on V&V studies to advance the utility of SHARC as a waterborne hazard fate and transport modeling and analysis tool in dynamic estuarine systems.

MARM 235

Reaction of hexabromocyclododecane with reduced sulfur species in methanol/water solutions

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The individual degradation rates of the three dominant isomers (α, β, γ) of hexabromocyclododecane (HBCD) with bisulfide were investigated at pH 9 in methanol/water solutions at two different temperatures. α-HBCD was reacting significantly slower with bisulfide than β-HBCD and γ-HBCD. Reactions of HBCD with all three isomers were found to be faster at 40 °C than at 25 °C. The experiments were performed in 20% water/80% methanol, 50% water/50% methanol and 80% water/20% methanol at 40 °C. It is indicated that solvent can affect the reaction and the second order rate constants of HBCD with bisulfide are larger with higher amount of water in solution. The much slower reaction of α-HBCD compared to β-HBCD and γ-HBCD could potentially explain why α-HBCD is in general found at higher concentrations in biological samples.

MARM 236

Investigating the photodegradability of personal care product ingredients for aquatic environmental fate assessment

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The aquatic environmental fate of a non-biodegradable non-sunlight absorbing fragrance chemical, Pamplewood, was assessed through an investigation of its photodegradability. A sensitive and reliable quantitative LC-MS method was developed to study its photodegradation kinetics. Its indirect photolysis rates under various indoor and outdoor conditions were measured. Although the measured rates varied, they collectively indicate that Pamplewood is intrinsically photolabile. Results from quencher experiments revealed that hydroxyl radical was the main reactive intermediate responsible for the indirect photodegradation of Pamplewood with a half-life of about 18 days in sunlit surface water based on the experimentally determined second-order rate constant ($8.48 \pm 0.19 \times 10^9$ $M^{-1}s^{-1}$). Moreover, photoproducts of Pamplewood were studied by GC-MS and total organic carbon (TOC) analysis. Complete mineralization of Pamplewood was observed when it was reacted with hydroxyl radicals in an aqueous solution. This approach can be applied to assess the aquatic environmental fates of other non-biodegradable non-sunlight absorbing personal care products ingredients.

MARM 237

Occurrence of pyrethroid and organochlorine residues in human milk from Nadia, West Bengal, India

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Despite the fact that most organochlorine pesticides are banned and restricted for use in India, residues of these compounds continue to be present in the environment. However these chemicals are gradually being replaced by pyrethroids. The present study was carried out to understand the impact of this change on human exposure. Concentration of pesticides belonging to organochlorines, pyrethroids and neonicotinoids were measured in fifty six human milk samples collected from Nadia district, West Bengal, India during 2013–2014. Analysis was carried out with the help of GC-MS/MS and LC-MS/MS using modified Quecher's method. The method was evaluated for 25 pesticides and typical recovery was found in the range of 90±10 %. However no measurable concentrations of neonicotinoids were found in the breast milk samples while organochlorines and three synthetic pyrethroid were found to be present. Among the organochlorines analyzed, DDTs (21.67 ngg^{-1} w/w average value) were the predominant contaminants, followed by HCHs (14.71 ngg^{-1} w/w average value). Pyrethroids detected were bifenthrin,

lambda cyhalothrin and permethrin (average value 3.68, 3.55 and 2.05 ngg^{-1} w/w respectively). Daily intake estimation of nursing infants was calculated and compared with acceptable WHO/FAO levels. Estimated daily intake showed that infants were exposed to OCs to a greater extent, particularly HCHs and lambda cyhalothrin above the acceptable limit. By comparisons with previous studies, we found that the organochlorines particularly DDT and HCH concentrations decreased over the period of time. These results identify the pesticide that, for sustainable use, requires further monitoring and identification of sources. This is one of the first studies to report pyrethroid concentrations in human milk in this region of India.

MARM 238

Functional π-organogelators based on T-shaped phenazines

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Much attention has been paid to developing low molecular mass organogelators (LMOGs) based on π-conjugated molecules since their fibrillar structures possess excellent potential in optoelectronic applications such as aggregation-induced emission, field effect transistors, organic solar cells, conducting nanowires, energy transfer, etc. Vigorous research efforts have been focused on the development of various types of π-LMOGs. In many cases, π-π interactions between flat, large π-cores serve as a driving force for the assembly, with additional intermolecular forces such as van der Waals and hydrogen bonding to enhance the gelation ability. The primary goal of our research is to develop versatile π-LMOGs that can withstand further chemical modifications for electronic property modifications. Creating new π-LMOGs is nontrivial, however further structural derivatization without compromising gelation ability is even more challenging. We have successfully developed T-shaped π-LMOGs in which dialkoxyphenazine is orthogonally connected with phenylene ethynylene (T-NP) or dithiophene (TH-P). The dialkoxyphenazine core serves as a gelation promotor while orthogonal substituents modify the electronic properties. T-NP series showed excellent gelation ability upon peripheral substitution with nitro groups. The fibrillation and electronic properties of T-shaped LMOGs will be presented along with theoretical correlations. In particular, unusual photophysical properties of certain T-NP molecule will be discussed. Finally, we fabricated both bulk and planar heterojunction organic solar cells (OSCs) with TH-P and PCBM as an electron donor and acceptor, respectively. Detailed study about the fibrillation effect on the performance of small-molecule-based OSCs will also be presented.

MARM 239

Mechanogelation of fuel mixtures with a bioderived small molecule gellant

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The development of novel sustainable gel alternatives to current products and processes calls for a new approach to old gelation techniques. Though for centuries gels have been made through thermoreversible heating and cooling processes, thixotropic gel systems may lend themselves to be formulated via mechanical induction. This technique is a continuation of the previously demonstrated shear-induced gelation, which uses shaking to form a gel from a sol. As mechanochemistry is the growing field which demonstrates the utility of shear forces in altering covalent bonds, likewise mechanogelation will prove to demonstrate the function of shear forces in altering the conformations of gelator molecules by capitalizing on their non-covalent interactions to afford functional gels. Using traditional ball and vibratory milling

techniques the gelation of a low molecular weight gelator and biodiesel/diesel mixtures is shown to afford robust thixotropic gels in relatively short shearing times (as little as 15 minutes shearing with 1 day setting). Having synthesized the small molecule gelator from waste biodiesel and a functional biobased glucoside the methods and product follow several principles of green chemistry and engineering. Resultant gels are comparable to heated and cooled systems, and demonstrate similar rheology. This safe and low temperature method may be used to induce gelation through shearing with temperature sensitive systems or in instances in which high temperatures are not desirable. Resultant gels may be used as solid fuels that do not spill, in fuel spill remediation, or in engines which may be built to run on sustainable fuel alternatives.

MARM 240

Synthesis and characterization of carbohydrate-based small molecular organogelators and hydrogelators

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Carbohydrates are abundant and renewable natural resources; various carbohydrate derivatives have been found useful in producing new functional advanced soft materials or biologically active compounds. For the past several years, we have synthesized and studied many series of monosaccharide derivatives and obtained new classes of carbohydrate based low molecular weight gelators (LMWGs). These compounds form unique reversible supramolecular gels that are useful in biomedical research and as advanced functional materials. We have systematically studied their structures and self-assembling proeprties and obtained knowledge on the structure features leading to effective gelation in polar organic solvents and water. In the design of functional LMWGs and for obtaining useful supramolecular hydrogels, it is desirable if the gelator molecules contain additional triggered mechanisms other than being thermally responsive. We have incorporated photosensitive functional groups including photolabile, and polymerizable functional groups, as well as pH responsive functions in the gelator design. Our recent research progress on the study of novel D-glucose and D-glucosamine derivatives will be reported. Their potential applications as soft materials for controlled release drug delivery will also be discussed.

MARM 241

At the intersection of low molecular mass organogelators and polymers

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This talk will discuss research on low molecular mass organogelators (LMOGs) to demonstrate (1) the utility of polymer thermodynamics to understand the fundamental solution behavior of LMOGs and (2) the application of LMOGs as additives to generate functional polymer materials. In the first topic, the solution phase behavior of *R*-12-hydroxystearic acid (12-HSA) will be presented. It will be shown that the supramolecular polymerization or aggregation of the 12-HSA in the molten state when coupled with a standard regular solution model provides a framework to explain the exceptional gelation ability of this compound in numerous solvents compared to other fatty acids. The potential importance of molar volume and entropy of mixing as a design parameter for the generation of new LMOG will be emphasized. In the second topic, blends of LMOGs and elastomers will be presented. It will be shown that the formation of a solid, load bearing LMOG network is able to convert a simple elastomer into a shape memory polymer (SMP), which are useful stimuli responsive materials. In the SMP an elastic deformation of the polymer network can be held or fixed by the resistance of the LMOG network to the elastic recovery of the polymer network. Recovery of the initial shape is triggered by heating the SMP above the melting temperature of the LMOG network. The relationships between the shape memory behavior and the blend characteristics to optimize the design of SMPs will be discussed.

MARM 242

Understanding molecular nuances of self-assembly of sorbitol-based molecular gelators in various solvents

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Since molecular gels require a balance between contrasting parameters, it is no surprise that solvent and gelator chemistry play an integral role in determining the importance of the different molecular interactions and the natures of the nano- and supramolecular structures. Optimal gelation is achieved when the solvent and gelator are unable to establish strong interactions (i.e., H-bonding, electrostatic interactions, pi-pi stacking, dipole-dipole, and London dispersion forces) and the SAFiN is comprised of thin entangled fibres. However, the forces governing assembly are often confounding and complex. Systematically, we will examine the effect of modifying the chemical structure of the gelator and observing the changes in Hansen Space that is effectively gelled.

MARM 243

Gels through surfactant self-assembly and through the use of the hydrophobic effect

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We describe two classes of gels with specific technological implications. The first class is a nanostructured organo-hydrogel formed through the self-assembly of the anionic surfactant, dioctyl sodium sulfosuccinate (DOSS), the zwitterionic lipid, phosphatidylcholine (PC) and the nonionic surfactant, polyoxyethyelene sorbitan monooleate (Tween -80). These systems form a clear gel containing equal volumes of water and a hydrocarbon phase and show an ordered structure ranging from inverse hexagonal to sheet-like lamellar and multi-lamellar vesicle type morphologies. Characterizations based on the complementary techniques of small angle neutron scattering, NMR, and cryo electron microscopy, clearly indicate structural transitions and the coexistence of specific structures. The gels are positively buoyant on water, break down on contact with oil and release amphiphilic components that stabilize oil-water interfaces creating emulsions that are stable for extended periods. Such gel dispersants offer significant advantages over existing systems for mitigating the impact of oil spills. The second class of gels is based on the hydrophobic effect, where long chain alkyl groups attached to the backbone of a biopolymer (chitosan) insert themselves into lipid bilayers of liposomes and cells, into oil droplets, or attach to hydrophobic surfaces such as carbon nanotubes, graphenes and carbon microspheres. The phenomenon leads to a gelation of liposomes, carbon based materials, and oil droplets resulting in new applications in drug and vaccine delivery and energy and separations technologies.

MARM 244

Development of drug-like inhibitors of Nek2 kinase

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NIMA-related kinase 2 (Nek2), a serine/threonine kinase is involved in mitotic regulation. It has been shown that aberrant activity of Nek2 can promote chromosomal instability and aneuploidy, two primary causes of tumorigenesis. Recent data suggests that Nek2 is overabundant in a highly invasive form of human carcinoma, triple negative breast cancer (TNBC). Our laboratory has identified a non-toxic novel Nek2 pharmacophore using the first whole animal model, developed in Drosophila *melanogaster*. Using this pharmacophore, a small library of potential Nek2 inhibitor candidates have been synthesized and screened against recombinant human Nek2 kinase. Efforts are currently underway, guided by SAR and computational models, to identify a selective and highly potent inhibitor of Nek2 kinase.

MARM 245

Use of the QuEChERS approach in the extraction of pesticides from imported fresh fruits and vegetables

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The U. S. Environmental Protection Agency (EPA) registers the use of pesticides and establishes tolerances on the maximum amounts of residues that are permitted in both imported and domestic foods shipped in interstate commerce. Early methods and procedures for determining pesticide residues were based on classical elemental analysis, spectrophotometric, biochemical, and biological methods. During the 1950s and early 1960s, chromatographic methods were employed, with greater sensitivity and the capability of distinguishing residues within a given class. The QuEChERS (Quick, Easy, Cheap, Effective, Rugged, and Safe) procedure was introduced by Lahotay & Anastassiades (2003) and is currently routinely used in this endeavor. The method entails extracting the food sample with acetonitrile, partitioning with a mixture of sodium chloride (NaCl) and magnesium sulfate ($MgSO_4$), followed by a dispersive solid phase extraction (dispersive SPE) cleanup with primary-secondary amine sample prep easy (PSA SPE) sorbent. Base-sensitive compounds are treated with the Lahotay modified QuEChERS method, that uses1% acetic acid/ acetonitrile extraction, partitioning with sodium acetate and $MgSO_4$, followed by a dispersive SPE cleanup. The results of these analytical procedures will be presented with emphasis on the difficulties encountered and comparative data obtained from various sources of the same food.

MARM 246

Use native plants/oils to synthesize novel antimicrobial surfaces

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In order to maintain a sterile environment and protect patients in a clinical setting from microorganisms can be a challenge. Previous research has been conducted where creating antimicrobial surfaces could minimize the growth of microorganisms e.g. bacteria, fungi, viruses. Challenges faced throughout the process of creating these surfaces include difficulty to industrialize, non-uniformity throughout the surface, and activity of the antimicrobial agent being lost by wiping off a given surface. Gelatin B are

peptides and proteins produced by partial hydrolysis of collagen extracted from the skin, bones, and connective tissues of animals, its molecular weight affects its viscosity, gel strength and other properties, such as emulsion stabilization, by also destroying certain chemical cross linkages present in collagen, the part of the connective tissue that in the skin helps in firmness, suppleness and constant renewal of skin cells. Beeswax is a product made from the honeycomb of the honeybee containing antibacterial properties, helping keep skin clean and reducing the risks of contamination and inhibited the growth of bacteria and fungus. Our work involves the utilization of Gelatin B and beeswax to incorporate and fuse with plants essentials oils in varying concentrations. Oils include: sage, thyme, Neem seed, yarrow, Propolis, black elderberry, ginger, turmeric, rosehip, Tamanu, dragon blood, and key lime. These new surfaces are tested against gram positive and gram negative bacteria.

MARM 247

Determining the total amount of oxygen consumption in effluent via carbonaceous biochemical oxygen demand (CBOD) and biochemical oxygen demand (BOD)

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Water from showers, rain, melted snow, and sidewalk washing travels into a whole new world through the remarkable systems of pipes in the New York's City sewer system, DEP (Department of Environmental Protection). The DEP is a wastewater treatment plants that removes most of the pollutants from wastewater before being released. One of the most commonly measured constituents of wastewater is the biochemical oxygen demand (BOD) defined as the amount of dissolved oxygen required for aerobic microorganisms (found in sewage) to decompose the organic matter in the wastewater. This value measures the degree of pollutant by identifying the decrease of dissolved oxygen the bacteria used to survive and consume the waste. If more oxygen is consumed than produced, DO (dissolved oxygen) will decrease and some aquatic life forms will weaken, migrate to a different location, or die. This test is used by government agencies to determine how efficient plants are and how effluent (released water from treatment plant) will affect receiving water. Carbonaceous biochemical oxygen demand (CBOD) follows the same procedure as BOD but the nitrifying bacteria in the sample are inhibited. Nitrifying bacteria consume nitrogenous materials (compounds with reduced forms of nitrogen) and add to the oxygen demand of the wastewater. Methods and procedures will be presented along with the importance of testing BOD/CBOD in the wastewater treatment facility.

MARM 248

ArcGis: Understanding city-wide infrastructural landscape and its environmental impact

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ArcGis (Geographic Information System) is a city's inter-agency mapping system used in Department of Environmental Protection for mapping standards. With the use of this system, DEP's Shoreline Survey Unit within the Compliance Monitoring Section (CMS) continues to verify and update the survey of the

nine basin areas. This procedure is conducted by comparing the print version of the existing positions of the discharge overflows, outfalls and all underlying connections against the existing system. The update to the system is performed manually and overrides all existing points that other agency uses. The survey of the nine basin areas resulted in the identification of 3,429 outfalls. The outfalls consist of 337 combined sewer overflow outfalls, 1,977 direct discharge outfalls, 118 general outfalls, 803 highway outfalls, 152 storm outfalls and 42 SPDES permitted outfalls. In identifying, updating and rectifying the sewer, sanitary, and combined connections the Department of Environmental Protection-Compliance Monitoring Section (DEP-CMS) uses a proprietary mapping system ArcGis to also enhance communication and management of the physical locations and classifications of the outfall size to the citywide officials for emergency and day-to-day operational management. Details for each individual process will be provided.

MARM 249

Investigation of *S*-oxidation of *m*- and *p*-substituted 2-phenyl-3-aryl-1,3-thiazolidin-4-ones with Oxone®

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S-oxidation of *m*- and *p*-substituted 2-phenyl-3-aryl-1,3-thiazolidin-4-ones with Oxone® was investigated. For all compounds evaluated, selective oxidation to the sulfoxide was realized using 3 equivalents of Oxone® at room temperature. Alternatively, the sulfone was prepared at high temperature by increasing the equivalents of Oxone® used; the extent of sulfone formation was affected by the substituent of the 3-aryl ring. The selectivity of the high temperature oxidation (the ratio of the sulfone to sulfoxide) was quantified by ^{1}H NMR.

MARM 250

A new synthesis of pyrroles using the Cadogan approach

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The Cadogan-Sundberg synthesis of indoles and carbazoles involves deoxygenation/cyclization of *o*-nitrostyrenes or *o*-nitrostilbenes with trialkyl phosphite. For example, 2-nitrostyrenes (nitro group on the benzene ring) and β-nitrostyrenes (nitro group on the alkene) are converted to indoles and 2-nitrobiphenyls to carbazoles using a reducing agent which produces either a nitrene or a nitroso intermediate. Triethylphosphite was the agent Cadogan discovered and Sundberg was responsible for the use of carbon monoxide with a Palladium catalyst (e.g. $Pd(OAc)_2$). The former is the simplest: one dissolves the nitro compound in triethylphosphite and refluxes the mixture until the starting material is consumed – usually within 2-24 hrs. This method of indole synthesis is similar to that of the Leimgruber-Batcho approach except there is no need to prepare a dinitrostyrene before reduction, thus avoiding an extra step. The aim of this research project is to investigate if the available methods of preparing indoles and carbazoles from nitro compounds are in fact applicable to the synthesis of pyrroles.

MARM 251

Macroporous TiO_2 photoanodes for high-efficiency PSI-based biohybrid photovoltaics

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Photosystem I (PSI) is a protein complex residing within chloroplast of photosynthetic organisms. It is being studied as a candidate for dye-sensitized solar cell (DSSC) because it converts solar radiation to electrons with near-unity internal quantum efficiency. One of the obstacles that hinder PSI from being a more widely used dye is its large size. It is difficult to get sufficient PSI loaded throughout the photoanode of DSSC, a layer of titania (TiO_2) nanoparticle coating, because the regular titania coating is mesoporous (pore size less than 50 nm). This presentation focuses on designing macroporous titania coatings with pore size as large as 1000 nm so that integration between titania coating and PSI would be enhanced. Sacrificial templating technique is employed to incorporate porosity into titania paste using oil-in-water emulsion and polystyrene latex as templating materials. The templated titania paste has been made directly from titanium dioxide powder. Then a titania coating has been produced on fluorine doped tin oxide (FTO) glass by doctor blading. The resulting coatings are uniform and crack-free. Scanning electron microscopy shows that the templated titania coatings have high porosity and interconnected meso and macro pores. They also demonstrate increased absorbance of PSI according to UV-Vis photospectroscopy. According to electrochemical analysis, using the designed macroporous TiO_2 film as a photoanode largely enhances the overall power and efficiency of PSI-based biohybrid photovoltaics due to the high integration of PSI and TiO_2.

MARM 252

Slp1 is a key component controlling early cardiogenesis in *Drosophila*

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Heart formation is very important in all organisms. Any abnormality during the process can affect the morphology and function of the heart, causing congenital heart defects. Therefore, the study of heart development may be beneficial to the prevention and therapy of human heart disease. Here we use Drosophila as an animal model to study heart formation. The structure of Drosophila heart is much simpler than the mammalian heart, but the transcriptional gene network is highly conserved between both organisms. BMP (Dpp) and Wnt (Wg) signaling induce specification of heart precursors from dorsal mesoderm. These two factors induce heart-specific genes, such as Tinman (Tin) and Dorsocross (Doc). Mutations in *sloppy-paired-1* (*slp1*), a gene required for proper segmentation during early stages of Drosophila embryogenesis also affect heart development, but the specific role has not yet been fully defined. Slp1, a member of the Forkhead family of transcription factors, represses expression of non-heart genes such as *bagpipe* (*bap*) (Lee & Frasch, Development, 2000), but it is not known whether Slp1 also regulates expression of heart-specific genes. We investigate the role of Slp1 by analyzing *slp1* mutant embryos using *in situ* hybridization (ISH) with heart (*doc1*), dorsal mesoderm (*tin*), and *wg*probes. Our data suggest Slp1 regulates the expression of *doc1* through *wg*. These results provide further evidence that *slp1* plays a key role in cell fate determination in heart development and lay groundwork for further studies on this process.

MARM 253

New modes of initiating cation radical cycloaddition dimerization and polymerization reactions

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We are reinvestigating the work of Bauld and coworkers with respect to cation radical cycloaddition polymerization and dimerization. Bauld's most easily oxidized monomers provide suitable substrates for testing our group's novel photochromic photooxidants' abilities to gate sensitivity to photoinduced charge transfer initiation of cation radical reactions of materials interest. Photochromes with long wavelength isomers (LW) capable of acting as photooxidants but with short wavelength isomers (SW) less capable of doing so are sought. This necessitates photochromes that revert only thermally and that have excited state reduction potentials that are more positive for LW than for SW. For instance, N-3-bis(*trans*-1-propenyl)carbazole should be able to be photooxidized by the long-wavelength isomer of our quinazolinespirohexadienone photochrome. Revised syntheses of Bauld's monomers and a comparative study of their initiation by chemical oxidants, direct electrochemical oxidation, conventional photooxidants and our novel photochromic photooxidants is underway.

MARM 254

Molecular encapsulation of sugar alcohols by arylamide foldamers: A computational chemistry study

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Recognition of sugars is one of the most challenging problems in host-guest chemistry, due to their subtle but consequential structural differences. We have developed computational tools to aid the design of molecular receptors selective for a variety of sugars and their derivatives. The poster will present the results of molecular dynamics (MD) simulations of foldamer encapsulated linear sugar alcohols. We focus on arylamide foldamer capsules, recently shown to encapsulate sugars with unprecedented selectivity and high affinity. For such foldamers, we have used MD simulations with appropriately modified torsional parameters to predict the needed sequence length, and thus the capsule cavity size appropriate for capturing the desired sugar alcohols. We will also present MD-derived conformations of encapsulated sugar alcohols and their interactions with the inner capsule wall.

MARM 255

Treatment of wastewater samples at the New York City-Department of Environmental Protection (NYC-DEP)

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The New York City Department of Environmental Protection (NYC-DEP) is responsible for cleaning the wastewater and protecting the environment in New York City. The Newtown Creek wastewater treatment plant in Brooklyn tests the treated wastewater from all 14 plants every day via its chemistry and microbiology research laboratories. When samples arrive in the lab they are separated into four different groups – acidified, non-acidified, processed solids and total solids. After they are tested for their pH value samples are composited according to an established flow sheet. Details of this procedure and examples of cases encountered daily will be described. The difference in the processing of Total Suspended Solids (TSS) and Total Solids (TS) using primary and secondary digesters that reduce the degree of pathogens during treatment will also be highlighted.

MARM 256

Exploring the formation of conglomerates for optical resolution

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The resolution of optical isomers by Louis Pasteur provided insight to a fundamental principle in organic chemistry. Chirality, or handedness, is an important consideration in chemistry with applications in medicines, separations, materials, biochemistry, and so on. An alternative to Pasteur's classical resolution is preferential crystallization of an enantiomer from a racemic mixture. One requirement for this is the formation of conglomerates. It has been previously reported that 2, 3-Bis-fluoren-9-ylidenesuccinic acid can be resolved into conglomerates. In our study, performed the synthesis of diethyl 2, 3-bis(fluorenylidene)succinate and investigate its ability to form homochiral inclusion crystals. This study will consist of two phases. In the first phase, the diester will be synthesized and its structure will be confirmed by NMR, MS and IR. During the second phase, the formed crystals will be tested for their enantiomeric purity.

MARM 257

Performance of a magnetic shape memory micropump

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Solid-state micropumps have constituted a promising market for point of care diagnostics, biomedical research and lab-on-a-chip test devices. Magnetic shape memory (MSM) alloy Ni-Mn-Ga elements have several desirable properties that make them attractive candidates for solid-state micropumps. Ni-Mn-Ga changes shape by up to 6% when exposed to a magnetic field. In this study, we constructed a micropump using a Ni-Mn-Ga MSM element, which was actuated by the magnetic field of a rotating diametrically magnetized cylindrical magnet. The magnetic field created a cavity on the MSM element which moved along the length of the MSM element and transported fluid. The MSM micropump successfully transported a drop of water from the fluid inlet to the outlet. We also observed multiple cracks form on the MSM element. Scanning Electron Microscope images of MSM element fracture surface exhibit ripples which may correlate with twins.

MARM 258

Degradation of an azo dye by single-walled carbon nanotube-ruthenium nanoparticles composites

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The integration of carbon nanotubes with nanoparticles into hybrid structures often possess unique structural and catalytic properties that are not available to the respective components alone, and thus, have been envisioned for many applications. Azo dyes are often used in textile industries which are lost in waste water during the dyeing procedure and causes great threats to aquatic life. Herein, a comparative study of the catalytic degradation of Congo red dye by single walled carbon nanotubes-ruthenium nanoparticle composites was performed. The composites catalytic properties were characterized by UV-Vis Spectroscopy.

MARM 259

Synthesis of a fluorenyl quinolone molecular switch

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Properly functionalized dithienylethenes show promise for light-induced switching processes. However, Cis-trans isomerization is known to compete with 6 π-electron ring closure, to prevent this competition, the ethane segment is usually combined in a (perfluorinated) cyclopentene. The focus of our research was the synthesis of perhydrocyclopentene (4), which serves as a suitable for large-scale alteration. Further functionalization of this compound is possible due to the chloro group, which is located at the 5-position of the thiophene rings. The chloro group was coupled to a p-type material (2,7-(bispinacolato diboron) fluorene) via Suzuki reactions for 24hrs. Next, it was coupled to a 8-quinolyl ligand.

MARM 260

Synthesis and photorelease study of glycine caged bis-1,2-(4-acetylphenylethynyl)-4,5-dimethoxybenzene, first-generation dendron phototrigger

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Glycine caged bis-1,2(4-acetylphenylethynyl)-4,5-dimethoxybenzene, the dendritic photoactive compound is synthesized for photo release study of the model drug. The terminal functionality of dendron, (1,2 dimethoxy benzene) provides the platform for connecting drug and targeting to molecules and the photo-trigger 1-(4 Ethynylphenyl)-ethanone, a cleavable linker which keep the drug carrier inactive until the light are absorbed. Once it's absorbed the proper light it releases the therapeutic drug through photocleavage of the anchor bond. The NMR spectra of the photoreaction shows the drug being released and the computational study before and during the synthesis supports the release mechanism based on the optimized molecular geometries and frontier orbitals of the different moieties of the caged dendron.

MARM 261

Aggregation propensity of (F ® L) mutants of hIAPP$_{22\text{-}29}$

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Amilyn, a 37 amino acid residue peptide, is co-secreted with insulin to control blood sugar levels in the body. Amyloid fiber formation has been linked to playing a significant role in Type 2 diabetes. A number of investigation aims to unravel the mechanism that triggers and propels amyloid formation. It has been speculated that the aromatic residues play an important role in the formation of amyloid fibers. We hypothesize that while aromatic rings play a role in amyloidogenesis, its absence does not necessarily prevent amyloid formation. We also hypothesized that the amylogenic propensity of the leucine mutants will depend on the structure of the leucine derivatives. To prove our points we prepared several mutants of NFGAILSS (hIAPP22-29), where the phenylalanine has been replaced by leucine or its derivatives (normal leucine, isoleucine and *tert*-leucine). The short peptide, hIAPP22-29, is derived from the 37 residue amyloid and is believed to be directly involved in amyloidogenesis. Phenylalanine and leucine (as well as its derivatives) share the same characteristics of being non-polar and have very similar hydrophobicity but they differ in that phenylalanine has an aromatic ring. We compared the behavior of our hIAPP22-29 mutants to the wild type using: turbidity or scattering measurements to detect opacity of the samples; circular dichroism (CD) to monitor changes in secondary structure; Raman and IR to further clarify whether they form parallel or antiparallel conformations; and TEM to see the fiber morphology. Results indicate that leucine mutant in general aggregated slower than the wild type which contains phenylalanine. Further, only mutants containing leucine or normal leucine forms aggregate while the iso- and tert-leucine do not. This led us to believe that a bulky group on the β-carbon, like in iso- and tert-leucine, appears to prevent aggregate formation. Results will be analyzed in terms of its mechanistic implications on the aggregation process.

MARM 262

Energy of the quasi-free electron in H_2, D_2 and O_2: Probing intermolecular potentials within the local Wigner-Seitz model

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We present for the first time the quasi-free electron energy $V_0(\rho)$ for H_2, D_2 and O_2 from gas to liquid densities, on noncritical isotherms and on a near critical isotherm in each fluid. These data illustrate the ability of field enhanced photoemission (FEP) to determine $V_0(\rho)$ accurately in strongly optically absorbing fluids (e.g., O_2) and fluids with extremely low critical temperatures (e.g., H_2 and D_2). We also show that the isotropic local Wigner-Seitz model for $V_0(\rho)$ – when coupled with thermodynamic data for the fluid – can yield optimized parameters for intermolecular potentials, as well as zero kinetic energy electron scattering lengths. *Acknowledgments: All measurements were performed at the University of Wisconsin Synchrotron Radiation Center, a facility that was primarily funded by the University of Wisconsin – Madison with supplemental support from facility Users and the University of Wisconsin – Milwaukee. This work was supported by a grant from the National Science Foundation (NSF CHE-0956719).*

MARM 263

Adenosine/guanosine preferring nucleoside ribohydrolase: From flavonoids to fragments

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Trichomoniasis, caused by the parasitic protozoan *Trichomonas vaginalis,* is the most prevalent, non-viral sexually transmitted disease. The parasite has shown increasing resistance to the current 5-nitroimidazole therapies indicating the need for new therapies with different mechanisms. Since *T. vaginalis* is unable to synthesize purine and pyrimidine rings *de novo*, it relies on salvage pathway enzymes such as adenosine/guanosine preferring nucleoside ribohydrolase (AGNH). The NIH clinical collection was screened for inhibitors of AGNH using ^{1}H NMR to monitor substrate hydrolysis. Five inhibitors that belong to a class of compounds known as flavonoids were discovered with IC_{50} values less than 10 μM. This finding validates AGNH as a druggable target. However, the flavonoids are poor starting points for drug design since they have relatively low ligand efficiencies. A fragment based approach might circumvent this limitation and lead to compounds better optimized for the ribose and nucleobase binding sites. The identification of several smaller fragments of the flavonoids that retain activity and have higher ligand efficiencies indicates the potential of a fragment-based drug design approach. This poster will describe our results to date and outline our project path plans.

MARM 264

An exploration of polycarbonate-diluent systems via FFCNMR

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Over the past century, advances in electronics and electrical components have led the way to some of the most advanced technology present today. With an ever increasing demand for advanced electrical components to match the needs of industrial and public interests, research on materials fit for such purposes is at the forefront of material science. Advances in dielectric materials are one example of highly sought research in this field, and methods of research vary in power and utility. Common techniques are dielectric relaxation measurements and NMR (Nuclear Magnetic Resonance) spectroscopy. A proposed method of study is the use of an NMR technique, in which the magnetic field is varied through the experiment, called fast field cycling (FFCNMR). Through this technique, the reaction of materials to external magnetic fields can be probed at a wide range of both field strengths and temperatures. This grants insight into the molecular activities of materials, which further allows for empirical prediction of their behaviour under varying environmental conditions. Polycarbonate is a well received and widely used polymer in industrial and manufacturing applications. It is also of potential interest as a high energy and power density dielectric for thin film capacitors. The effect of additives on polycarbonate can thoroughly be studied via FFCNMR. In this particular research, the addition of the diluents 2-Adamantanone and 1-Adamantanecarbonitrile to pure Polycarbonate are studied in field strengths varying from 0.8MHz (relative to protons) to 35MHz, from temperatures of -100 to 155°C. It is surmised that the diluents facilitate polymer structural mobility in such a way as to enhance the dielectric properties. FFCNMR provides a powerful means to investigate the extent and nature of the polymer chain dynamics.

MARM 265

Fabrication of core-shell, transition metal nanowires as catalysts for glucose sensors

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Over 9.3% of the U.S. Population suffers from Diabetes Mellitus. Therapy relies on accurate determination of serum glucose levels. There has been a recent interest in developing enzyme-free sensors for measuring blood glucose concentration because they are more robust and easier to produce than sensors based on the glucose oxidase enzyme. Current limitations of enzyme-free detectors are their dependence on expensive platinum (Pt) metal and their low selectivity for glucose among other species such as urea and amino acids in biological fluids. To overcome existing limitations, we have designed a new class of electrocatalysts consisting of inexpensive transition metal cores coated with precious metal shells for the glucose oxidation reaction. The proposed sensing platform is designed to increase cost-effectiveness since the precious metal content is localized only at the catalytic interface. Transition metal nanowires were created using an ambient, solution-based method, allowing for control of both wire composition and aspect ratio. We have also successfully developed approaches to deposit thin precious metal shells on the surface of the transition metal nanowires with control over the composition and thickness of the shell. Our synthetic methods allow us to tune the composition and structure of the catalytically active surface sites, which we expect will allow for higher overall catalytic activity and selectivity for glucose.

MARM 266

Determining secondary structure and binding capacity for small molecules of cartilage oligomeric matrix protein constructs for the treatment of osteoarthritis

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Osteoarthritis (OA), a degenerative joint condition, can be attributed most commonly to traumatic injuries and degradation due to age. Symptoms arise in response to the thinning of articular cartilage between bones, caused by the chondrocytes' imbalance between synthesis and degradation of extracellular matrix (ECM) components, resulting in a decrease of the synovial fluid's viscosity and therefore an increased chance of the bones grinding against one another. The degradation of the cartilage ECM can be directly linked to the small molecule, all-*trans* retinoic acid (ATRA), indicated by significantly high levels present in the synovial fluid of OA affected joints. ATRA is capable of upregulating the expression of matrix metalloproteinase-13 (MMP-13), in addition to downregulating the expression of collagen type II. The effects of ATRA on the joints can be inhibited by BMS493, a pan-retinoic acid receptor inverse agonist. However, free BMS493 can be easily degraded and hence presumably has rapid clearance in physiological conditions. Moreover, BMS493 has low solubility in aqueous buffers. Therefore, the coiled-coil motif of cartilage oligomeric matrix protein (COMPcc), a non-collagenous glycoprotein biomaterial, is proposed to be used as a drug delivery vehicle herein. COMPcc self-assembles into a homopentamer possessing a hydrophobic cavity which been reported to bind to several hydrophobic ligands, such as vitamin A, vitamin D_3, ATRA and curcumin (CCM), and thus is anticipated to be able to encapsulate BMS493. As BMS493 does not exhibit fluorescence properties, we perform a competition assay with BMS493 and curcumin-bound COMPcc to determine its binding capacity and molecular configuration in the presence of the small molecules.

MARM 267

Transition metal-based, core-shell nanowire electrocatalysts for cost-effective fuel cells

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The main goal in this research project is to develop new and more cost-effective catalysts for Polymer Electrolyte Membrane Fuel Cells (PEMFCs). PEMFCs are promising devices for power generation with low environmental impact because they use hydrogen gas as its fuel and produce water as its only byproduct. The hydrogen oxidation reaction (HOR) and the oxygen reduction reaction (ORR) are catalyzed by platinum or other precious metal nanoparticles supported on carbon catalysts. However, high catalyst and precious metal loadings are required because of slow reaction kinetics and poor long-term durability. Recent reports have shown that one-dimensional and core-shell nanostructures are significantly better catalysts for fuel cells. Aiming to further reduce the high costs of platinum catalysts, first-row transition metals will be used as inexpensive core materials on which we have deposited thin precious metal layers. The target core-shell nanowires are synthesized by an efficient method that is beneficial because it employs green chemistry, relies on non-toxic solvents and is performed under ambient conditions. We expect that tuning the size and composition of the core and the thickness and composition of the shell will allow us to produce a highly active fuel cell catalysts with low platinum loadings.

MARM 268

Methodology testing on complex substrate, ethisterone

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Various methodology to functionalize alkynes involving iron (III) and gold (III) catalysts are currently in development in our lab. The substrate scope of the methodology will be expanded to include more complex alkynes, beginning with the progestin, ethisterone, which consists of a fused ring system with various substituents. In order to prevent the interference of the substituents with the desired alkyne functionalization reaction, countermeasures must be taken such as acetylation of the propargyl alcohol. Successful functionalization of ethisterone will allow access to many of its analogs, opening the opportunity to screen for any changes in biological activity and study of its mechanism of action.

MARM 269

The purification and analysis of distinct porphyrin molecules

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The goal of this research is to purify the meso-substituted isomers of p-anisaldehyde, p-tolualdehyde and p-pyridinecarboxaldehyde porphyrins that are synthesized by a modified Adler method. These compounds are separated using column chromatography. Different silica gel and chloroform/methanol mixtures were used based on the type of porphyrin being purified. For the tolyl and methoxy porphyrins, a 60Å mesh silica size was used. The tetra-tolyl porphyrin separated with 100% chloroform, while the tri tolyl porphyrin used a 5% methanol/chloroform mixture. The tetra-methoxy was obtained with 100% chloroform and the tri methoxy porphyrin required a 2% methanol/chloroform mixture. The silica used for pyridine porphyrin was a 150Å mesh. The tetra pyridine was obtained with 100% chloroform and the

mono-pyridine porphyrin required a 2% methanol/chloroform mixture. Purity was tested by TLC, UV-Vis, and NMR. For the tolyl porphyrin, the average percent yield was calculated to be 5%. The methoxy porphyrin average percent yield was 4.77%. The pyridine porphyrin average yield was 5.4%. These molecules will be incorporated into liposome carriers for use in the destruction of cancer cells.

MARM 270

The infrared optical measurements of hyperbolic metamaterials

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Metamaterials are artificial structures that are used to obtain unique optical properties. The Law group focuses on metamaterials in the Infrared. We grow Indium- Arsenide (InAs) metamaterial samples using molecular beam epitaxy. The doping density and fill factor of the InAs samples varied allowing us to tune the optical properties. The samples were measured using Fourier Transform Infrared Spectroscopy (FT-IR). FT-IR enables us to obtain reflection, transmission, and absorption properties of our samples. We were also able to test for negative reflection. We observed metamaterial behavior in our samples in reflection, and transmission. We tested our samples through negative refraction test which shows light bending backwards. This is conclusive evidence that our samples are acting as hyperbolic metamaterials. In the future we will tune the optical properties by adjusting the sample structural properties. In future we will continue to develop our metamaterial that can lead to revolutionary improvements in biomedical imaging and engineering, as well as cloaking.

MARM 271

Development of cathepsin S inhibitors using Ugi reaction

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Cysteine Cathepsin S (CatS) of the Clan C1 cysteine proteases is a lysosomal protease that has been found to be expressed in the cells of the auto-immune system, such as macrophages, B cells, and dendritic cells. Cystein cathepsins degrade biological molecules not only intracellularly but extracellularly as well. Out of the 11 cysteine cathepsins that have been discovered, Cathepsin S (Cat S) is a dominant member which can function in a wider pH range. The aberrant over expression of CatS in the Homo sapiens has been linked to a variety of diseases associated with an elevated immune response. As a result, by making use of targeted inhibition of CatS, much benefit could be gained in treating diseases such as asthma, and emphysema. In this investigation a small library of compounds were synthesized by making use of the Ugi Four-Component Reaction. Ugi-4CR, while having its economic and ecofriendly advantages can prove as a successful synthetic methodology. The synthesized library is currently being screened against recombinant CatS, and it is anticipated that a highly potent and selective CatS inhibitor will emerge from this study. Aisha Ashfaq and David Salazar are participants in the NIH Bridges to the Baccalaureate Program at Queensborough Community College.

MARM 272

Cytotoxic and cytostatic effects of single-walled carbon nanotubes on triple-negative breast cancer cells

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Single-walled carbon nanotubes (SWCNTs) are sp^2 hybridized carbon structures that possess unique chemical and physical properties. Since their identification in 1991, numerous biomedical applications including drug delivery and photodynamic therapy have been proposed. However, the data on cytotoxic effects of unfunctionalized single walled carbon nanotubes varies with exposure time and cell type as well as other variables. In this study we used the triple negative breast cancer cell line, 468 to investigate the cytotoxic and cytostatic effects of SWCNT treatment. Triple negative breast cancer cells serve as a model to study triple negative breast cancer, a disease in the treatment options are limited due to a lack of cell surface hormonal receptors. Therefore there is a great need for novel therapies including carbon nanotube based therapies. Several assays were employed namely trypan blue exclusion assay to (determine the number of viable cells), MTT, a colorimetric assay to (assess cell metabolic activity) and Hoechst nuclear staining (an indicator for apoptotic cell death). Our trypan blue data revealed little to no effect on cell viability in concentrations 2.5-200 µg after a 24 hour exposure. The MTT results show that cell viability decreases at concentrations as low as 2.5 µg suggesting an effect on the aerobic respiratory metabolism. Further Hoechst staining indicates an increase in apoptotic death. The results show that although the trypan blue assays show little or no effect on cytotoxicity, SWCNT treatment may be affecting 468 metabolic pathways. Further studies will investigate the changes in 468 cellular oxidative stress after single walled carbon nanotube treatment.

MARM 273

Tracing marine particulate organic carbon from primary production to sedimentation

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Phytoplankton are primary producers of oceanic organic carbon, most of which is recycled back to CO_2 as their detritus sinks down the water column. A small fraction of organic carbon, however, persists and is ultimately buried in marine sediments. This sedimentary carbon sink is a crucial mode of removal of CO_2 from the atmosphere. Many previous studies have shed light on the chemical composition of dissolved organic carbon. Far fewer studies have examined the chemistry of particulate organic matter (POM) in the oceans, due to the analytical complexity of measuring heterogeneous environmental solids. We seek to analyze the chemical composition of POM that persists to sedimentation. Using Attenuated Total Reflectance-Fourier Transform Infrared Spectroscopy (ATR-FTIR), we analyzed fresh phytoplankton, partially degraded phytoplankton, and highly degraded sedimentary particles to trace the fate of particulate organic carbon from primary production through sedimentation. We examined isolated membranes of different phytoplankton species, including the coccolithophore *Emiliana huxleyi*, the diatom *Thalassiosira* sp., and the green alga *Tetraselmis* sp. We also analyzed *Tetraselmis* membranes that had been subjected to a range of oxidative treatments, as a representation of partially degraded phytoplankton. Sediment trap samples from deep in the water column of the Arabian Sea provided an endmember for highly degraded oceanic particulates.

The ATR-FTIR spectra reveal a variety of organic carbon functionalities in fresh phytoplankton, some of which are affected by the introduction of oxidants. An aromatic peak around 3013 cm^{-1} appears in fresh samples of *E. huxleyi* and *Tetraselmis* sp. This peak persists after H_2O_2 oxidation of *Tetraselmis* but

disappears upon NaOCl treatment. Alkane C-H peaks at 2800 to 3000 cm^{-1} and 1400 cm^{-1} to 1450 cm^{-1} also decrease in intensity with the introduction of oxidants. Sediment samples show few organic carbon functionalities, with only small alkane and protein peaks (amide I and amide II, at approximately 1650 cm^{-1} and 1550 cm^{-1}, respectively) remaining. These likely represent remnants of cellular glycoproteins that persist through the degradation process and are destined for burial in the sediment.

MARM 274

Atomic force microscopy measurements of single-walled, carbon-nanotube treated MDA-MB 468 cells

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Biomedical applications of single walled carbon nanotubes (SWCNT) have the potential to expand treatment options for cancer patients. However biosafety studies are currently inconclusive. These studies have been limited by technical issues related to the hydrophobic nature of the nanotubes. The diameter (1.5 nm) of the nanotube should allow passage through cellular gap junctions and ion channels but aggregation of the nanotubes in aqueous solutions decreases cellular uptake in *in vitro* studies. These carbon rich structures could be associating with and adversely affecting cellular components. Coating single walled carbon nanotubes with collagen has been shown to facilitate cellular uptake thus allowing for such intracellular associations to be investigated. In this study, MDA-MB 468 cells were treated with collagen coated SWCNT. Atomic Force Microscopy was used to measure the Young's modulus of the cells. Young's modulus indicates the degree of flexibility which in turn can be correlated with changes in the actin cytoskeleton. Actin cytoskeletal rearrangement is a key event in the metastatic process. The results suggest differences in the measures and therefore collagen coated single walled carbon nanotubes treatment may be affecting the cytoskeleton of these cells. Future studies will expand the investigation to include other types of cancer cells as well noncancerous cells and may reveal potentially novel cancer treatments.

MARM 275

Reactivity of vanadium and molybdenum oxide species on oxide supports in microwave assisted gas-phase oxidation of 3-picoline

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Silica- and titania-supported vanadium oxide binary and promoted with molybdenum oxide tertiary catalysts as well as the individual oxides were studied in synthesis of an important product and a valuable vitamin nicotinic acid by heterogeneous vapor phase oxidation of 3-picoline in presence of oxygen, nitrogen, and water at the temperature in the reactor about 250°C. Two sources of energy were used to heat the reactor: classical conventional and microwave. Microwave dielectric heating application made a positive contribution to the catalytic systems by increasing the selectivity for nicotinic acid and decreasing energy consumption. The highest specific activity and selectivity for nicotinic acid were discovered when microwave energy was applied to individual vanadium oxide as a catalyst. By using conventional energy, vanadium oxide was the least active and selective. Molybdenum oxide was found to

be a good promoter when it was present in a catalyst at the concentrations much lower than the concentration of vanadium oxide.
All effects are discussed with regard to the molecular structure, dispersion, and microwave absorbance ability of the studied catalysts.

MARM 276

Characterization of the putatively heterodimeric proteinaceous ichthyotoxin of *Pterois volitans*

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The growth in applications of the field of toxicology has increased interest in researching the components and mechanisms of venoms. A type of lionfish, *Pterois volitans*, contains a venom that causes intense pain, fever, and swelling in humans and is composed of a proteinaceous toxin with α and β-subunits. The symptoms may be due to an increase in intracellular calcium ion concentrations, which could suggest potential pore-forming properties in the *P. volitans* toxin, also found in stonefish toxin. The amino acid sequence of the *P. volitans* toxin has been derived; however, the quaternary structure of the protein toxin has yet to be characterized. Understanding the structure of the toxin will provide clues as to the mechanism of toxicity. The process of characterizing of the proteinaceous toxin of *P. volitans* has commenced with extraction and partial purification of the toxin, assessment of pore-formation using the liposome assay, and biophysical analysis of the toxin under varying conditions. The confirmation of pore-forming properties along with a detailed structure of the protein toxin will provide insight as to the role of the protein structure in the process of toxicity and reveal any correlations between the symptoms the toxin causes and the effect of the toxin on cells. Future research would involve crystallization of the toxin to determine the structure. The research could also lead to medical applications in the form of an antivenom, medicinal delivery system, or cell-specific lysis treatment.

MARM 277

New complexes of mes-BIAN in vanadium chemistry

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Bis(imino)acenaphthenes (BIAN) are a useful class of sterically demanding and structurally rigid α-diimine ligands. To-date, a large number of interesting BIAN complexes of late transition metal or main group elements have been reported. However, structurally characterized BIAN complexes of vanadium are currently absent from the literature. Herein, we describe the preparation and structures of several novel 1,2-bis(2,6-diisopropylphenyl-imino)acenaphthene (dipp-BIAN) and 1,2-bis(2,4,6-trimethylphenyl-imino)acenaphthene (mes-BIAN) complexes of vanadium. mes-BIAN is a bidentate ligand that has two nitrogen atoms each having lone pair of electron, which can be donated to form two coordinate bonds to a metal center. Consequently, the metal center is held more tightly in the presence of a bidentate than in the presence of a monodentate. mes-BIAN can also have multiple charges on it, facilitating transformation involving redox processes at metal centers, thus increasing the potential of their complexes to act as highly active catalysts.

MARM 278

Amyloid formation of hIAPP12-18

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The formation of insoluble amyloid deposits formed by Human Islet Amyloid Polypeptide (hIAPP) has often been a source of controversy. In order to clarify the misconception, an investigation is ran on 12-18 region of hIAPP, evidence is shown that the pi-electron distribution plays a role in self-assembly of hIAPP. Various peptide analogs containing electron withdrawing groups (EWG) and electron donating groups (EDG) have been synthesized on PHE- 15 and characterized largely using turbidity measurements. The unique peptide with various groups are run for approximately two weeks, to measure for aggregation. The aggregation of these peptides indicates the presence of large concentrations of Beta-pleated sheets. To confirm the formation of Beta-pleated sheets, circular dichroism is run with amylin for each of the various groups on PHE-15. The formation of amyloid is inhibited; is caused by various electron-donating groups on PHE-15, whereas electron-withdrawing groups cause aggregation in the terminal end of hIAPP.

MARM 279

Characterization of antibiotics and lipid vesicles in aqueous ionic liquid solutions

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Ionic liquids are increasingly being used in multiple biomedical and pharmaceutical applications such as drug delivery, protein solubilization, enzyme activity modulation, antimicrobial additives. Recently, ionic liquids have been utilized as antimicrobial compounds. We extended these findings in combination with traditional antibiotics to explore potential synergistic ionic liquid-antibiotic effects. In this study, we investigated the effects of antibiotic-ionic liquid combinations on synthetic lipid vesicles which are representative models for cellular membranes. Ionic liquids such as $BMIBF_4$, BMICl, and EMIAc were characterized in aqueous solution in combination with antibiotics such as polymyxin, nisin, and tetracycline. Antibiotics, ionic liquids, and lipid vesicles were characterized with Raman and IR spectroscopy. Vesicle shrinkage analyses and calcein assays were also used to study the antibiotic-ionic liquid combination on the stability of lipid vesicles. Antimicrobial efficacy assays were also performed using traditional MIC measurements and MIC assays designed to investigate synergistic interactions. Our results demonstrate that ionic liquids induce significant osmotic stress on vesicle systems however have more subtle effects on antimicrobial activity.

MARM 280

The determination of gallic acid present in juice and tea beverages using high-performance liquid chromatography

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Oxidative processes in our bodies produce free radicals, which may cause harm to our otherwise good health. Antioxidants, such as polyphenols, which are present in beverages inhibit the oxidation of biomolecules. The Gallic Acid Equivalence Method measures the total amount of antioxidants in the wine industry. Gallic acid, which is used as the standard for the measurement of the total antioxidant content, was found to quench free radicals by getting itself oxidized, thereby reducing cell damage. A procedure for the measurement of the total concentration of gallic acid present in various beverages was measured by High Performance Liquid Chromatography (HLPC). A standard gallic acid calibration curve was first prepared and further used to measure the amount of gallic acid present in commercially available tea and juice beverages. All samples were also allowed to be air oxidized for a week to semi-quantitatively measure the decomposition of the gallic acid originally present during that time frame. A comparison between various brands of beverages will be presented in addition to highlighting the differences between the drinks.

MARM 281

Determination of the total amount of antioxidants via the Folin Ciocalteau method

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The total phenolic content present in fruit, tea and coffee beverages was determined via the Folin-Ciocalteau method in a way similar to the one used by the wine industry. This procedure uses the Folin's phenol reagent that oxidizes the polyphenols in the beverages into the corresponding polyquinones. The reduced phosphomolybdate/ phosphotungstate reagent produces a blue color that allows the microscale visible spectrophotometric determination of polyphenolic antioxidants originally present in the beverage. The results were expressed as Gallic Acid Equivalents and the measurements were made using the Beer-Lambert's Law. This method was extended to several commercially available beverages as well as tea bags and instant coffee samples. A semiquantitative measurement of the antioxidants' decomposition after seven days was also determined giving an estimate of the percentage of air oxidized decomposition of the polyphenols.

MARM 282

Novel regio- and chemoselective aminolysis of epoxides with primary amines under mild conditions

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ß-amino alcohols are a common pharmacophore among pharmaceuticals and natural products. There is a high demand for advancements of more efficient and cost effective methods for their synthesis. The chemoselective ring opening of epoxides with primary amines is a direct and convenient way of arriving to these potent therapeutic scaffolds. Previous attempts are typically met with over N-alkylation, causing a need for inorganic Lewis acids, high excess of amine, or sterically hindered substrates. We propose a general method for the region- and chemoselective ring opening of epoxides with unhindered primary amines using mild conditions and a low stoichiometric excess of amine.

MARM 283

Synthesis of 1,3,4,5-tetrasubstituted pyrazoles from substituted hydrazines and β-ketoesters

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Pyrazoles are highly conserved molecular scaffold among natural products and commercial drugs. Although many methods are available, few provide the pyrazoles scaffolds with multiple synthetic handles for further modifications. We have found that substituted hydrazines and β-ketoesters under basic conditions provide tetrasubstituted pyrazoles with high yields and selectivities. This reaction shows that alkyl β-ketoesters selectively provide the respective pyrazoles while aromatic β-ketoesters furnish the expected pyrazolone. The scope of this reaction extends to a wide variety of substitution patterns on the hydrazine and the β-ketoesters. These highly substituted pyrazoles scaffolds are poised to work as building blocks for the synthesis of pharmacologically relevant scaffolds.

MARM 284

Exploration of the conformational states in EMIM FSA and EMIM BF_4 ionic liquids

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High Pressure Nuclear Magnetic Resonance (NMR) is used to study the local dynamics and related conformational states of 1- ethyl-3-methylimidazolium (EMIM) bis(fluoromethylsulfonyl)amide (FSA) and EMIM tetrafluoroborate (BF4), ionic liquids. Measurements of NMR spin lattice relaxation times and self-diffusion coefficients as a function of pressure reveal changes in the cation and anion local conformations. Calculated activation volumes determined from the spin lattice relaxation times data show smaller value for the cation compared to the anion. This suggests differences in the short-range local motions. Activation volumes determined from self-diffusion coefficient data shows similar values, indicating comparable long-range motions. These results suggest an optimization of packing that is afforded by increasing pressure.

MARM 285

Synthesis and stabilization of a protein-based magnetically-functionalized biomaterial

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Protein-based biomaterials are promising for drug delivery applications, such as cancer treatment. While their biological synthesis provides advantageous biocompatibility, ensuring the structure and stability of the agents *in vivo* is required. Here, we present a technique to stabilize protein fibers capable of carrying hydrophobic small molecules such as curcumin, which maintains anti-inflammatory and anti-neoplastic properties, as a basis for a magnetically-functionalized biomaterial.

We employ the N-terminal coiled-coil domain of the Cartilage Oligomeric Matrix Protein (COMPcc), which is a non-collagenous extracellular matrix glycoprotein found in cartilage, tendons, and ligaments. COMPcc is comprised of a heptad repeat pentamerization domain maintaining a partitioned hydrophobic pore capable of binding small hydrophobic, chemotherapeutic agents. Our variant of COMPcc, dubbed Q, has been engineered to maintain patches of positive and negative charges along the protein surface that result in optimal lateral fiber formation on the nanoscale. Circular dichroism suggests that Q fibers demonstrate improved thermostability in comparison to the parent protein, COMPcc. Curcumin is then bound to these fibers allowing for the further self-assembly into microfibers. Curcumin-bound fibers demonstrate fluorescence, allowing for visualization by fluorescence microscopy. A chemical crosslinker, bis(sulfosuccinimidyl) suberate (BS3), is used to covalently link the protein amine groups of the fibers to further stabilize the curcumin- bound microfibers. These stabilized fibers show great promise as a stable protein-based drug delivery vehicle and have subsequently been assessed for their ability to template iron oxide particles, thereby creating a therapeutic agent detectable by magnetic resonance imaging.

MARM 286

Preparation of porphyrin embedded liposomes for *in vitro* cellular studies

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Liposomal carriers are used for many commercial drugs to facilitate entry of a drug past the membrane into the cell. They are effective because they have two regions, a hydrophilic and a hydrophobic which prevents degradation inside the body as well as promotes entry into the cell. The purpose of this study is to develop a method by which meso substituted porphyrins will be enclosed in a liposomal system. Preparation of the liposomes with different porphyrins was done by an injection method using L-a dipalmitoyl phosphatidylcholine (DPPC) in a pH 7.4 phosphate buffer. The porphyrins are dissolved in a THF/ethanol solvent before injecting into the DPPC buffer system. The resulting liposomes are dialyzed overnight to remove any excess organic solvent. The liposome/porphyrin solution is processed through a 0.25 μm Millipore syringe filter to sterilize the solution before administration into cell cultures. The exact location of the porphyrin inside the liposomes we are preparing is not known at this time.

MARM 287

Drug-carrying protein ferrofluid for theranostic applications

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Iron-based magnetic nanoparticles exhibit unique features given their nanoscale size and superparamagnetic properties, which allow them to be directed to and maintained at desired anatomical regions by a magnetic field. The templation of drug-carrying protein materials to these nanoparticles results in a ferrofluid with potential as a dual therapeutic and diagnostic, or theranostic, agent monitored by magnetic resonance imaging. Our system is based on the pentameric coiled-coil domain of the Cartilage Oligomeric Matrix Protein, dubbed COMPcc. This non-collagenous extracellular matrix protein contains a hydrophobic core capable of carrying small therapeutic molecules such as doxorubicin and curcumin, a derivative of turmeric with anti-neoplastic properties. Q, an engineered variant of the protein COMPcc, self-assembles into functional nanofibers as a result of patches of surfaces charges distributed axially along the protein. These fibers subsequently form mesofibers upon curcumin binding. Through the use of residue-specific incorporation of the non-natural methionine analog, azidohomoalanine, we have synthesized an azide-functional variant, Q-AHA. The azide group of this residue is capable of [3+2] alkyne-azide cycloaddition, a form of click chemistry, to attach it to an alkyne-functionalized iron oxide-templating peptide called CMms6. The carboxyl-terminus of the Mms6 protein, or CMms6, is found in magnetotactic bacteria and is capable of binding iron salts and organizing the crystallization of iron oxide nanoparticles. Performing click chemistry between protein Q and alkyne-functionalized CMms6 permits this drug-carrying construct to template iron oxide nanoparticles, creating a ferrofluid that is susceptible to magnetic field (see Figure of iron oxide-bound protein under local magnetic force) for potential theranostic applications

MARM 288

Identifying the product of the reaction between chromotropic acid and formaldehyde

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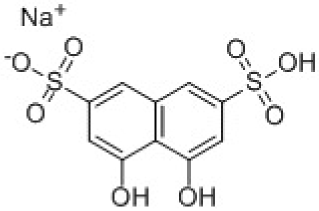
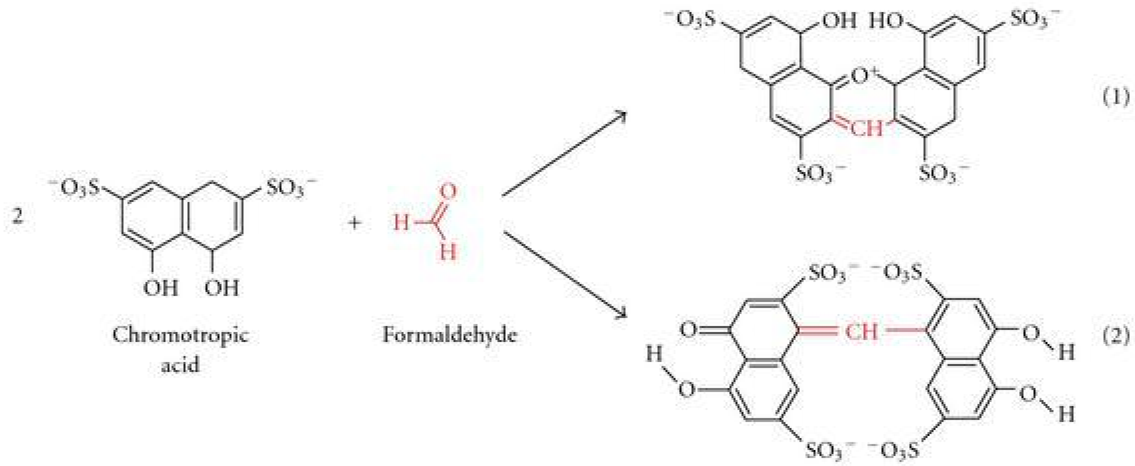
Experimental analytical methods were used to study the products of the reaction of formaldehyde and chromotropic acid. While this reaction has been used to determine formaldehyde in solution the reaction dynamics are not yet well understood. A better understanding of the product and the reaction dynamics will allow chemists to further refine analytical methods for the detection and quantitation of formaldehyde.

UV-visible spectroscopy was used to determine the concentrations of analytes in solution and FT-IR was performed on all the reactants as well as on the product solution. Concurrently, molecules that have been proposed as products of the reaction in the literature were modeled in this work with Density Functional Theory. The resulting calculated UV-visible spectra was compared to the experimental determination, and confirmed visual inspection while the vibrational frequencies of the two products were correlated with the FT-IR experimental determination for the product solution. Continuing work with column chromatography to isolate analytes of the reaction and NMR and GC will complement the obtained results.



Structure of Chromotropic Acid



Two proposed structures formed from the chromotropic acid and formaldehyde reaction.

MARM 289

Refractive index of malonic acid measured by zoom-in method

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Recently we have developed a method for determining the refractive index of solid compounds: the zoom-in method. The zoom-in method was based on the observation that the refractive index of a liquid remains unchanged with the addition of a solid if the refractive index of the solid is the same as the liquid. To choose two qualified solvents, a preliminary test was conducted using 3-8 different solvents: one showed an increase and the other underwent a decrease in the refractive index with the addition of malonic acid. Solutions of varying concentration (% mass) were prepared with the two solvents selected, and the refractive index of each prepared solution was measured. The value was compared to the refractive index of the same solution with malonic aicd dissolved in it (10% mass) until two values were matched. The matched value was the refractive index of malonic acid.

The refractive index of malonic acid has been determined by the zoom-in method by three sets of solvent systems: DMSO/THF, BzOH/THF, and BzOH/n-PrOH. In BzOH and THF solvent system, the refractive index of malonic acid was found to be the same as a 41% BzOH solution in THF, having a refractive index of 1.461(1). The same procedures were repeated with two other solvent systems, and the refractive index was measured as 1.458(1) and 1.455(1) which were close to the result obtained from BzOH/THF system. The zoom-in method turned out to be a useful system in measuring the refractive index of solid compounds.

MARM 290

Determination of the refractive index of benzoic acid measured by extension method

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The extension method which was developed based on the observation of a good linear relationship between the percent mass of solution (solid solute and liquid solvent mixture) and its refractive index has been used to determine the refractive index of solid compounds such as fatty acids and ionic compounds. In the system, a plot of refractive index vs percent mass was obtained in low concentration ranges (0 - 24%), and the line of the linear plot was then extrapolated to 100% mass (*i.e.* pure solid) where the refractive index of the solid was calculated.

The extension method has been further applied to measure the refractive index of benzoic acid because it showed good solubility in various organic solvents such as DMSO, ethanol, methanol, and THF. In the experiment, a linear plot was obtained between the refractive index and % mass of benzoic acid in a solvent, and a first order linear equation was calculated based on the plot. By applying 100 to the % mass variable (100% mass means pure solute, the solid compound) in the linear equation, the refractive index of benzoic acid was indirectly determined for the solvent.

Based on the data measured in DMSO solution of benzoic acid, a linear equation (e.g. $y=0.000690x + 1.476774$) was obtained, then a value of 100% was applied to get the refractive index of benzoic acid, which was 1.546. After two more trials, 1.546(1) was determined as the refractive index of benzoic acid in DMSO.

MARM 291

Thermodynamic study of esterification using a microwave reactor

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Microwave reactor is a new technology and has become an invaluable tool adopted in many areas of science laboratories due to the convenience including temperature, pressure and power controls. Application of a microwave reactor was further extended to the thermodynamic study of esterification reaction with the merit of a convenient temperature control of a microwave reactor.

The equilibrium constants of the esterification reaction between acetic acid and isopropanol at the temperatures of 50 - 90°C were determined from the initial and equilibrium concentrations of acetic acid through the acid-base titration using a 0.5M NaOH solution. Thereafter, the thermodynamic data (ΔH and ΔS) of the reaction were calculated from the linear relationship between the equilibrium constants obtained ($\ln K$) and the equilibrium temperatures ($1/T$). Similarly, the thermodynamic data of the esterification reaction between acetic acid and n-propanol were also obtained using a microwave reactor. The obtained data were compared to the data calculated from the acetic acid/isopropanol reaction.

This result will extend the usage of microwave reactor to a tool of the thermodynamic study which can be easily added to an undergraduate laboratory curriculum. Application a microwave reactor will make the thermodynamic study easy, simple and faster due to the convenience of the temperature control of the instrument and its safety feature.

MARM 292

Synthesis of thiol-substituted, water-soluble phthalocyanines conjugates

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Phthalocyanines (Pcs) can be efficient photosensitizers for photodynamic therapeutic (PDT) treatment of variety of cancers because they have strong absorption in the red region of the optical spectra and so can photosensitize the formation of singlet oxygen species the formation of which is important to cause cell death. Since the red light penetrates deeper into tissues, Pcs can be efficient PDT agents. Aqueous insolubility and ease of aggregate formation are problems often encountered with Pcs in biological systems. In order to evaluate the effect of substitution on the efficacy of phthalocyanines, a few of thiol substituted water-soluble phthalocyanines were prepared by reaction of the commercially available hexadecafluorophthalocyaninato zinc(II) by controlled nucleophilic substitution of the peripheral fluoro groups in the presence of potassium fluoride or potassium carbonate in dry dimethylsulfoxide (DMSO).

MARM 293

Detection of *Salmonella* in foods via microbiological methods

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The ability of microorganisms to grow and reproduce in foods has been a growing concern for many years. Microorganisms may cause spoilage or chemical changes in the food and injury or death to the individual. The Food and Drug Administration (FDA) sets scientific standards on testing foods for various contaminants. The Microbiological methods listed in the Bacterological Analytical Manual (BAM) are an example that lists all the analytical methods used for the detection of pathogens (bacterial, viral, parasitic, yeast and mold) and microbial toxins. Salmonella will be the focus of this presentation. Media production, food preparation, isolation and identification of Salmonella comprise the microbiological method will be discussed in detail.

MARM 294

Cleaning and protecting the municipal water via New York City's wastewater treatment system and the DEP shoreline survey unit

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In order to sustain the supply and demand of water usage for all New York City residents, the Department of Environmental Protection (DEP) has fourteen wastewater treatment plants located throughout the five boroughs of the city (Bronx, Brooklyn, Manhattan, Queens and Staten Island). Each treatment plant recycles wastewater from the sanitary sewer lines (from homes, businesses, schools) where the resulting clean water is discharged back into the rivers. A detailed five step process regarding the treatment of wastewater will be presented. Likewise the New York City DEP Compliance Monitoring Section (CMS) is comprised of two sectors – Industrial Pretreatment Program (IPP) and Shoreline Survey Unit (SSU). SSU aggressively pursues field investigations necessary to locate and terminate illegal contaminated discharges to the city waters from outfalls throughout the tristate area. Different investigational methods will be examined and also presented.

MARM 295

Synthesis of x-shape molecules as electron acceptors in organic solar cells

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The C_{60} fullerene based acceptor readily accepts electrons from a wide range of donor materials and exhibits high electron mobility. However, fullerene is not an ideal material due to its weak absorption and very deep LUMO level. Therefore there is a clear need for alternative acceptor materials. We propose to synthesize X-shape molecules as electron acceptors via strain and Hückel aromaticity as the driving forces. The molecule's bottom half is a fluorene unit, and the top half is a fused heterocyclic ring. Both motifs are twisted along a central double bond. We have synthesized our first target in four synthetic steps. This red compound shows intense green fluorescence. Its structure was preliminarily confirmed by H-NMR and C-NMR. The synthesis of this compound has been scaled up, and the last step's yield was improved from 22% to 87% by extending reaction time. With nearly 400mg in hand, its optical & electrical properties are under further pursuing.

First target dissolved in dichloromethane

MARM 296

Synthesis and photorelease study of glycine caged bis-1,2-(4-acetylphenylethynyl)-4,5-dimethoxybenzene, first generation dendron phototrigger

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Glycine caged bis-1,2(4-acetylphenylethynyl)-4,5-dimethoxybenzene, the dendritic photoactive compound is synthesized for photo release study of the model drug. The terminal functionality of dendron, (1,2 dimethoxy benzene) provides the platform for connecting drug and targeting to molecules and the photo-trigger 1-(4 Ethynylphenyl)-ethanone, a cleavable linker which keep the drug carrier inactive until the light are absorbed. Once it's absorbed the proper light it releases the therapeutic drug through photocleavage of the anchor bond. The NMR spectra of the photoreaction shows the drug being released and the computational study before and during the synthesis supports the release mechanism based on the optimized molecular geometries and frontier orbitals of the different moieties of the caged dendron.

MARM 297

Applications of tridentate and tetradentate tripodal ligands in bioinorganic and organometallic chemistry

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Multidentate ligands have received considerable attention due to their ability to tailor the steric and electronic properties of a metal center. The research presented will focus on recent applications of various tridentate and tetradentate tripodal ligands, as illustrated by (i) the *tris*(3-t-butyl-5-methylpyrazolyl)hydroborato ligand, [$\text{Tp}^{\text{t-Bu,Me}}$], which features a [$N_3$] donor array, (ii) the *tris*(2-mercapto-1-t-butylimidazolyl)hydroborato ligand, [$\text{Tm}^{\text{t-Bu}}$], which features an [S_3] donor array, and (iii) the *tris*(2-pyridylthio)methyl ligand, [Tptm], which allows the formation of new types of atrane compounds. An illustration of the reactivity to be discussed is provided by the ability of the zinc hydride compound, [Tptm]ZnH, to serve as a catalyst for a variety of transformations, including the hydrosilylation of aldehydes, ketones and carbon dioxide.

MARM 298

Hydrogen bonding in reverse micelle surfactants

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This talk will describe the formation of reverse micelles that form with the use of hydrogen bonding cationic surfactants that are paired with anionic sugar acids and other carboxylate containing molecules as counterions. The resulting structures are uniform and stable under ambient conditions. Hydrogen bonding interactions between cationic amphiphiles and their counterions promotes reverse micelle formation and in many cases eliminates the need for cosurfactants. One member of this class of cationic surfactants is hexadecyldimethylammonium acetamide which forms amide-carboxylate hydrogen bonds with glucuronate in chloroform. Related systems will be described.

MARM 299

Mechanistic investigation of catalytic and biocatalytic iron porphyrin carbene formation

*Rahul Khade, **Yong Zhang**, zhanguiucedu@gmail.com. Chemical Biology and Biomedical Engineering, Stevens Institute of Technology, Hoboken, New Jersey, United States*

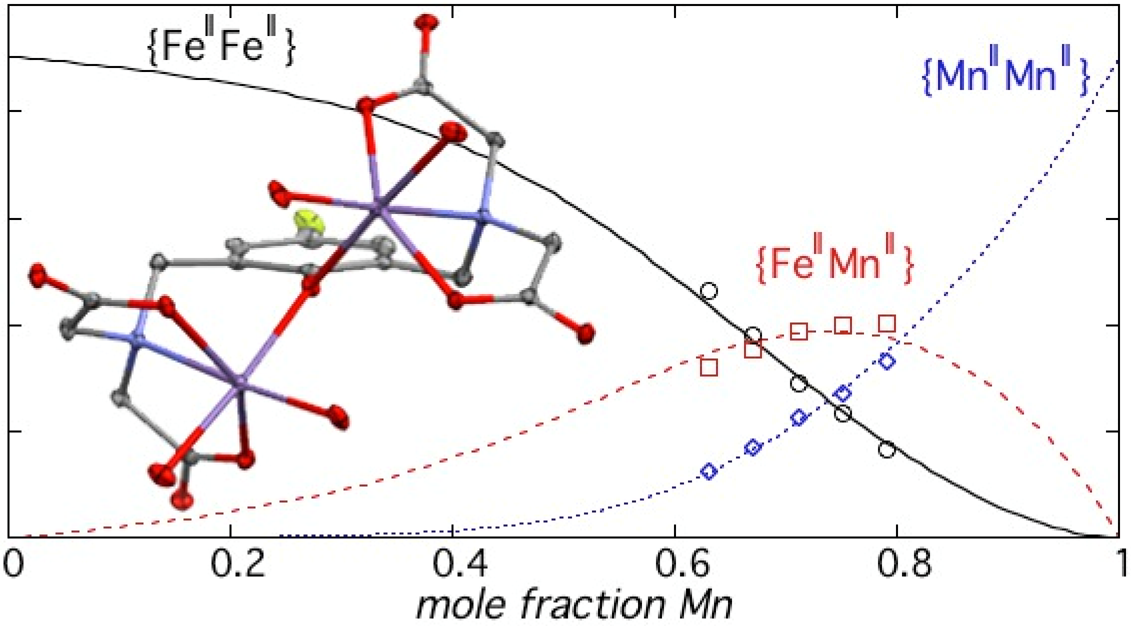
Iron porphyrin carbenes (IPCs) are important intermediates involved in various chemical reactions catalyzed by iron porphyrins and engineered heme proteins, as well as in the metabolism of various xenobiotics by cytochrome P450. However, there are no prior theoretical reports to help understand their formation mechanisms and identify key information governing the binding mode, formation feasibility, and stability/reactivity. Following our recent quantum chemical investigation of their Mössbauer, NMR, geometry, spin state, charge, and MO properties to resolve the major resonance structure for reactivitiy, a systematic quantum chemical study was performed to investigate the effects of carbene substituent, porphyrin substituent, and axial ligand on IPC formation pathways. Results not only are consistent with available experimental data, but also provide a number of unprecedented insights into electronic, steric, and hydrogen bonding effects of various structural factors on IPC formation mechanisms. These results shall facilitate research of IPC and related systems for sustainable chemical catalysis and biocatalysis.

MARM 300

Enhanced stability of heterobimetallic clusters as a driving force for cofactor assembly in dinuclear metalloproteins

***William D. Kerber**, will.kerber@bucknell.edu. Chemistry, Bucknell University, Lewisburg, Pennsylvania, United States*

The relative stability of bimetallic clusters supported by the dinucleating ligand F-HXTA (5-fluoro-2-hydroxy-1,3-xylenediamine-tetraacetic acid) has been investigated by fluorine NMR. Equilibrium binding of Fe(II)/Mn(II) mixtures to F-HXTA is a chemical model of cofactor assembly in the R2 subunit of class Ic ribonucleotide reductases (R2c) and R2-like ligand binding oxidases (R2lox). As predicted by the Irving-Williams series, F-HXTA forms more stable complexes with Fe(II) than with Mn(II), although the difference is relatively small due to a hard-soft acid-base mismatch between the polycarboxylate ligand and the divalent metal ions. A greater than statistically expected amount of the heterobimetallic complex is present at equilibrium, indicating a favorable interaction specific to the Fe/Mn metallation state. This appears to be a general phenomenon and was subsequently observed for heterobimetallic Fe(II), Zn(II) and Mg(II) complexes of F-HXTA. The importance of cluster stability for selective cofactor assembly in R2c/R2lox and other dinuclear metalloproteins will be discussed.



MARM 301

Heterolytic C-H and N-H/O-H activation by first-row transition metal complexes

*Sumit Chakraborty[1], Ruibo Xu[1], Paige Piszel[1], Cassandra Hayes[1], R. Tom Baker[2], Sarina Bellows[1], **William D. Jones**[1], jones@chem.rochester.edu. (1) Chemistry, University of Rochester, Rochester, New York, United States (2) Chemistry, University of Ottawa, Ottawa, Ontario, Canada*

Several first row transition metal catalysts employing iron, cobalt, and nickel with non-innocent ligands have been synthesized and their ability to catalyze dehydrogenation of alcohols and amines, as well as their ability to hydrogenate ketones and quinolines, has been comparatively evaluated. The scope and mechanism(s) of these reactions have been examined. Also, the use of an alcohol dehydrogenation catalyst along with an Aldol condensation catalyst has led to a new route to convert ethanol directly and cleanly to 1-butanol.

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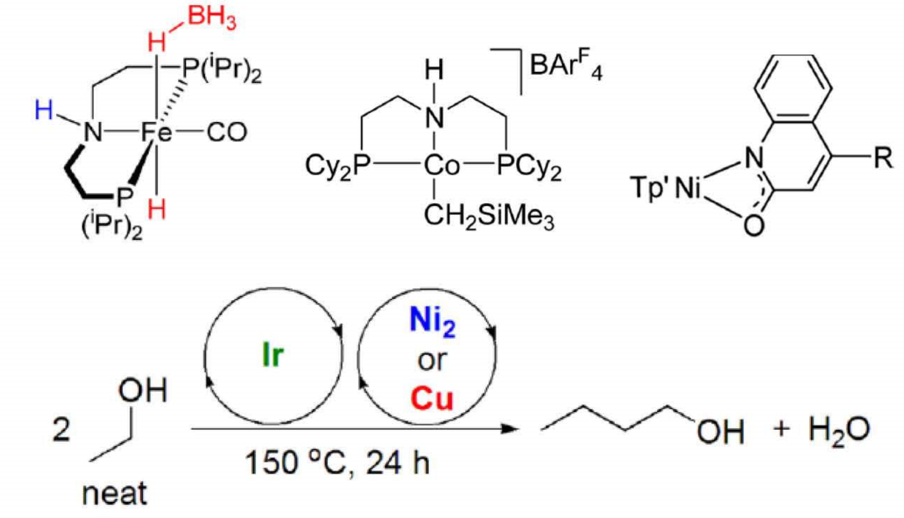

MARM 302

Carbon monoxide activation by first-row transition metal cyano carbonyls

***Jianfeng Jiang**, jiang@yu.edu. Chemistry, Yeshiva University, New York, New York, United States*

Carbon monoxide can be oxidized by oxygen gas or other oxidants catalyzed by nickel cyano carbonyls in basic solution at ambient temperature. A prototype CO-powered fuel cell was constructed based on this nickel cyano carbonyl catalyzed oxidation. In the presence of polymeric CO-coordinating double metal cyanides ($M(H_2O)_2Fe(CN)_4(CO)_2$ (M = Mn, Fe, Co and Cu), $ZnFe(CN)_4(CO)_2$, $Fe_2[Fe(CN)_4(CO)_2]_3$, carbon monoxide can be activated by heat to undergo a series of interesting reactions. CO reacted with nitrogen oxides to produce CO_2 and N_2 at 200 – 300ºC under 1 atm pressure.

MARM 303

Reactivity of low-valent iron and cobalt complexes of hydrotris(pyrazolyl)borate ligands modified with ferrocenyl substituents

***Daniel Cummins**, dccprime@udel.edu, Glenn P. Yap, Klaus H. Theopold. Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States*

Due to their ease of synthesis and their tendency toward making coordinatively unsaturated complexes, pyrazole substituted tris(pyrazolyl)borate (Tp) ligands serve as excellent scaffolds for activating small molecules such as dioxygen. Our group has previously reported various TpM^I-L complexes, where M is Co, Fe, and Cr, and L is either N_2 or CO, which react with oxygen atom transfer reagents to give intramolecular C-H bond activation products. This presentation will describe substitutionally labile, low valent cobalt and iron complexes of ferrocenyl modified Tp ligands, taking advantage of the ferrocene fragment's exceptionally strong C-H bonds to resist intramolecular C-H bond activation. The synthesis, structural characteristics, and reactivity of these complexes toward oxygen transfer reagents, such as dioxygen and pyridine-N-oxide, as well as nitrene transfer reagents, such as alkyl azides, will be discussed.

MARM 304

New mixed-valence copper cyanide polymers.

***Peter W. Corfield**, pwrc@earthlink.net, Alexander Sabatino, Emma Cleary, Joseph Michalski, Phuong Luu. Chemistry, Fordham University, Bronx, New York, United States*

The mixed-valent compound $Cu_4(CN)_5meen_2$, where meen is N-methylethylenediamine, crystallizes as a neutral three-dimensional polymer, with Cu atoms bridged by cyanide groups. $Cu(II)meen_2$ moieties occupy holes in the polymeric network, but are covalently linked to the Cu(I)CN network by a cyanide bridge. A second three-dimensional polymer is the salt $LH.Cu_2(CN)_3$, where LH^+ is the N,N-diethyl-2-hydroxyethan-1-aminium ion. This compound crystallizes as an anionic three-dimensional CuCN polymer, with the cations occupying holes in the structure without any covalent interaction with the CuCN network. In this compound, the expected stabilization by the ligand of some copper(II) atoms did not occur, and all the copper atoms are univalent. The synthesis and structural characterization of these new polymers reflect progress in our goal of the rational synthesis of mixed-valence copper cyanide frameworks. We will compare them with previously reported structures.

MARM 305

Versatile cobalt pincer catalysts for cross coupling reactions via a "hydrogen-borrowing" strategy

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Precious metal catalysis plays a major role in most of crucial organic transformations and pharmaceutical manufacturing processes. However, the scarcity, cost and toxicity of precious metals can be problematic, making them less attractive for widespread and large-scale commercial applications in industry in the future. The replacement of precious metals with cheap and earth abundant elements is, therefore, an ultimate goal of sustainable chemistry. Catalytic acceptorless dehydrogenation is an efficient and atom-economic method that has found applications in both organic synthesis and hydrogen storage. Remarkably, the acceptorless dehydrogenation methodology that initiates a hydrogen transfer process ("hydrogen-borrowing") has been elegantly utilized to carry out a range of C-C and C-N coupling processes which is "green" and generate no waste, especially when earth abundant metals are used as catalysts in recent years. In our precious work, we have developed a novel cobalt(II)-pincer catalyst which is highly efficient for homogeneous (transfer) hydrogenation of alkenes, aldehydes, ketones, and imines under mild conditions. The ability of the same catalyst in driving acceptorless dehydrogenation of alcohols and N-heterocycles has been also established. To extend this research, we present the applications of cobalt catalysts in mediating efficient C-C and C-N coupling reactions via a "hydrogen-borrowing" mechanism.

MARM 306

Do TFSA anions slither? Pressure exposes the role of anion conformational exchange in self-diffusion

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Multi-nuclear (^{1}H, ^{2}H, and ^{19}F) magnetic resonance spectroscopy techniques were applied as functions of temperature and pressure to the study of selectively deuterated 1-alkyl-3-methylimidazolium (alkyl = ethyl (EMIM) or butyl (BMIM)) bis(trifluoromethylsulfonyl)amide (TFSA) ionic liquids (ILs). Studies of relaxation times gave information about changes in the structure of the ILs with temperature and pressure. Most significantly, the pressure dependences of the ionic self-diffusion coefficients in EMIM TFSA revealed that the displacements of the cations and anions are uncoupled, with the TFSA anions being more affected by increasing pressure as supported by a larger activation volume (24 ± 4 cm^3/mol) compared to that of the EMIM cations (15 ± 1 cm^3/mol). This dramatic difference is unique among the nine imidazolium ILs for which such data is available. A less pronounced effect is seen in BMIM TFSA, but for all other cases the activation volumes for the anion and cation are similar. Increasing pressure may lower the mobility of the TFSA anion by hindering its interconversion between trans and cis conformers, a process that published MD simulations suggested would be coupled to diffusion. The effect is visible in EMIM TFSA due to the small cation size. The high-pressure diffusion data provide clear experimental evidence for the MD prediction.

MARM 307

Structure of silicon-substituted ionic liquids

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Small changes in the composition of ionic liquid anions or cations can have profound effects on viscosities and diffusivities. Changes as small as a single atom substitution of silicon for carbon have led to viscosity changes of up to 740 %. In order to find out that how this viscosity change is related to the change of ionic liquid bulk viscosity, we studied a series of ionic liquids with cations have silicon-containing functional groups by both X-ray scattering and molecular dynamics simulations. We compared their structures with a non-silicon ionic liquid. We found that substituting a carbon atom by silicon will lead to a small left shift of the adjacency peak in structure factor, and a smaller charge-charge correlation peak. This leads to weaker inter-ion interactions, which is also correlated with the low viscosity of these ionic liquids.

MARM 308

Tuning the physical properties of ionic liquid mixtures

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The need for improved energy storage capability in devices like batteries and supercapacitors has prompted the use of ionic liquids (ILs) as alternatives to organic solvents, due to their attractive properties such as low vapor pressure, high conductivity and thermal stability. Despite the advantages of ILs in battery applications there are still factors that pose difficulties in finding an IL with optimal transport properties. Binary mixtures of ILs are being widely explored because they provide additional means of tuning IL properties. We have designed IL mixtures that incorporate structural features (such as alkoxy side chains and dications) that are known to reduce viscosity and/or increase conductivity. Mixtures containing 80-90% by weight *N*-ethoxyethyl-*N*-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide with 10-20% of ILs containing monocations or dications combined with the same NTf_2 anions were designed. A series of such binary IL mixtures were synthesized and characterized for their physical properties. Results reveal that mixing ILs can extend their useful properties to greater limits. We observed a depression of the glass transition temperatures, extending the lower operating temperature limit of these IL systems.

MARM 309

Structures and stabilities of proteins in aqueous ionic liquid solutions: Unfolding kinetics and thermodynamics studies

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Recent years have seen a dramatic increase in the utilization of ionic liquids for biomedical and biochemical applications. Ionic liquids in aqueous solution have been added to protein solutions to increase solubility, prevent aggregation, modulate enzyme activity, and enhance antibiotic activities. The nature of proteins in aqueous ionic liquid solutions remains an open field of fundamental research seeking to elucidate interactions between ionic liquids and proteins and the effects of these interactions on protein stabilities, structures, and conformational dynamics. We have characterized the structures and stabilities of model proteins myoglobin, BSA, and red fluorescent protein in different ionic liquid solutions. We have used protein-melting experiments to quantify protein stabilities, unfolding kinetics experiments to characterize conformational dynamics, and HDX-MS experiments to probe protein structures. By comparing results in

the presence and absence of ionic liquids we can understand how these novel additives interact with to stabilize or destabilize different protein structures.

MARM 310

Ionic liquid solutions for dissolving cellulose

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Cellulose, a component found in plants, and cellulose derivatives are used to produce paper, fibers, coatings, films, and biofuels. However due to extensive hydrogen bonding within the polymer, cellulose is insoluble in water and most organic solvents. Traditional processes used to dissolve cellulose require the use of expensive, toxic and/or corrosive chemicals. Ionic liquids (ILs), organic salts that have melting points below 100 °C, may be a greener alternative for dissolving this biopolymer. In this report, we explore the use of quaternary ammonium salts that may be ionic liquids, dissolved in various solvents for the dissolution of cellulose.

MARM 311

A proton-transfer reaction and an esterification reaction in ionic liquid EMIMOAc

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Acetate-based ionic liquids (such as 1-ethyl-3-methylimidazolium acetate, EMIMOAc) demonstrated potentials in the applications for CO_2 absorption and electrochemical reduction, chemical separation and extraction of HF or acetic acid, and the Fischer esterification of alcohol, amine, and starch. Strong or weak organic acids can be dissolved in EMIMOAc and yield interest proton-reach acidic ionic liquids solutions. We have use a series of spectroscopic methods (FTIR, Raman, NMR), calorimetry, and vapor pressure, viscosity, and conductivity measurements to characterize the solution properties of the acid solutions in EMIMOAc. Unique proton transfer and esterification reactions are observed in many of these acidic solutions with carboxylic acids or sulfonic acids as solutes.

MARM 312

Photocatalyzing multi-electron, multi-proton conversions: An excited-state acid-base process

***Harry D. Gafney**, harry.gafney@qc.cuny.edu, Edward C. Look, Daiki Okamoto. Chemistry and Biochemistry, CUNY Queens College, Flushing, New York, United States*

Photocatalyzing multi-electron, multi-proton reactions lies at the heart of solar energy conversion. Achieving photocatalysis with low-cost, abundant, thermodynamically-robust materials and with visible light, however, remains a significant scientific challenge. Different metal oxides have been known to photocatalyze the reduction of CO_2 to CH_4 for more than a quarter century, yet these systems, including the tungsten oxide doped nanoporous silicas described here, continue to require UV excitation and methane yields remain frustratingly small. Photoexcitation is thought to populate the oxide conduction band, but how that one-photon, one electron process converts into the eight electron, four proton reduction of CO_2 is not clear. This presentation will focus on a different model; an excited-state acid-base mechanism.[1] Two forms of tungsten oxide, which appear to be W(VI) 0xides that differ in their aggregation and hydration, have been found to be emissive when adsorbed into porous Vycor glass. Spectroscopic and O_2 quenching data indicate that the emissive states are triplet ligand to metal charge transfer, ^{3}[LMCT], states. In spite of their low energy, 2.6 to 3.1 eV, emission quenching experiments confirm that these states are quenched by H_2O, CO, CO_2 and NH_3. Consistent with the proposed excited state acid-base model, the energetics of the different quenching process indicate that quenching occurs by an acid-base mechanism.

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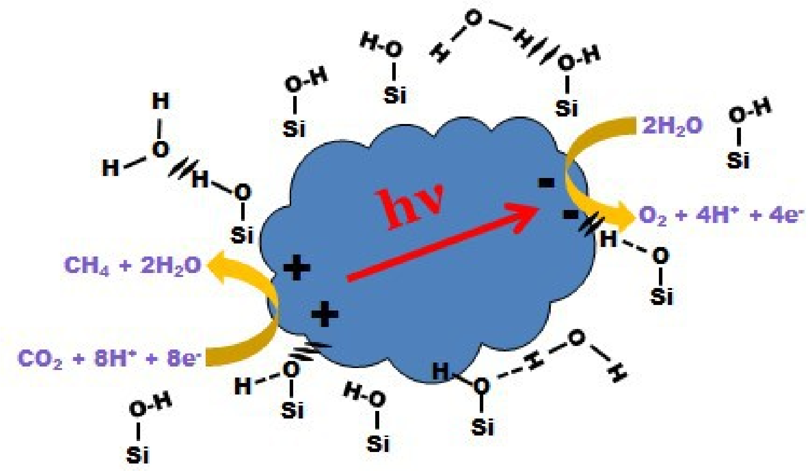


MARM 313

Synthesis and characterization of Fe doped single-phase multiferroic

Frederick A. Pearsall[2,3], *pearsall.frederick@gmail.com, Stephen O'Brien*[1]*. (1) Chemistry, The City College of New York, CUNY, New York, New York, United States (2) Chemistry, The City College of New York, New York, New York, United States (3) Chemistry, The Graduate Center of the City University of New York, New York, New York, United States*

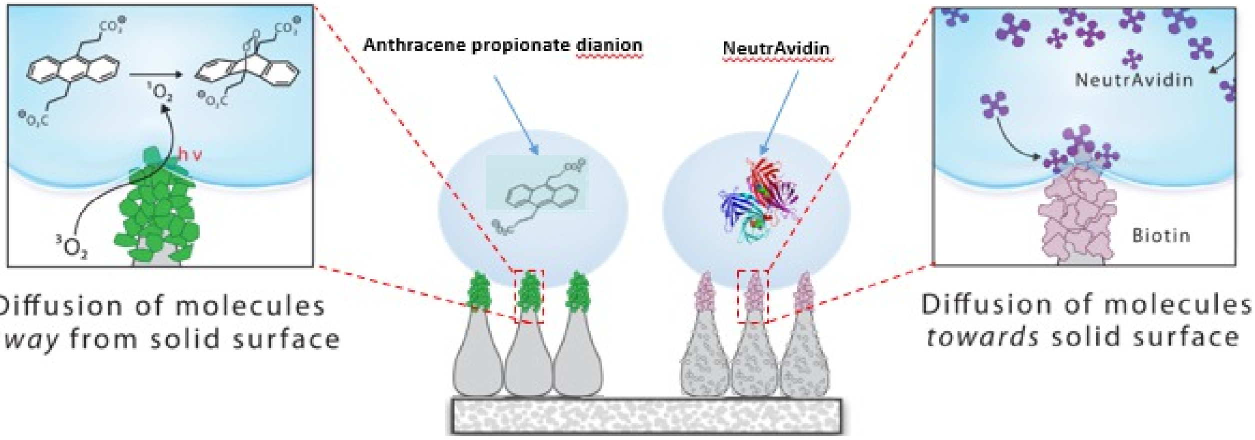
Discovery of new complex oxides that exhibit coupled ferromagnetic and ferroelectric properties is of great interest for the design of functional magnetoelectrics, in which research is driven by the long-term technological prospect of controlling ferromagnetic hysteresis with an electric field and vice versa. Multiferroics offer opportunities for sensors, 4-state logic, and spintronics. Single-phase coupled multiferroics are of theoretical interest due to the possibility of a quantum character in such coupling. $BaMn_3Ti_4O_{14.25}$ (BMT-134) is a recently discovered single-phase multiferroic complex oxide exhibiting antiferromagnetic and ferroelectric behavior. In an attempt to exhort a room temperature ferroic order response, BMT-134 was doped with Fe at varying degrees. Using a chemical solution processing approach two distinct variations of nanocrystals were synthesized; $BaMn_{3-x}Fe_xTi_4O_{14.25}$ with x = 1, x = 2. All variants were found to belong to the same hollandite crystal class as BMT-134 and Fe was shown to be incorporated into the crystals of each, proportional to the precursor ratios. Using EDS and XPS, elemental composition was determined qualitatively and iron content was corroborated with precursor amount. Impedance analysis was performed on pellets of the material to determine the effect of iron doping on dielectric strength and dissipation factor. TEM and SEM techniques were used to determine size distribution and morphology of the nanoparticles and of their packing within pellets. Due to the porous nature of arrayed nanoparticles, 0-3 nanocomposites were fabricated, using high k polymers to in infiltrate inherent void space allowing for a more stable dielectric over the frequency range of 100Hz - 2MHz.

MARM 314

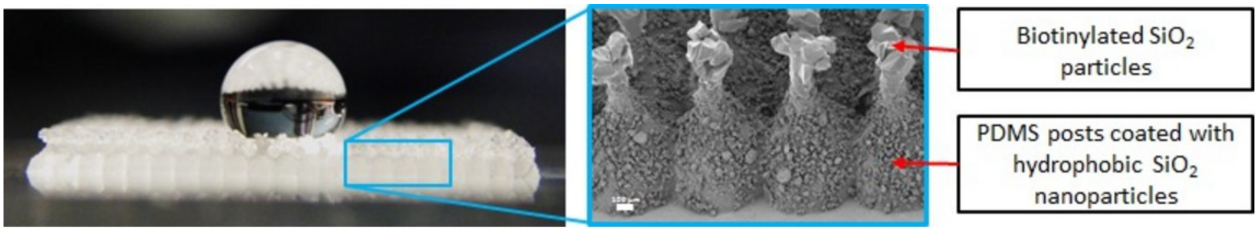
Reactions in individual droplets on a superhydrophobic surface: Effect of convection

Yang Liu[1,3], *liuyangtongji@gmail.com, Xiaoxiao Chen*[1], *QianFeng Xu*[1], *Alexander Greer*[2,3], *Yuanyuan Zhao*[1,3], *Alan M. Lyons*[1,3]. *(1) Chemistry, College of Staten Island, Staten Island, New York, United States (2) Chemistry, Brooklyn College, Brooklyn, New York, United States (3) Chemistry, The Graduate Center of the City University of New York, New York, New York, United States*

On a superhydrophobic surface, an aqueous droplet can maintain its quasispherical shape without wetting the surface. This geometry creates a nearly isothermal microscale container in which chemical reactions and analysis can be conducted using small volumes (<10 μL) of reagents. Due to their small size and thermal isolation from the substrate, convection in these droplets is suppressed and so mixing within these micro-containers occurs only by diffusion. In this paper, we present a method to induce, control and quantify convective mixing within small size droplets poised on multifunctional superhydrophobic surfaces. We prepared superhydrophobic surfaces using a 3D printing process to create arrays of PDMS posts onto which functionalized nanoparticles were partially embedded. On these surfaces, an aqueous droplet was placed and imaged using a high speed camera to quantify convection. By modifying the functionality of the nanoparticles, two reactions were studied. In one system, singlet oxygen was generated by illuminating sensitizer particles such that singlet oxygen was generated at the solid liquid interface. Anthracene dipropanate dianion dissolved in the drop trapped the single oxygen and the concentration change was measured by UV spectroscopy. In a second system, the protein binding interaction between NeutrAvidin (dissolved in the droplet) and biotin (bound to the surface) was quantified using a fluorescently labeled protein. The binding profile was plotted as a function of time, and the kinetic rate constant was calculated. By comparing the rates with and without convection, we show that the reactions are limited by diffusion in static droplets and that convection leads to significantly higher reaction rates.



Schematic of the two reactions studied in droplets on functionalized superhydrophobic surfaces.



Side view of a 10μL water droplet on a functionalized superhydrophobic surface; inset shows SEM image of PDMS posts with particles partially embedded into the surface.

MARM 315

Nanocrystalline solar oxide perovskites derived from potassium niobate $KNbO_3$ by gel collection

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Inorganic materials synthesis techniques that can approach low temperature routes akin to chemical solution processing are attractive for their ability to prepare oxides, traditionally derived from high temperature ceramic processing, which can offer thin film integration options more compatible with modern device platforms such as spray coated or printed devices (2D, 3D) and flexible electronics. A chemical solution processing method (Gel Collection) based on sol-gel chemistry was used to obtain a set of perovskite compounds of the formula $[KNbO_3]_{1-x}[BaNi_{0.5}Nb_{0.5}O_{3-d}]_x$, called KBNNO, known to be a class of visible light absorbing ferroelectric photovoltaic materials, with a tunable bandgap as a function of x. The materials produced were fully crystallized and with a nanocrystalline morphology. Control over the composition of KBNNO was based on the synthesis of nanocrystalline potassium niobate $KNbO_3$ (KNO) via potassium and niobium ethoxides, with subsequent chemical reaction of complimentary barium and nickel alkoxides and methoxyethoxides. Characterization by TEM, SEM, XRD, and EDS confirms structure and composition. Frequency dependent dielectric measurements, performed on KNO-PFA (poly fufuryl alcohol) and KBNNO-PFA nanocomposites, show stable effective dielectric constants of 41.18, 70.84, 94.04, and 108.32 for KNO, KBNNO $x = 0.1$, 0.2, and 0.3 respectively at 1 MHz. Using a modified Kerner model, it is estimated that the dielectric constant of the individual nanoparticles of KNO, KBNNO $x = 0.1$, $x = 0.2$, and $x = 0.3$ are 150, 400, 270, and 240 respectively. Following the introduction of Ba and Ni, a transition from the original orthorhombic *Amm2* unit cell ($x = 0$) to a more complex atomic arrangement in cubic *Pm3m* ($x > 0.1$) is observed. This synthetic route to KBNNO, previously only synthesiszed by solid state processing at 1050-1200 °C, provides a lower temperature (< 525 °C) approach to doping ferroelectric $KNbO_3$ with Ba and Ni, which inserts Ba^{2+} onto the *A*-site, and Ni^{2+} onto the *B*-site with the addition of oxygen vacancies for charge compensation.

MARM 316

Identifying corrosion protection and breakdown mechanisms of corrosion preventative compounds (CPCs), and investigating new corrosion protection technologies

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Corrosion Preventative Compounds (CPC's) are used to protect bare metal surfaces where permanent coatings cannot be applied. For Navy aircraft (our focus), CPCs are used to protect copper rich aluminum alloys from pitting corrosion. The mechanism behind that protection is not well understood. Typical CPCs for naval application are formulated with a base oil, a corrosion inhibitor and other additives. The oil is used as a moisture barrier and carrier for the other additives. The corrosion inhibitor is added to organize on the surface in a specific fashion to protect it from pitting corrosion; otherwise, active corrosion sites are exposed to corrosive elements such as chloride ions and oxygen. We have

separately investigated the effect of each component (oil and inhibitor), as well as formulations of differing concentrations of inhibitor, for corrosion initiation on bare aluminum as a means to investigate the protection mechanism.

In addition to the mechanistic study, we have evaluated two different novel materials as replacements for current CPC technology. We show that fluorinated organic oil and surfactants can be affixed to the copper rich aluminum alloy surface and provide a large increase in the pitting corrosion potential. Furthermore, recent literature has shown films comprised of alternating layers of polymer and graphene oxide polymers to exhibit very low oxygen permeability. Because oxygen is necessary for corrosion, we have explored the relationship between reduced oxygen transport across these layers and delayed corrosion initiation.

MARM 317

Co(II) containing anionic clays: Structure and particularities

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Hydrotalcite-like compounds, also called anionic clays or layered double hydroxides, with the formula $[M(II)_{1-x}M(III)_x(OH)_2](CO_3)_{x/2}H_2O$, where M(II) = Co(II), Ni(II) and/or Mg(II) and M(III) = Al(III) and Cr(III) have been synthesized and characterized. These compounds consist of layers of M(II) and M(III) cations which are octahedrally co-ordinated by six oxygen anions, as hydroxides. These layers have a similar layered structure to that of natural brucite $Mg(OH)_2$. The substitution of M(III) cations into the brucite-like hydroxide layer leads to an overall positive charge on the octahedral layer, the overall electrical neutrality being maintained by the presence of anions, which are typically carbonate, in the interlayer region between the metal hydroxide layers, where water molecules also exist. Lamellar compounds with hydrotalcite-like structures have been used as ion exchangers, catalysts, and catalyst precursors after being calcined at fixed temperatures. Cobalt-containing hydrotalcites, in particular, have been used for several applications including as precursors to prepare Fischer–Tropsch catalysts, removal of SO_2 and NO_x. When cobalt hydrotalcites are submitted to thermal treatment, a part of the divalent cobalt is oxidized to the trivalent state, probably due to the easy formation of the cobalt spinel, Co_3O_4. Layered compounds with the above-described structure have been synthesized by coprecipitation for various combinations of divalent and trivalent cations, such as Co(II), Ni(II) and Mg(II), along with Al(III) and Cr(III). The prepared structures have been investigated by X-Ray diffraction, FTIR spectroscopy and BET surface area analysis. Each M(II)/M(III) combination led to unique features of the obtained materials.

MARM 318

Droplet microfluidics in industry

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Droplet microfluidics is a versatile technology with a broad range of applications in industrial research. At BASF, microfluidics has developed into a core competency of the formulation research group. As a formulation tool, the technology can produce both single emulsions (droplets) and double emulsions (core-shell systems). The technology can produce highly monodisperse droplets with a fine control of physical properties, while using very small volumes of liquid reagents. A diverse array of product divisions within BASF capitalize on microfluidic technology, including home and personal care, catalysts, agriculture, and pharmaceuticals.

MARM 319

Origins of defects in organo-halide perovskites examined by time-resolved photoluminescence spectroscopy

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The performance of solution-processed, organo-halide perovskite semiconductors as the active layer in optoelectronic devices is reminiscent of thin-film materials such as single-crystal GaAs and polycrystalline CIGS but is rather anomalous for semiconductors deposited from solution. In order to further refine the electronic properties of perovskite semiconductors, we report an investigation of the relationship between chemistry in precursor solutions, processing conditions, and charge traps in perovskite films. Using a combination of time-resolved photoluminescence spectroscopy, materials characterization, and systematic variation of chemical composition, we find that the precursor concentration of tetraiodoplumbate is strongly correlated to the density of charge traps in films – suggesting that the band-edge electronic structure of perovskites is influenced by iodoplumbate complexes formed in solution preceding film casting. Furthermore, we demonstrate the principal advantage of two-step methods for the deposition of organ-halide perovskite films arises from their prevention of iodoplumbate species being formed during perovskite formation rather than their improved film morphology. Our findings elucidate the solution-phase chemical equilibria that determine the final concentrations of defects in organo-halide perovskite films and provide a framework to consider new chemical processes for further refinements of the electronic properties of perovskite materials.

MARM 320

Structural properties of iron in organic vs. non-organic *Brassica oleracea*

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Structural properties of iron in plants may vary depending on the soil conditions on which plants were grown and treatments, such as fertilizer or pesticides, given to the plants. When vegetables are grown in the contaminated soil, many unwanted chemicals become incorporated into the chemical composition of the. This study will serve to clarify some issues concerning the structure of iron in Brassica Oleracea plants. Mossbauer spectroscopy is a valuable method to probe structural properties of iron. We will present the results obtained on organic and non-organic Brassica Oleracea using the Mossbauer spectroscopy.

MARM 321

Melting gels and their anticorrosive properties on magnesium alloy AZ31B

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Hybrid glasses obtained from the consolidation of melting gels have shown promising results in reducing corrosion rates for magnesium alloy AZ31B. Magnesium and its alloys are attractive materials for aerospace and automotive applications, largely due to their low density, high strength, good thermal and electrical conductivity, and low elastic modulus. The replacement of 1 m^3 of aluminum with magnesium results in a weight reduction of 1,000 kg. The downside of Mg and its alloys is their tendency to oxidize. The purpose of this study is to show that melting gels are good barrier layers in a corrosive medium such as 0.35 and 3.50 wt. % NaCl solutions. Melting gels were prepared using a mixture of a mono-substituted alkoxide, for example, methyltriethoxysilane (MTES), and a di-substituted alkoxide for example, dimethyl-dimethoxysilane (DMDES). Because of their low glass transitions temperatures, melting gels are easy to process by pouring or dipping, while their viscosities are low. Once the melting gels were coated onto the Mg alloy AZ31B , the coatings were converted to hybrid glasses by consolidation at temperatures between 135 and 160°C. Two important properties of melting gels make them usable as anticorrosive coatings; one is their high hydrophobicity and second is their lack of porosity. To quantify these properties, the surface of the coatings was analyzed using contact angle and BET surface area measurements. All samples are hydrophobic with q> 90°. Their structure was investigated using FT-IR, ^{29}Si NMR and SAXS. Their morphology was investigated using SEM. Electrochemical analysis (Anodic Polarization and Electrochemical Impedance Spectroscopy) was performed in 0.35 and 3.50 wt. % NaCl solutions. Taken together, the results show a significant improvement of corrosion resistance, with no change in impedance after 100 days.

MARM 322

Determination of soil pH dependence of structural properties of iron in plants

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Different types of green leafy vegetable plants were grown under controlled soil with different pH values from 4 to 9. The amount and structural properties of iron were measured using X-ray absorption near edge structure spectroscopy. The amount of iron absorbed by plants depends on the soil pH and the value slightly varies with the type of the plant. The main absorption edge energy position remains the same in different type of plants indicating similar electronic environment around iron atoms regardless of the type of the plant and soil pH.

MARM 323

Structural investigation of Nickel oxide thin films using synchrotron x-rays

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Recently there has been a very high demand for small scale magnetic storage devices. The industry sector has consistently demanded sub micron or even nano-meter scale magnets. Magnetic thin films often contain several layers of coating. For the purpose of this study, we prepared thin film magnets by spin coating a precursor containing nickel into a glass substrate. The thickness of the films was controlled by the spin rate. Precursor films on the substrate were then annealed to 600^0 C for 3 hours in air. The micro structure of iron in the films was investigated using the X ray Absorption Near Edge Structure (XANES) and pre-edge feature that appears before the main absorption edge.

MARM 324

Self-assembly with boron-containing polymers: New luminescent, sensory and stimuli-responsive materials

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The incorporation of boranes into polymers has recently developed into a promising new direction in materials science.[1] Notable examples include boronic acid-functionalized polymers for use as sensory materials, luminescent boron diketonate- or bodipy-functionalized polymers for medical imaging, and carborane-functionalized polymers for optoelectronic applications.[2] We have embarked on a research program that takes advantage of chain growth polymerization techniques to prepare boron polymers of well-defined architecture. The resulting amphiphilic structures in turn undergo self-assembly into nanostructured materials. In this presentation recent work on the development of new borinic acid and arylborane polymers, their self-assembly and applications as sensory and stimuli-responsive materials will be introduced.[3] We will also describe redox-active hybrid materials that utilize boron-based polymeric ligand architectures for binding of transition metal complexes.[4]

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MARM 325

Scattering mediated hot-electron transfer: A new paradigm for light-driven energy transfer

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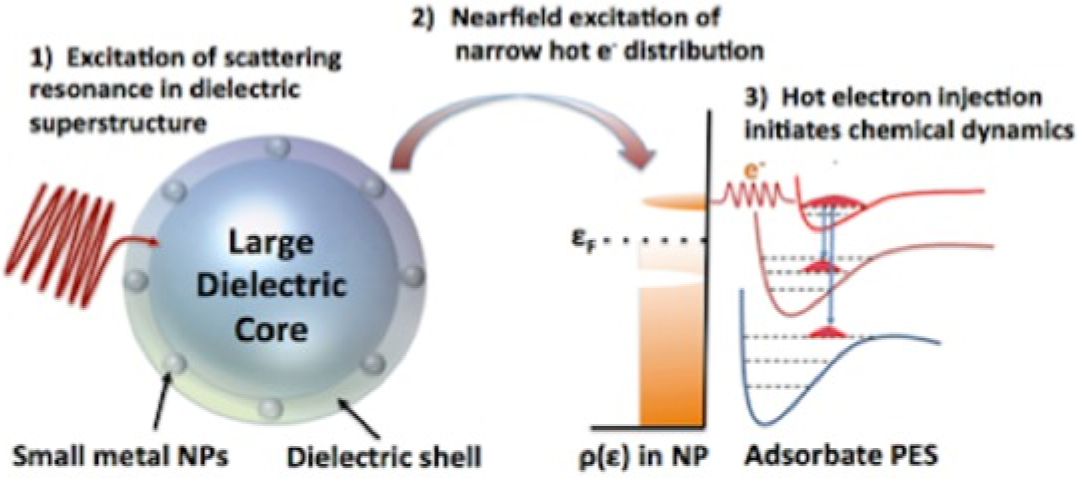
This talk will highlight recent results aimed at elucidating a new paradigm of light-driven energetic electron transfer that we call “Scattering Mediated Hot-Electron Transfer” (SMHET).
Light-driven energetic electron transfer has attracted considerable attention as an emerging paradigm for

photocatalysis and solar energy conversion. Localized surface plasmon resonances (LSPR) in noble metal nanoparticles have been widely used as the optical resonance for initiating energetic ("hot") electron transfer; however, several fundamental impediments for widespread utilization of LSPR for photocatalysis or solar energy conversion have been identified. In particular, the energy distributions of hot electrons derived from LSPR are broad and difficult to control; moreover, the rapid decay of these energetic electrons limits their transfer efficiency. Additionally, the most promising materials for LSPR are noble metals, which are not earth abundant or cost-effective.

We propose an entirely new mechanism of light-driven energetic electron transfer, called Scattering Mediated Hot-Electron Transfer (SMHET), which can potentially circumvent all of these fundamental limitations. We show results suggesting that SMHET can be enabled by engineered hybrid nanostructures whose majority materials are made from cheap and abundant dielectric materials, for example, silicon dioxide, polystyrene, or polycarbonate. While the presence of broad-band absorbing materials (i.e. metals) is crucial to this phenomena, we will demonstrate that non-precious metals can give rise to the effects we associate with SMHET. We will also highlight the tunability of scattering resonances supported by the majority dielectric structures, both in terms of their resonance frequency and bandwidth, and describe how we envision this can impact efficiency and selectivity of photocatalytic reactions initiated by SMHET. We will conclude by discussing how we envision these predictions can be experimentally realized in practical structures.



Schematic of the proposed Scattering Mediated Hot-Electron Transfer mechanism and illustration of an engineered nanostructure that can support this phenomenon.

MARM 326

Crystallite size dependency of the pressure and temperature response in nanoparticles of ceria and other oxides

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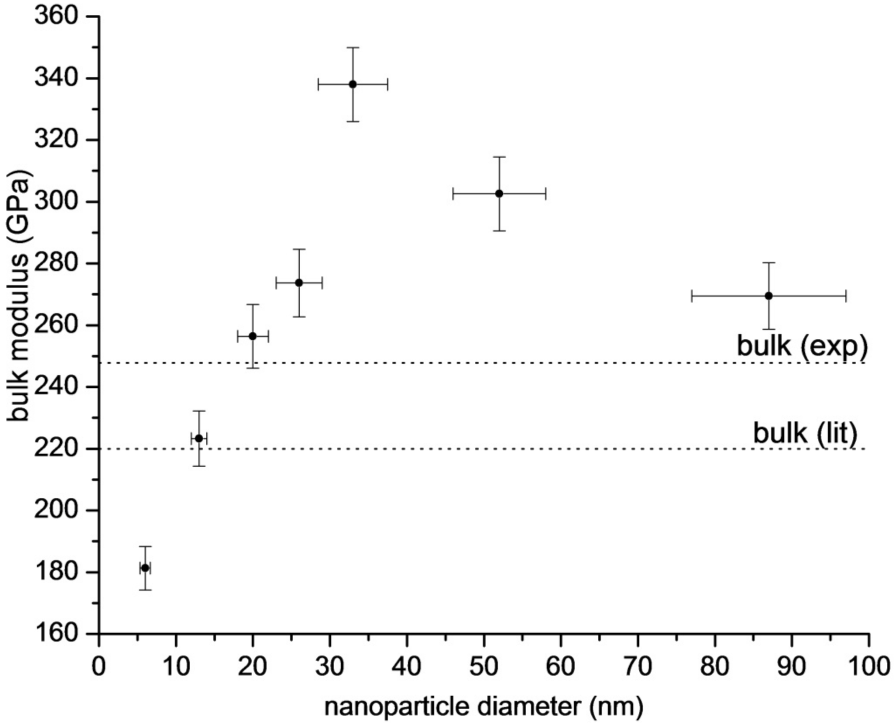
As nanotechnology develops and becomes more prominent, it is increasingly important to understand the details of how ionic bonding changes for very small crystallites. In comparison to bulk materials, it has long been known that smaller crystallites of metal nanoparticles have decreased lattice parameters, whereas smaller crystallites of metal oxide nanoparticles have increased lattice parameters. Many explanations for this phenomenon rely on a pressure response that is constant across all crystallite sizes. This work described here shows that for ceria nanoparticles, the response of the lattice to hydrostatic pressure is dependent on crystallite size and in fact stiffness has a peak at an intermediate crystallite size near 30nm. These results are complemented by detailed thermal expansion studies across crystallite sizes, and rationalized with the Grüneisen parameter that relates thermal expansion to bulk modulus. A similar set of results will presented for magnesia nanoparticles, whose crystallites have a different structure from ceria, and the potential impact of such bonding changes in small crystallites for heterogeneous catalysis will be explored.



Ceria bulk modulus as a function of crystallite size.

MARM 327

Synthesis of polyrhodanine-supported noble metal nanoparticles and their role in catalysis

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Polyrhodanine has attractive properties of antimicrobial agents and heavy metal absorbent. It has various other biological activities ranging from antidiabetic, antiviral, anticonvulsant and the presence of three different heteroatoms on the Rhodanine act as very good absorbent centers. Metal nanoparticles tend to congregate during the catalytic process unless they are well protected, however the protection or stabilization should not affect the catalytic ability of the nanoparticles. We have synthesized polyrhodanine supported noble metal nanoparticles (Ag, Au) and investigated their catalytic properties. The role of electrolytes on the morphology and the catalytic properties of Polyrhodanine metal nanoparticles composite was also examined. It has been observed that the change in concentration of the electrolytes changes the rate of catalysis as it can either make the nanoparticle catalytically inert by preferential absorption on the surface of the catalyst or can reduce the fermi potential of the metal particle and accelerate the catalytic process.

MARM 328

Dynamic peptide libraries

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Active materials are of great interest in supramolecular chemistry due to their ability to respond according to the environment. Herein, we report on the effect of environmental changes (salts, metals, solvent, pH, binders) on the supramolecular aggregation of dipeptides using biocatalytic self-assembly. Different dynamic peptide libraries (DPL) were investigated screening the sequence series of the amino acid building blocks (FF, LL, WW – FF + LL, FF + WW). Their supramolecular polymerization was analyzed using High Pressure Liquid Chromatography (HPLC) and further characterized using a variety of spectroscopic (fluorescence, Circular Dichromism, FT-IR) and microscopic (AFM, TEM) techniques. Peptide synthesis was carried out using solid phase peptide synthesis. The peptides were assembled from N-terminus to C-terminus beginning with the initial FMOC-Arg(PbS)-Wang resin. The peptides were analyzed using LC-MS (Liquid Chromatography-Mass Spectroscopy) and HPLC.

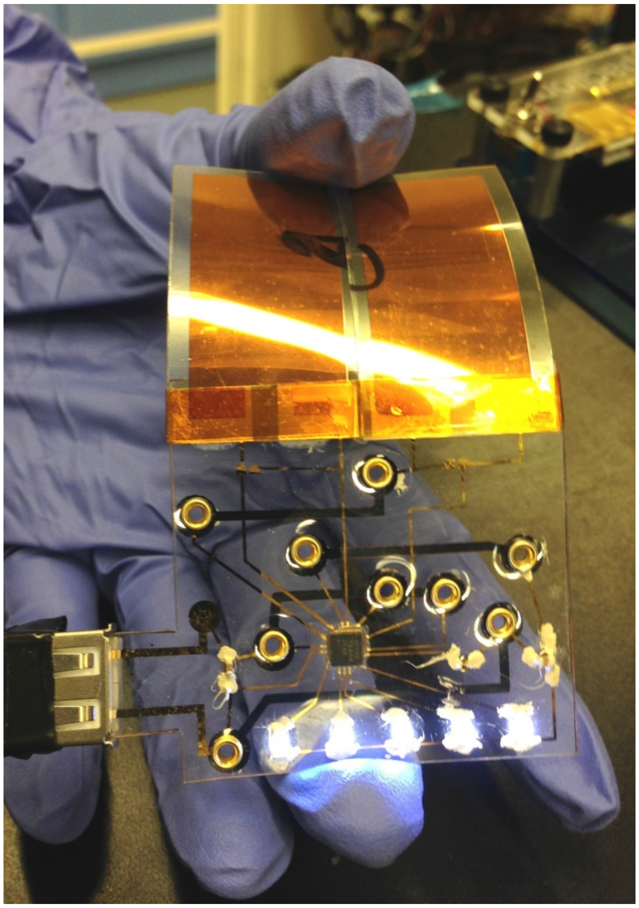
MARM 329

Nanochemistry and power technology: The design of printed nanocomposite capacitors for power electronics

Limin Huang[3,6], *Shuangyi Liu*[4,6], *Shyuan Yang*[2], *Barry Van Tassell*[5], *Eli Leland*[5], *Daniel Steingart*[1], *Ioannis J. Kymissis*[2], ***Stephen O'Brien***[5,6], *sobrien@ccny.cuny.edu. (1) Mechanical and Aerospace Engineering, Princeton University, Princeton, New Jersey, United States (2) Electrical Engineering, Columbia University, New York, New York, United States (3) South University of Science and Technology of China, Shenzhen, Guangdong, China (4) Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences, Chongqing, Sichuan, China (5) Energy Institute, City University of New York, New York, New York, United States (6) Chemistry, City College of New York, New York, New York, United States*

The topic of high efficiency power conversion in electronics and electrical engineering is considered indispensable to the role it plays in renewables integration, and ultimate influence over electricity consumption. I will give an overview of our project, called metacapacitors, that attempted to unite nanochemical approaches to designing capacitors optimized for applications in high frequency DC-DC power conversion. Within the context of a university consortium, we prepared prototypes aimed to improve efficiency, functionality and form factor of off-line power converters suitable for LED solid-state lighting, with a long term view to developing an attractive technology platform for load management and

power conversion across a broad range of applications. Based on integrated switched-capacitor (SC) topologies, the project adopts an integrated approach from materials to devices to circuits. We designed capacitors based on high-dielectric nanocrystals, that can be prepared using high throughput microfabrication/nanotechnology techniques, ink deposition and multilayering. The capacitor dielectric, a nanocomposite composed of $(Ba,Sr)TiO_3$ nanocrystals in polyfurfuryl alcohol (BST/PFA, $k > 20$, 100Hz - 1 MHz , loss < 0:01 , 20 kHz), targets a high volumetric capacitance density and ripple current capability. The methodology for preparing the capacitor dielectric films relies on a novel method to prepare complex oxides, followed by evaporatively driven self-assembly into thin films. I'll review rational synthetic design, multigram scaling, and dispersion formulation design, as well as recent advances in the synthesis and characterization of relevant complex oxides.



Two printed thin film Metacapacitors integrated with a commerical converter IC on a flexible substrate. The capacitors were made from printable BST colloidal dispersions of nanocrystals.

MARM 330

Solvent effects on the crystal structure formation of perylene diimide derivative

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Here we present the polarized absorption spectra of the perylene diimide derivative, N,N′-Bis(3-pentyl)perylene-3,4,9,10-bis(dicarboximide) (B2). This molecule has been used as a model system to control the degree of crystal growth as a function of growth conditions. Crystals of B2 were fabricated by evaporation of chlorobenzene, toluene, and tetrahydrofuran solvents. The resulting crystals were analyzed microscopically and spectroscopically. The resulting spectrum for the crystals made from the chlorobenzene solution were compared to the solution state spectra to monitor the degree of intermolecular electronic coupling. The solid phase spectrum shows both a large bathochromic shift (2200 cm^{-1}) and a smaller hypsochromic shift (600 cm^{-1}) compared to the spectrum of B2 in solution, which indicates the presence of two aggregate states. The lower energy portion of the film spectra has an absorption polarization ratio of 1.0 while the higher energy spectrum has a polarization ratio of -0.2. The polarization dependent isosbectic point is at 520 nm (19200 cm^{-1}). In contrast, the crystals made from the tetrahydrofyran solution show a larger degree of crystal formation, but the spectra do not show an appreciable polarization ratio. The bathochromic shift is also less pronounced (630 cm^{-1}), indicating a weaker degree of electron coupling in these crystals. AFM and x-ray results confirm the differences of crystal formation in these structures on the nanometer and sub-nanometer scales. These results exemplify the interplay between crystal growth propagation, solubility, and molecular alignment in these materials.

MARM 331

Molecular helices as electron acceptors in fullerene-free organic solar cells

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Despite numerous organic semiconducting materials synthesized for organic photovoltaics in the past decade, fullerenes are widely used as electron acceptors in highly efficient bulk-heterojunction (BHJ) solar cells. None of the non-fullerene bulk heterojunction solar cells have achieved efficiencies as high as fullerene-based solar cells. Design principles for fullerene-free acceptors remain unclear in the field. We herein introduce a series of helical molecules as highly efficient electron acceptors. The molecules are constructed by fusing perylene diimide (PDI) units together with a two-carbon bridge. They have relatively high electron mobilities, good electron-accepting ability, and LUMO levels similar to those of $PC_{61}BM$ and $PC_{71}BM$. By varying lengths of the ribbons and controlling film morphology in BHJs, we achieved a power conversion efficiency > 8% which was a record high for non-fullerene BHJs. Femtosecond transient absorption spectroscopy revealed both electron and hole transfer processes at the donor−acceptor interfaces, indicating that charge carriers are created from photogenerated excitons in both donor and acceptor phases. This study describes a new motif for designing highly-efficient acceptors for organic solar cells.

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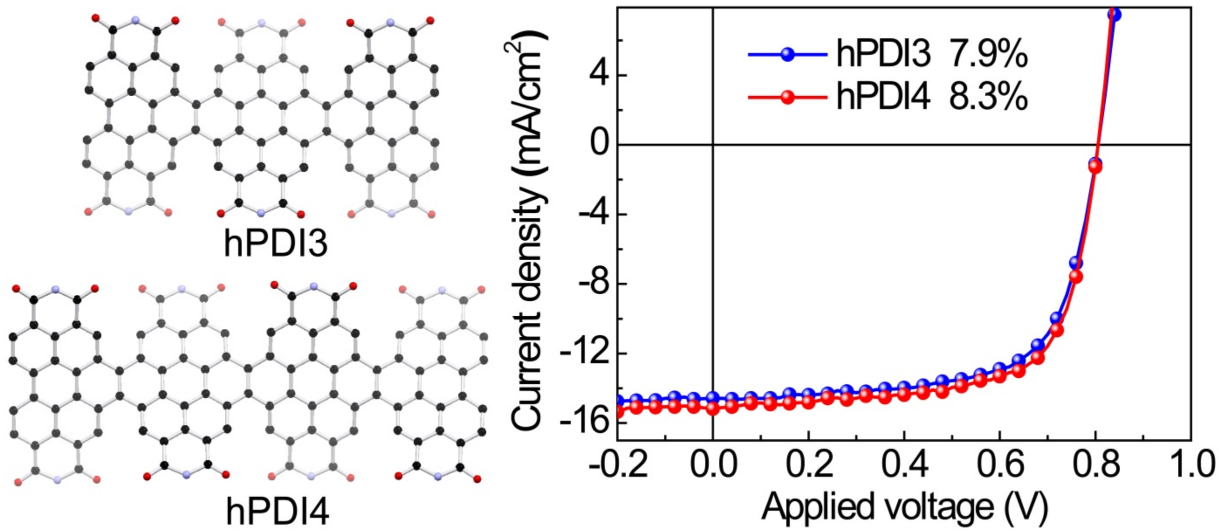

Helical molecular acceptors in fullerene-free organic solar cells

MARM 332

Effect of nanoconfinement on the crystallization and stability of metal-halide perovskites

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Current record efficiency solid-state dye-sensitized solar cells comprise metal-halide perovskites deposited from solution onto highly disordered mesoporous titanium dioxide (m-TiO_2) layers. These m-TiO_2 layers contain nanopores that confine perovskite crystallization to the tens to hundreds of nanometer length scale. To understand the effect of nanoconfinement on the crystallization process, we employed two-dimensional x-ray diffraction to systematically study how the extent of nanoconfinement affects the crystallization of methylammonium lead halide ($MAPbI_3$) in the uniaxially-aligned pores of anodized aluminum oxide (AAO) templates. MAI/PbI_2 mixtures co-dissolved in N-N-dimethylformamide (DMF) or dimethyl sulfoxide (DMSO) were spin coated onto AAO templates with characteristic pore sizes ranging from 20 to 200 nm in diameter. 2D x-ray diffraction patterns revealed that these mixtures form a highly oriented intermediate crystalline phase incorporating solvent molecules in the nanopores of the AAO templates. The experimental diffraction patterns closely matched those predicted by previously reported unit cell parameters of PbI_2:DMF and PbI_2:DMSO crystals, with the exception of a doubling in the *c* axis length in both cases. Interestingly, the intermediate crystalline phase was oriented with alternating planes of PbI_2 and solvent molecules parallel to the long axis of the AAO pores, with the extent of orientation dependent on the nanopore diameter. Conversion of the intermediate crystalline phase to $MAPbI_3$ crystals was subsequently induced via thermal annealing. This conversion process was accompanied by a complete loss of preferred crystal orientation with respect to the long axis of the pores. Time-dependent measurements revealed that converted $MAPbI_3$ crystals confined within the AAO nanopores were stable in air for a period of two weeks. In comparison, unconfined $MaPbI_3$ crystals deposited on flat SiO_2 substrates degraded completely over the same time period.

MARM 333

Fabrication of single crystal organic field-effect transistor using hexatriacontane as a dielectric interlayer

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Single crystal field-effect transistor (SCFET) has been considered as the best way to achieve the highest charge carrier mobility attributed by its defect-free charge transport. Yet, it has been challenging to eliminate defects and charge traps at the interfacial layers of devices. In this study, we tried to eliminate these inefficiency of devices by adding hexatriacontane($C_{36}H_{74}$) interlayer between organic semiconductor and silicon dioxide (SiO_2) dielectric layer. We fabricated organic field-effect transistors using single-crystal rubrene ($C_{42}H_{28}$) as a semiconductor material and hexatriacontane and silicon dioxide as dielectric layers. Electrical properties of devices were measured and the effect of hexatriacontane interlayer was investigated. Significant improvement in hole mobility, on/off ratio, and working voltage was achieved when the device was thermally annealed at 50 °C. After the annealing process, the mobility was increased by 2.5 times and the on/off voltage ratio was increased by 100 times. As for the working voltage, it showed a decrease of approximately 1.5 times compared to the results of a regular device without hexatriacontane interlayer. Mainly attributed by solid-solid transition of hexatriacontane layer, hexatriacontane epitaxy was formed on crystalline rubrene surface and eliminated charge traps, which resulted in higher device performance. Selected area electron diffraction (SAED) of rubrene-hexatriacontane interlayer also showed the growth epitaxy of hexatriacontane.

MARM 334

Integration of high-purity carbon nanotubes into electronic devices

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Due to their exceptional electronic properties, carbon nanotubes (cnt) are leading candidates to be employed as channel materials in future nanoelectronic devices. A key bottleneck to realizing device integration is the sorting of carbon nanotubes, namely the isolation of high-purity, semiconducting cnt solutions. This talk will describe our efforts in using polymer-based sorting methods to isolate high-density and high-purity semiconducting cnt solutions. We explore the dependence of starting material and polymer to cnt ratio on the effectiveness of the separation. We confirm optically and electrically that the semiconducting purity is greater than 99.99% through several thousand individual device measurements. In addition to single-cnt devices, thin-film transistors were also fabricated and tested. Due to the high purity of the solutions, device switching (\textasciitilde 10^5 I_{ON}/I_{OFF}) was observed at channel lengths below the percolation threshold (500 nm). Operating below the percolation threshold allows for devices with much higher current densities and effective mobilities as transport is now the result of direct transport as opposed to hopping between cnts.

MARM 335

Tuning the dynamics of triplet excitons from singlet fission in functionalized pentacene films by controlling molecular order

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Recent reports have demonstrated that incorporating organic singlet fission sensitizers into solar cells is a potential method for boosting photoconversion efficiencies. To this point, most singlet fission studies investigate how triplet exciton generation is determined by gross changes in electronic coupling attained through chemical modifications or crystal polymorphs. However, the impact of variations in film morphology on both triplet exciton generation and decay remain unclear, yet they are critical for optimizing exciton harvesting efficiency. Here, we use a combination of x-ray diffractometries along with a variety of steady-state and time-resolved optical spectroscopies to study the effects that molecular order and film morphology have on triplet exciton formation and decay rates for a functionalized pentacene. We develop a new microscopic model showing that subtle variations in molecular order determine not only triplet generation rates but also order-of-magnitude changes in triplet lifetime following singlet fission. Our results show for the first time that it is possible to tune triplet exciton yields and lifetimes of singlet fission sensitizers by controlling film processing conditions.

MARM 336

Catalytic reduction of carbon dioxide in artificial photosynthesis

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Artificial photosynthetic systems exploit a variety of photochemical transformations with the ultimate result of efficient conversion of the photon energy into chemical bonds. The reduction of carbon dioxide using protons and electrons derived from water is one of the important chemical processes leading to the formation of carbon-containing fuels. The major scientific challenges associated with chemical reduction of CO_2 are demanding thermodynamics, slow reaction rates and selectivity towards the desired products. The rational design of a catalyst which can promote low energy pathways and boost selectivity and reaction rates is required for alleviating these challenges. Metallic cathodes have been known as simple and robust electrocatalysts for CO_2 reduction for several decades; however their practical application was limited mainly by high overpotentials and low selectivity for CO_2 reduction compared to hydrogen evolution. It has been demonstrated recently that the efficiency of metal electrocatalysts toward CO_2 reduction can be substantially improved by creating a highly structured nanoscale surface morphology. In our work, we discovered a novel approach for the production of high surface area halide-modified nanoporous silver electrocatalysts fabricated by a facile oxidation-reduction method in the presence of chloride anions in an aqueous medium. A current density of 10mA cm^{-2} can be achieved at the overpotential of only 0.53 V with the current efficiency still remaining at 95%. Combined surface spectroscopy, electrochemical and theoretical investigations indicate that the adsorbed halides play critical role in lowering overpotential and increasing the selectivity of CO_2 reduction towards production of CO.

The work at Brookhaven National Laboratory was carried out under contract DE-SC0012704 with the U.S. Department of Energy and supported by its Division of Chemical Sciences, Geosciences, & Biosciences, Office of Basic Energy Sciences.

MARM 337

Plasmonic photocatalysts for CO_2 conversion

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Development of effective, low cost catalysts that uses renewable energy, such as sunlight, for CO_2 conversion has attracted significant attention. We have investigated various nanomaterials to enable CO_2 conversion driven by visible light illumination. One such example is the use of plasmonic Au nanoparticles to generate heat under plasmon resonance excitation, which in turn leads to CO_2 conversion on ZnO catalyst particles. One advantage of the plamon heating enabled photocatalysis is that it allows the selectivity of the products to be easily controlled by simply adusting the light illumination intensity. In addition, due to the highly localized heating nature, the bulk of the reactor remains at room temperature even as the catalyst is heated to severl hundred degrees Celcius, eliminating the need for heat manangement as required for conventional thermally driven catalysis processes. Furthermore, the catalysts are robust with no need for the addition of hole scavengers which are frequently utilized in semiconductor based photocatalysts. More recently, this approach is tested in a larger scale, continuous flow reactor that may be more relevant to practical deployment of plasmonic photocatalysts. If time permits, a discussion on the prospect of achieving carbon negative CO_2 conversion will be presented.

MARM 338

Surface and interface properties of photoelectrocatalysts for solar fuels

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A surface science approach can greatly advance understanding of the structure and reactivity of photoelectrocatalysts for solar fuels. This involves experiments using well-defined model catalysts under controlled conditions and utilizing a range of spectroscopic techniques for characterization of surface and interface properties and the nature and reactivity of surface-bound species. We report on several of our recent studies, which include investigations of the effects of dopant incorporation on the structural and chemical properties of the α-Fe_2O_3(0001) surface for water oxidation catalysis, facet-dependent activity and stability of Co_3O_4 nanocrystals towards OER, and the interaction of water with GaP(110), a semiconductor that is known to enable selective CO_2 reduction to methanol in aqueous solutions of CO_2 and nitrogen-containing heteroaromatics. For water oxidation on α-Fe_2O_3, we found that Ni doping in thin films of model catalysts caused a new termination for the films and induced formation of more stable surface-bound OH groups. For the Co_3O_4 system, we used the well-defined morphologies of nanocubes and nanooctahedra to demonstrate that the (111) surfaces vastly out-perform the (100) surfaces for OER activity (overpotential and current density). Finally we have spectroscopically identified*in situ* the surface-bound species on GaP(110) associated with exposure to water using ambient pressure photoelectron spectroscopy (APPES). These observations on model systems afford further analysis and discussion of the role of surface-bound species in mechanisms for catalyzed water oxidation and CO_2 reduction.

MARM 339

Stabilizing electrodeposited catalytic particles on metal-insulator-semiconductor (MIS) photoelectrodes for water electrolysis

***Daniel Esposito**, de2300@columbia.edu, Natalie Labrador. Chemical Engineering, Columbia University, New York City, New York, United States*

Photoelectrodes based on the metal-insulator-semiconductor (MIS) architecture are a promising approach to achieving photoelectrochemical energy conversion with both high efficiency and good stability. Within this design, an ultra-thin insulating layer is positioned between the semiconducting absorber layer and the catalytic metal layer. The insulator helps to protect the semiconductor from corrosion while still allowing for efficient electron transport between the metal and semiconductor by quantum mechanical tunneling. By this means, the stability and light absorption properties of the semiconductor may be decoupled. In this talk, electrodeposition is explored as a potentially low-cost and scalable means of depositing ultra-low loadings (1 to 20 ng cm^{-2}) of Pt nanoparticles onto SiO_2-covered p-Si photoelectrodes. As-deposited MIS photoelectrodes are found to be highly unstable, but this issue can be overcome through application of a thin secondary insulating layer. This talk will focus on the mechanisms by which stability and efficiency are enhanced when the electrodeposited MIS photoelectrodes are coated with a secondary insulating layer

MARM 340

Photoelectrochemical water-splitting with a $SrTiO_3$:Nb / $SrTiO_3$ n^+-n homojunction structure

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We report pulsed laser deposition (PLD) of epitaxial $SrTiO_3$ (STO) thin films on Nb doped $SrTiO_3$ (STO:Nb) single crystal substrates for photoelectrochemical (PEC) water splitting. X-ray diffraction (XRD), angle-resolved photoelectron spectroscopy (XPS), transmittance electron microscopy (TEM) and scanning electron microscopy equipped with energy dispersive X-ray spectroscopy (SEM-EDX) were employed to characterize the samples. Epitaxial growth and stoichiometric of Sr/Ti of STO thin films were achieved by optimizing the introduced oxygen partial pressure (p_{O2}) under a substrate temperature of 750 ^oC. The Nb diffusions from STO:Nb substrate to the deposited STO thin films were observed by angle-resolved XPS and cross-sectional TEM EDX-mapping. Evaluation of these samples as photoanodes shown that the incident photon-to-current efficiency (IPCE) were highly affected by the p_{O2} during sample preparations. The STO:Nb substrate worked as electron collector. The diffusive Nb shortened the effective STO thickness of the photoanodes, resulting in different IPCE performances of the STO/STO:Nb photoanode with a homojunction structure.

MARM 341

Super-resolution imaging of single-nanorod photoelectrocatalysis

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Photoelectrochemical water splitting devices represent a sustainable technology to generate hydrogen, a carbon-free chemical fuel. Device-level measurements have not revealed nanoscale strategies to interface their key components: catalysts and semiconductors. I will discuss our approach that combines single-molecule super-resolution reaction imaging and sub-particle-level photocurrent measurements to identify optimal oxygen evolution catalyst deposition sites on individual nanorod photoanodes. Our discovery leads to an activity based strategy for rationally engineering photoanodes with minimal amounts of catalysts.

MARM 342

Hydrogen production using Ag-Pd/TiO_2 bimetallic catalysts: Is there a combined effect of surface plasmon resonance with the Schottky mechanism on the photo-catalytic activity?

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A series of Ag-Pd/TiO_2 catalysts have been prepared, characterized and tested for H_2 production activities from water in the presence of organic sacrificial agents. The synergistic effect of metallic properties (plasmonic and Schottky mechanisms) was investigated. XPS results indicated that silver is present in the form of its oxides (Ag_2O and AgO) at 0.2-0.4 wt. % loading while palladium is present as PdO and Pd metal at similar loading. However, metallic character for silver particles increases while that of palladium metal particles decreases with increasing their % in the investigated range (0-1 wt. %). HRTEM results coupled with EDX analyses indicated the presence of two types of Ag containing particles (large ones with about 4-6 nm and smaller ones with ca. 1nm in size). Palladium was only found forming Ag-Pd alloy/composite with a wide size distribution range between 10-60 nm. Both particles are composed of silver and palladium, however. Optimal photocatalytic H_2 production rates were obtained for catalysts with a palladium to silver ratios between 4 and 1.5 in the case of bimetallic catalysts. In addition, H_2 production rates showed linear dependency on plasmonic response of Ag. The study demonstrates that increased H_2 production rates can be achieved from an understanding of plasmonic and Schottky properties of metals loaded on top of the semiconductor.

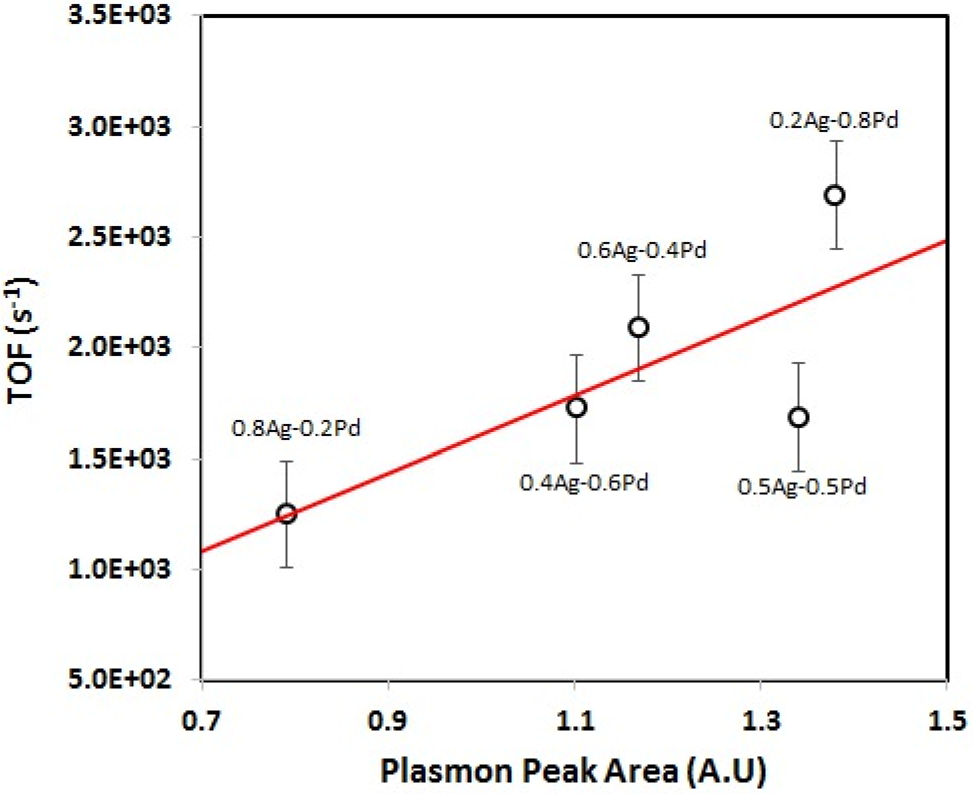

Fig. Turn over frequency (TOF) as a function of Plasmon peak area over Ag-Pd/TiO_2 photocatalysts.

MARM 343

Quantitative analysis of blends and copolymers of polyvinyl acetate (PVAc) using Fourier transform infrared spectroscopy (FTIR) and elemental analysis (EA)

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Fourier transform infrared spectroscopy is one of the most important instrumental techniques used to study the molecular structure of organic polymers. As part of our efforts to increase instrumental use in the undergraduate chemistry laboratory we have developed a quantitative FTIR experiment for use in our analytical and instrumental courses. The objective of the experiment is to determine the % composition of PVAC in copolymers and blends with polyethylene (PE) and n-vinyl pyrrolidone (PVP).
We report on the experimental methods used and the results obtained on examining the quantitative FTIR and elemental analysis of a series of ethylene vinyl acetate (EVAc) copolymers. The EVAc copolymers ranged from 10% to 80% of PVAc. Copolymers and blends of n-vinyl pyrrolidone – polyvinyl acetate ranging from 20 to 70% PVP were also analyzed.

MARM 344

Morphological studies of ring-substituted polyanilines by first and second-year undergraduates

***David M. Sarno**, dsarno@qcc.cuny.edu, Jean Hwang, Derek Perry. Chemistry, Queensborough Community College of CUNY, Bayside, New York, United States*

Polyaniline (PANI) and its derivatives belong to a class of intrinsically conductive polymers having unique electronic and optical properties. Many aspects of their study are well-suited to undergraduate research because they are easily synthesized, they are environmentally stable, and they are readily characterized by FTIR, UV-Vis, and SEM. Our work is focused on the synthesis and characterization of partially sulfonated PANI nanofibers (SPANI) and poly(*o*-toluidine) porous microspheres (POT). The negatively charged sulfonate groups on SPANI nanofibers can attract positively charged metal nanoparticles, and such high surface area composite materials may be used in sensors and other devices. However, sulfonation also imparts water solubility, which can significantly degrade the desirable nanostructure. To avoid this, we have modified a previously published method to partially sulfonate preformed PANI nanofibers via nucleophilic substitution with sodium metabisulfite. We are currently attempting to exert more control over the extent of sulfonation by limiting the availability of reactive sites on the PANI backbone. Porous POT microspheres may be useful as electroactive microreactors, scaffolds for catalysis, and encapsulants for drug delivery. The polymer, initially synthesized as an irregular granular material, undergoes a total morphological transformation when 4M NH_4OH is added to the crude product mixture. We have found that this is highly dependent on the amount of unreacted *o*-toluidine (OT) monomer in the system and we propose that the rapid change to an alkaline environment creates a water-in-oil-in-water double emulsion. The spheres are formed by insoluble OT droplets that dissolve the granular POT, and the pores are formed by water droplets trapped in the polymer matrix. Our current focus is to understand and control the size of the porous spheres. The development of our methods and the preparation and characterization of these materials as carried out by first and second-year undergraduates will be discussed.

MARM 345

Silicone chemistry in undergraduate laboratory and research courses

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Silicones and siloxanes provide excellent materials for demonstrating core concepts in general, inorganic and polymer chemistry, as well as introducing topics that are generally overlooked in traditional curricula, such as crosslinking and basic mechanical properties. As relatively safe, biocompatible, non-toxic materials, silicones are ideal for handling by both beginning and advanced undergraduate chemistry students. Herein, the many fundamental principles present in siloxanes are highlighted to show their versatility as teaching tools in the general chemistry classroom. Additionally, the design of a relatively simple, straightforward and tangible experiment suitable for an advanced inorganic laboratory course, which highlights the polycondensation of inorganic compounds and organometallic catalysis (hydrosilation), is described to expand on the traditional “silly putty” experiment. Finally, the use of silicones in two undergraduate research projects is presented focusing on their capabilities as inorganic surface modifying agents and various materials which can be easily made from them.

MARM 346

PUNK: An online resource for integrating polymer science into the undergraduate curriculum

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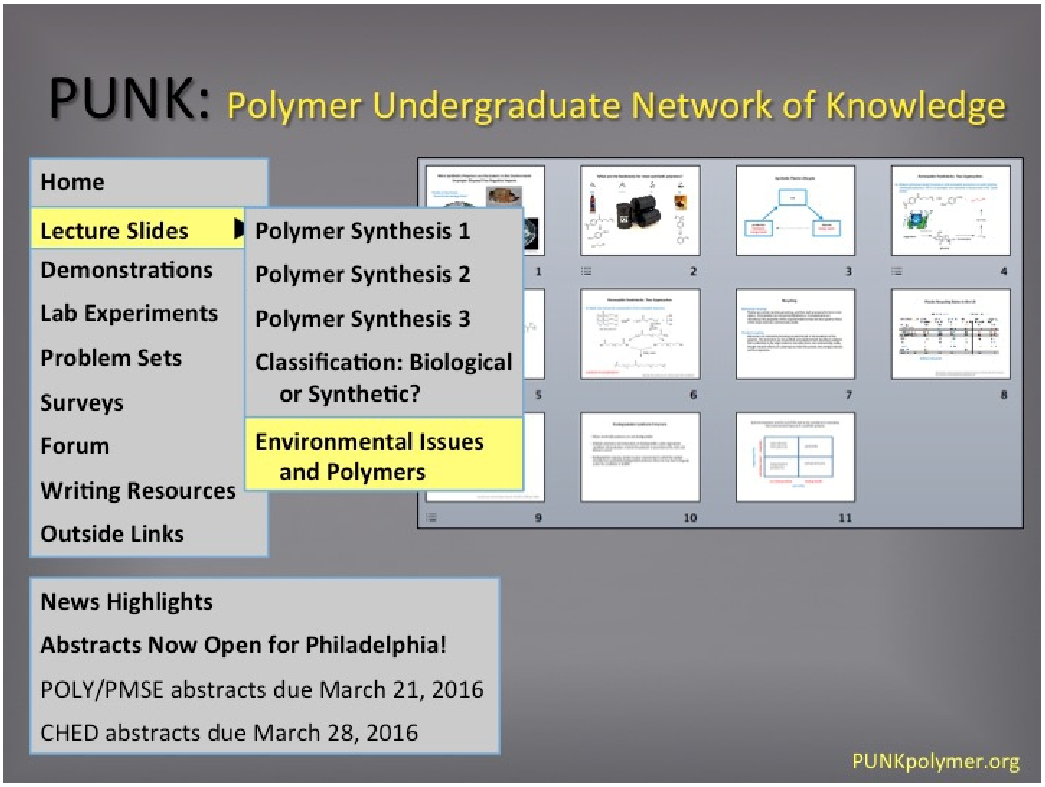
The 2015 ACS Guidelines for Bachelor’s Degree Programs now require that some course time be devoted to the introduction of polymers (synthetic and/or biological) and the discussion of meso-and nanoscale materials. Polymer Undergraduate Network of Knowledge, PUNK, is designed to be an online resource for the polymer community to assist in those teaching currently established courses or looking to create a new polymer course. Offering course content from lecture slides and laboratory experiments to textbook reviews and sample writing assignments, PUNKpolymer.org will serve to fill the knowledge gaps in polymer science by providing content that will be accessible for both introductory and upper level courses. This presentation will introduce the website (debuting spring 2016) and its contents. The audience is encouraged to bring their requests for content, and their ideas for contributions.



PUNK: Polymer Undergraduate Network of Knowledge

- Home
- Lecture Slides
  - Polymer Synthesis 1
  - Polymer Synthesis 2
  - Polymer Synthesis 3
  - Classification: Biological or Synthetic?
  - Environmental Issues and Polymers
- Demonstrations
- Lab Experiments
- Problem Sets
- Surveys
- Forum
- Writing Resources
- Outside Links

News Highlights

Abstracts Now Open for Philadelphia!

POLY/PMSE abstracts due March 21, 2016

CHED abstracts due March 28, 2016

PUNKpolymer.org

MARM 347

Industrial role-playing to replace the traditional laboratory experiment: Formulating nail polish

Naphtali O'Connor, *naphtali.oconnor@lehman.cuny.edu. Chemistry, Lehman College, Bronx, New York, United States*

The role of the laboratory in the modern classroom is to teach lab skills and re-inforce the lecture. Implied in this is the preparation of students for the chemical industry or graduate school. However the formulaic design of labs does a poor job of preparing students for a life in industry. Most labs are designed with a hypothesis or question and a known answer. It is the job of the student to achieve this answer. The purpose of labs are further complicated by interactions with students that have previously taken the course or the availability of information on the internet.

Herein is described our preliminary work towards developing an investigative model for laboratory design where students ‘role-play’ as industrial research chemists. Within this premise the laboratory experiment resembles the duties of a research scientist in an industrial setting. The objectives of this experimental model are to **1.** Providing insight and prepare students for a career in Industry, **2.** Introduce students to the scientific process particularly as it pertains to product development and **3.** Equipping students with the opportunity to develop logical, systematic problem solving skills that can be deployed in any career. With this model, laboratory experiments are replaced with ‘Scenarios’. Within a scenario students are given a task similar to that of an industrial chemist. For example, the development or improvement of a product. We demonstrate the prototype of a scenario experiment where students will utilize latex materials to develop films for commercial products in a similar setting to that of a chemical industry research scientist. As a proof-of-concept we targeted the commercial product nail polish. In this scenario, students must first determine the attributes of a good nail polish. Then students are given a series of latex materials to determine their glass transition temperatures and particle size. These properties play a role in their film forming ability and the physical attributes of the films. The student then prepares films from binary latex solutions and optimized these formulations to obtain the model properties of a nail polish. The student then connects how the latex particle properties are connected to the film properties and how a research chemist might utilize this information to produce film forming products.

MARM 348

Accommodating individuals with disabilities in the chemistry lab: Focus on students accompanied by service dogs

***Sally J Ramp**, joeyramp@yahoo.com. Neuroscience, University of Illinois, Mahomet, Illinois, United States*

The question of access for individuals with disabilities is widely debated in higher education, especially among STEM major administrators and professors. Individuals with disabilities are underrepresented in the STEM major demographic as a whole. Within the field of chemistry there is resistance among some scholars and departmental administration to look beyond a person’s disability and look to what changes can be made, primarily within the chemistry laboratory, to accommodate and allow equal access to coursework and research opportunities, while still meeting safety regulations and following appropriate safety protocol. This resistance is detrimental and borders on exclusion; this leads to the discouragement of students with disabilities to choose or apply for majors within the School's of Chemical Sciences. As a current student with a disability and a service dog, seeking a degree in Neuroscience and having a prior career in Research and Development, I present from a unique perspective. This presentation focuses on the issues of equal access for students with disabilities in teaching and research laboratories, with special attention to these students accompanied by a service dog. Specifically, I will be looking at the safety concerns of having a service dog in a laboratory, including discussion of current working solutions. Input from a current professor of Organic Chemistry, regarding the thought, time requirement and lab reconfiguration required to accommodate a service dog team is included in this presentation. Service dogs are being utilized to mitigate many different disabilities and are becoming a more visible presence on college campuses. This presentation, by closely examining the working model I have developed that meets both federal ADA regulations and meets safety requirements in chemistry laboratories, sheds new light on the rarely acknowledged issue of disability exclusion, primarily service dog exclusion in chemistry laboratories and what can be accomplished through open and informed dialogue.

MARM 349

Twenty-first century digital science access tools: Opening doors of opportunity for the blind to promote hands-on learning

***Cary A. Supalo**, cas380@gmail.com. Independence Science, West Lafayette, Indiana, United States*

In this interactive presentation, the newest in a line of talking scientific data logger technologies to be used in the chemistry laboratory classroom will be described and demonstrated. This twenty-first century technology will empower students who are blind or visually impaired to experience a more engaging science curriculum through hands-on learning in wet chemistry labs. Hands-on engagement is well-established as leading to increased interest in Science, Technology, Engineering, and Mathematics subject areas. Additionally, the first text-to-speech enabled organic chemistry drawing tool will be demonstrated.

This new multi-sensory science learning tool scaffolds students' understanding of organic chemistry structures.

MARM 350

Preparing students with disabilities for the challenges of graduate school: Thoughts from a REU program

Karl S. Booksh*, kbooksh@udel.edu, Sharon Rozovsky, Joseph P. Smith. Chemistry and Biochemistry, University of Delaware, Newark, Delaware, United States*

Students with disabilities continue to be an underrepresented and understudied demographic in science, technology, engineering and mathematics (STEM) fields. In the 25 years since the passage of the Americans with Disabilities Act (ADA) we have experienced improved educational services for students with disabilities in K-12 and post-secondary education. However, post-secondary institutions are seeming focused on accessibility for mobility and sensory impaired students while unprepared for the influx of students with learning, psychological, or social disabilities. Consequently there has not been an ultimate improvement in post-secondary outcomes; the percentage of STEM doctorates earned by people with disabilities has remained flat for 25 years. The statistics regarding the students with disability pipeline will be presented along with some theories regarding the major loss points and ideas for improving the performance and persistence of students with disabilities in STEM. In this context, the outcomes from a research experience for undergraduates program in chemistry and how the students were affected through their educational journey will be presented.

MARM 351

Service dogs in the academic laboratory

Patricia A. Redden*, predden@saintpeters.edu. Chemistry, Saint Peters University, Jersey City, New Jersey, United States*

The use of service dogs by individuals with disabilities is increasing, and their presence in the chemistry laboratory raises issues of compliance with the Americand with Disabilities Act (ADA), the needs of the individual chemist, and concerns about the safety of the dog and of other individuals in the laboratory. This paper addresses these issues and gives some guidelines for discussion with the dog's partner about the feasibilty of having the dog present during laboratory.

MARM 352

Nanoscience in the undergraduate curriculum: Introducing students to tiny miracles

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The field of nanoscience has generated a lot of interest and funding since the turn of the century and courses in nanoscience and nanotechnology have been introduced in the undergraduate curriculum across the country. At Susquehanna University, the ACS-certified Chemistry Department first offered Nanoscience as a Special Topics Elective in 2006. The course has been offered three more times since, and is open to all science majors. The format has varied from traditional lecture/lab to a hybrid

lecture/discussion/workshop format. Interdisciplinary connections between chemistry, physics, biology and material science are investigated through readings, discussions and laboratory activities. Major topics include the formation and implementation of nano-structured systems, the physics behind their unique properties, synthesis and detection of nanoparticles, their current roles in technology, medical applications, ethical implications, and the future impact of such systems on society, industry and the environment. Students are expected to read, discuss and formally present literature articles, engage in debate about the ethics and promise of nanotechnology research and write an original proposal. Laboratory activities include synthesis and characterization of nanoparticles (ex. Gold, silver and zinc oxide), applications (ex. Solar cells with titanium dioxide, SERS), and tools of nanoscience (lithography and microcontact printing).

MARM 353

Nanomaterials education for CUNY science and engineering undergraduates

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A strong need for the availability of engineers and scientists educated in the field of nanotechnology was identified in 2003. The increasing number of nanomaterials and nanotechnology related articles in both the public sector and in the scientific literature at the time indicated the interest in the field and the need for a mature perspective amongst young scientist, engineers and the general public. Exposure of students at all levels in Science and Engineering as well as non-Science and non-Engineering majors was deemed necessary to prepare the US for the interdisciplinary nature of nanoscience and -technology.
Thirteen years later, we report about the outcomes of and lessons learned from educational activities carried out over a ten-year time frame with funding from the National Science Foundation's NUE initiative at the City College of New York, a senior college of the City University of New York. A coherent modular nanomaterials course was created that reflects the interdisciplinary nature of nanomaterials. The course has been taught eight times since its inception in spring of 2007 both at the undergraduate and graduate level. The course content was designed with a modular structure such that the modules can be used as independent units. In addition to implementing and teaching the course at CCNY, we have also collaborated with six CUNY community colleges and will discuss difficulties and opportunities we have encountered in the implementation of nanomaterials education.

MARM 354

Integrating nanotechnology in CUNY Hostos Community College: Successes and challenges

Mohammad Sohel, *msohel@hostos.cuny.edu. Natural Sciences, CUNY Hostos Community College, Bronx, New York, United States*

As progress for nanotechnology research and development picks up speed, more and more universities are beginning to offer degree programs in nanotechnology. These programs now range from minor and majors in nanotechnology to Masters' programs to PhD's in any number of nanotechnology-related fields. The presentation aims at the integration of nanotechnology education in the early years at City University of New York's junior and senior colleges in a two-stage implementation process. The proposed program has three major objectives: (a) Curriculum design, condensation and refocusing of course and laboratory components (b) analysis and optimization of the implementation process as a pilot study for future teaching material and (c) creation of a pipeline for a diverse group of research-trained students from junior to senior college across CUNY with the following goals: to familiarize and initiate excitement and interest in the "nano" area by providing affective, knowledge and skill based training integrating POGIL as a group learning component. Along with class criteria, pre- and post- surveys were conducted which showed increasing special interest and eagerness about this new frontier of science among our science and engineering students. Also, students were tracked to their interest and career goals to understand the impact of the exposure.

MARM 355

Introduction of a nanoscience lecture and laboratory course into an undergraduate curriculum at a community college

Tirandai Hemraj-Benny, *themrajbenny@qcc.cuny.edu. Chemistry, Queensborough Community College, Bayside, New York, United States*

Nanoscience is an emerging and exciting field. There is an increased interest in educating undergraduates about this growing discipline. At Queensborough Community College, The City University of New York, a lecture course was first introduced into the curriculum to satisfy the scientific world requirement for graduation. Many science and non-science majors took this writing intensive course over two semesters. The format now incorporates a laboratory component where students will have the unique opportunity to obtain hands-on experience in using an Atomic Force Microscope and a Scanning Electron Microscope, not common at most community colleges. The synthesis of nanomaterials, the tools used to characterize these materials and societal impacts of nanomaterials and nanotechnology (such as ethical, legal and environmental implications) are discussed in this lecture and laboratory combination.

MARM 356

Involving undergraduate students in nanoscience research at a community college

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Queensborough Community College (QCC) is predominantly a minority and Hispanic serving institution situated in Queens, New York. In the chemistry department at QCC, I have mentored several undergraduate students in nanoscience research involving simple synthetic strategies in making single-walled carbon nanotubes-metal nanoparticle composites for catalytic and mechanical applications. These undergraduate students have given several oral and poster presentations at both local and national ACS meetings. Some of these students have also had the unique opportunity to participate in Research Experience for Undergraduates (REU) Summer Programs. In addition, their research findings have been published in peer-reviewed journals.

MARM 357

Synthesis of biologically interested heterocyclic compounds

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This presentation highlights our recent effort on the development of green reaction and separation techniques for the synthesis of diverse heterocyclic scaffolds through the integration of atom economic multicomponent reactions (MCRs), step economic one-pot synthesis, energy efficient microwave reactions, and straightforward fluorous solid-phase extraction (F-SPE) for the synthesis of compound libraries with substitution, skeleton, and stereochemistry diversities. The compounds have been submitted for screening against different drug targets for to the discovery of several leads such as **UMB-32,** a novel BRD4 bromodomain inhibitor.

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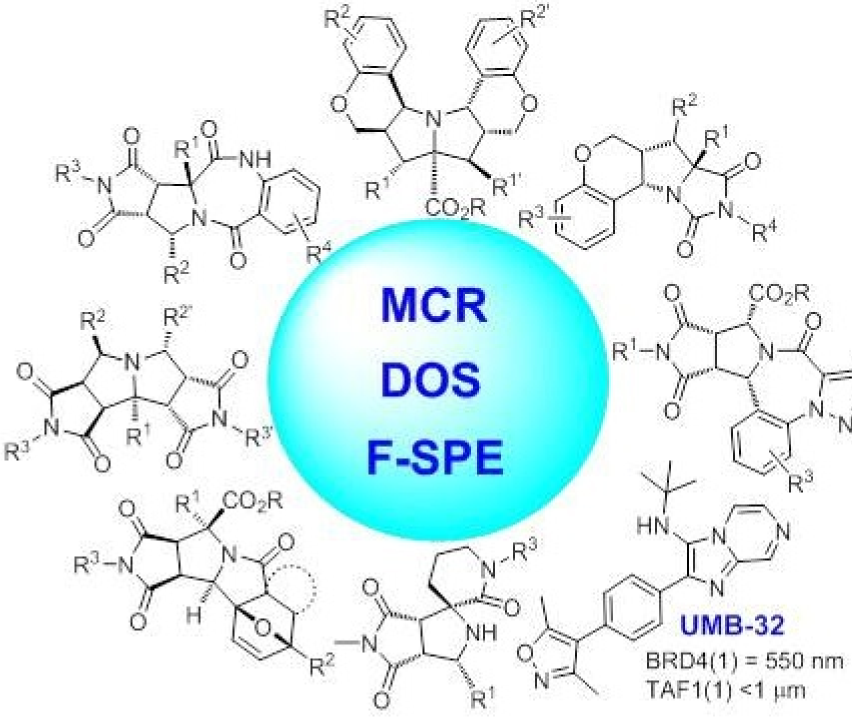


Synthesis of diverse heterocyclic molecules

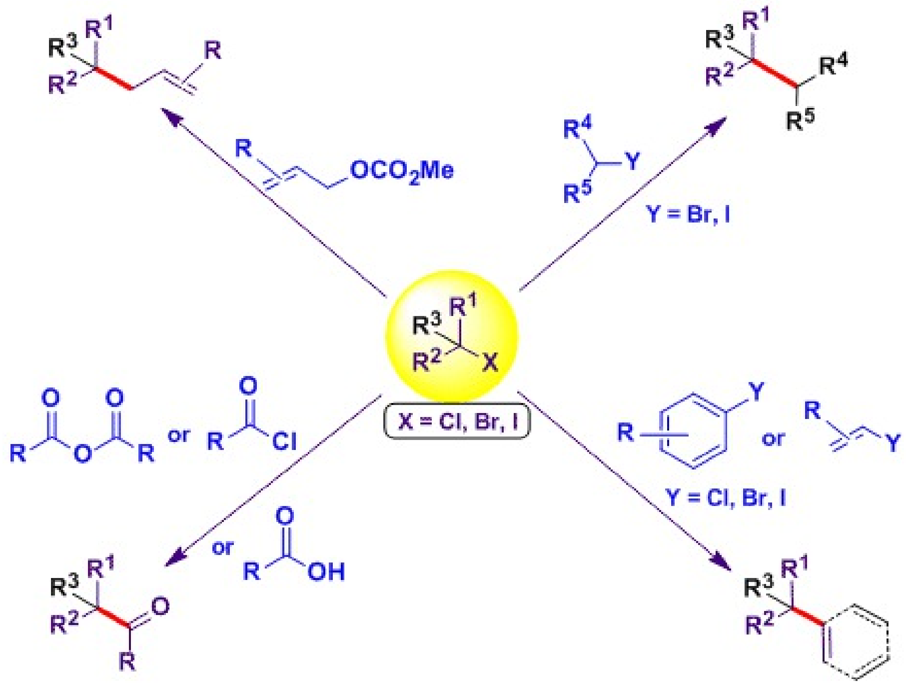
MARM 358

Nickel-catalyzed reductive coupling of alkyl halides with other electrophiles

Hegui Gong, *hegui_gong@shu.edu.cn. Chemistry, ShangHai University, ShangHai, ShangHai, China*

Ni-catalyzed reductive cross-coupling of alkyl halides with other electrophiles have been successfully developed. The formation of C(sp3)-C bonds can be readily achieved from the coupling of alkyl halides with other alkyl and aryl halides, allylic carbonates and acid derivatives. The reactions feature excellent functional group tolerance and broad substrate scope under mild conditions. Recently, the reductive coupling strategy has been successfully applied to the sterically more demanding unactivated tertiary

alkyl halides. The coupling with acids and aryl halides allows efficient synthesis of acylated and arylated quaternary carbon compounds without pre-preparation of organometallic reagents (Figure 1).



MARM 359

Dual cross-coupling involving α-amino radicals generated from organotrifluoroborates

***Mirna El Khatib**, elmirna@sas.upenn.edu, Gary A. Molander. Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania, United States*

Direct access to complex, enantiopure benzylamine architectures using a synergistic iridium photoredox/nickel cross-coupling dual catalysis strategy has been developed. α-Amino radicals are generated by visible light photoredox-based oxidation of R-BF_3K and are captured in nickel catalysis forming C(sp3)C(sp2) bond.

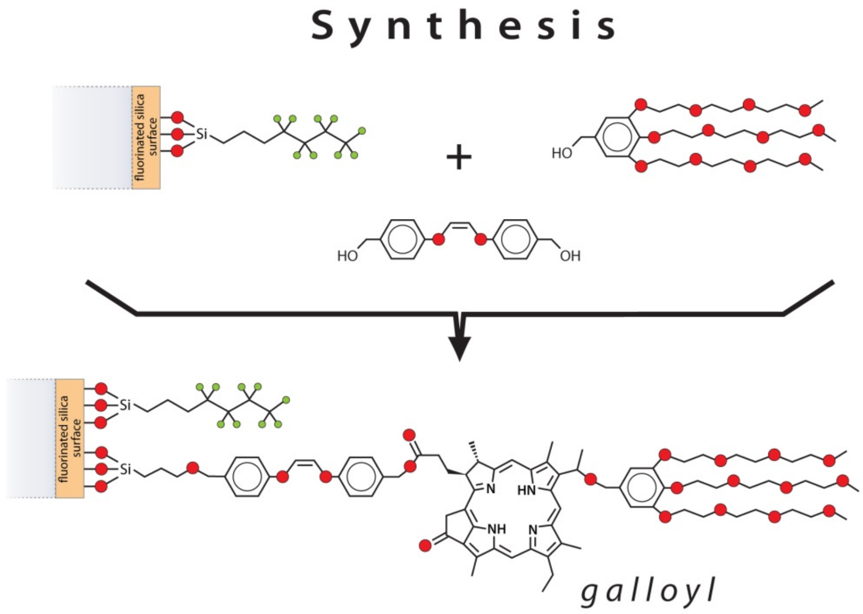
El Khatib, M.; Serafim, R. A. M.; Molander, G. A. "*α-Arylation/Heteroarylation of Chiral α-Amino Radicals via Synergistic Iridium Photoredox and Nickel Cross-Coupling Catalysis*" **2015**, *Angew Chem., Int. Ed.* **2015**, *128,* 262.

MARM 360

'All-in-one' photodynamic device: Synthesis of a poly(ethylene glycol) galloyl sensitizer tip

***Ashwini A. Ghogare**[2,1], ashwinighogare_86@yahoo.com, Alexander Greer[2,1]. (1) Chemistry, Brooklyn College of the City University of New York, Brooklyn, New York, United States (2) Ph.D. Program in Chemistry, Graduate Center of the City University of New York, New York, New York, United States*

Synthesis of a specialized silica tip an all-in-one photodynamic therapy (PDT) device capable of delivering all components necessary for photodynamic therapy, has been described. Oxygen, light and a cleavable tripolyethylene glycol (PEG)-galloyl pheophorbide sensitizer are simultaneously delivered by the silica tip, where the tip was synthesized in six steps. A comparison of synthetic steps to reach PEGylated sensitizers bound to fluorinated silica and a previously reported Teflon/polyvinyl alcohol (PVA) nanocomposite, was made. The hydrolytic stability of the attached PEGs and the extent to which the PEG groups enhance solubility will also be discussed. The new triPEG-galloyl sensitizer has the potential for use in intraoperative pointsource photodynamic therapy which aims for precision treatment of residual disease.



Schematic of the synthesis of a poly(ethylene glycol) galloyl sensitizer attached photoactive silica tip.

MARM 361

A facile conversion of alkynones to enaminones and its synthetic application

Yu Chen, *yu.chen1@qc.cuny.edu. Chemistry & Biochemistry, Queens College, Flushing, New York, United States*

Enaminones are a group of versatile and frequently employed C3 synthons in synthetic organic chemistry, especially in the synthesis of heterocyclic compounds. Its preparation has attracted the synthetic organic chemists' interest for decades. Our group has recently discovered a facile synthetic route for the preparation of enaminones by converting simple alkynone compounds to isoxazoles/5-hydroxy-2-isoxazolines followed by FeCl3-catalyzed ring opening reactions. This synthetic route is highly regioselective and promises facile synthesis of a variety of enaminone derivative compounds. A detailed reaction mechanism as well as the application of this new synthetic method in the preparation of interesting heterocyclic compounds will be discussed.

MARM 362

The role of organized water in mediating ligand-protein interactions

***Jonathan D. Gough**, jonathan@jonathandgough.com. Chemistry, Lehman College, New York, New York, United States*

The displacement of water from the surface of a protein, by a binding partner (ligand), provides a contribution to its binding free energy. However, despite these contributions, it is rare for all waters to be displaced within said binding site. In fact, in many cases, crystalized waters are present and mediate interactions between a protein and ligand. Some waters are critical for ligand binding. From a ligand docking perspective, they are considered part of the binding site topography; water in HIV-1 protease and acetylcholine receptors have been targeted to increase inhibitor affinity. The structure of water in β2 adrenergic receptor played an important role in describing the mechanism of receptor activation. As water organizes itself within these complex proteins, it effects protein structure, function and mediates ligand protein interactions. Therefore, the exploration of the thermodynamic properties of these molecules provides insight about protein function and activity. Here we applied solvation thermodynamic mapping techniques, which rely heavily on Inhomogeneous Solvation Theory, on a series of drug binding proteins. We will discuss the role of water and water networks in protein ligand interactions, in addition to shedding insight regarding how to treat water in the context of docking experiments.

MARM 363

Multiscale simulations to characterize the blood-brain barrier tight junctions

***Shikha Nangia**, snangia@syr.edu. Biomedical Chemical Engineering, Syracuse University, Syracuse, New York, United States*

Although discovered more than 100 years ago, the blood-brain barrier remains an unresolved scientific challenge. It is widely accepted that the blood-brain barrier is the brain's security system that allows entry of essential nutrients while blocking potentially harmful substances. The selectivity of the BBB is critical in maintaining the homeostasis of central nervous system, yet the BBB is a major hurdle in treating neurodegenerative diseases, such as Alzheimer's and Parkinson's. Specialized physical barrier called "tight junctions" present between adjacent endothelial cells act as molecular gatekeepers in regulating paracellular traffic at the blood-brain interface. Understanding the molecular basis of the tight junction selectivity has been difficult using experimental methods. In my research group, we are characterizing molecular interactions responsible for the tight junction assembly using multiscale molecular dynamics. The molecular insights from this research have propelled us a step forward towards solving the blood-brain barrier puzzle, and consequently are aiding in designing novel therapeutics to treat the brain-related ailments.

MARM 364

Molecular interactions of complex biological systems in rare and orphan diseases

***Kenny Nguyen**[1,2], nguyenk6@chop.edu, Lifeng Tian[1], Dong Li[1], Michael March[1], Renata Pellegrino[1], Charlly Kao[1], Patrick Sleiman[1,3], Hakon Hakonarson[1,3]. (1) Center for Applied Genomics, The Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States (2) Proteins and Disease Research Affinity Group, The Children's Hospital of Philadelphia, Philadelphia, Pennsylvania, United States (3)*

Department of Pediatrics, Perelman School of Medicine, University of Pennsylvania, Philadelphia, Pennsylvania, United States

The Center for Applied Genomics (CAG) at The Children's Hospital of Philadelphia (CHOP) is one of the largest and foremost institutions of its kind in the world. CAG has recently integrated molecular modeling and simulation in its precision and translational medicine pipeline to elucidate and observe the structure, dynamics, and energetics of systems at a tractable spatiotemporal resolution. A core mission at CAG is to identify the genetic basis and function of diseases – common, rare, and orphan – in children and translate those findings into novel therapeutics. However, there are between 7,000 and 8,000 known rare and orphan diseases in the world. About 4% of those have effective drug therapies. There are over 25 million people that are affected by a rare and orphan disease in the United States alone. About one in every 12 newborn children is affected by it. It is important to note that about 10% of all rare and orphan disease patients in North America come through CHOP; therefore, CAG contains an infrastructure for such cases. Of the many systems in the pipeline, cystatin C (CST3), CXC chemokine receptor type 1 (CXCR1), and palmitoyl protein thioesterase 1 (PPT1) will be shown where the disease and system can be structurally linked through chemistry and high performance computing (HPC), as well as continue to reduce the immense gap for effective therapeutics.

MARM 365

A grand canonical ensemble approach to solution interfaces: Inference of the concentration gradient

***Mark N. Kobrak**, mkobrak@brooklyn.cuny.edu. Chemistry, Brooklyn College -- CUNY, Brooklyn, New York, United States*

It is well-known that surface-active molecules in solution form a concentration gradient in close proximity to the interface. However, the nature of this concentration gradient remains poorly understood. In this work, we develop a simple thermodynamic model of the interface that permits inference of the concentration gradient. The model is similar in spirit to the Gibbs isotherm, but exploits the properties of an equilibrium system in a way that links the lengthscale of the concentration gradient with the concentration of the solute in the bulk liquid and the surface tension of the solution. The results may be of use in identifying the optimal surface morphology for applications in heterogeneous catalysis and electrochemistry.

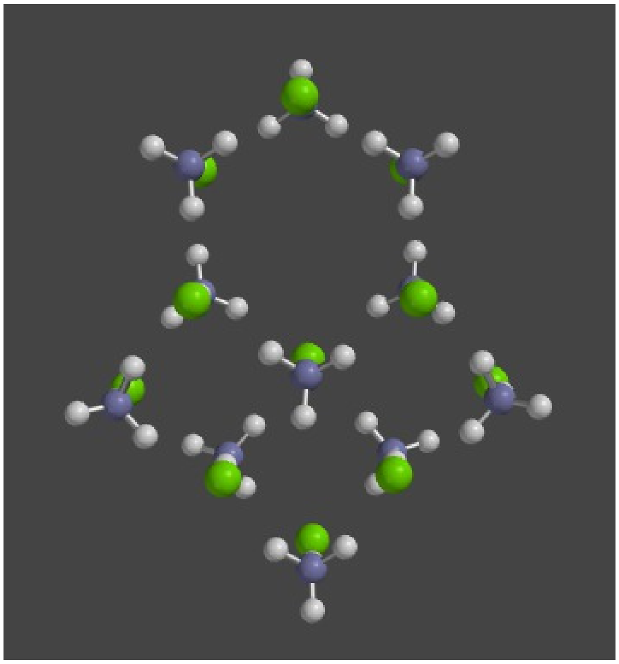
MARM 366

Mag-walking Monte Carlo and quantum mechanics predictions of structures and interaction energies of ammonium halide clusters

***Robert Q. Topper**, topper@cooper.edu, John J. Biswakarma, Vlad Ciocoi. Chemistry, The Cooper Union, New York, New York, United States*

Contributions from different intermolecular and interionic forces, as well as variations in bond energies, may produce size-dependent variations in the structures of molecular clusters formed from acid-base chemistry. The growth patterns of ammonium chloride, bromide and fluoride clusters are considered using quantum molecular modeling and “mag-walking” simulated annealing Monte Carlo calculations. Simulated annealing is used to identify local and global minima of the particles. Second order Moller-Plesset (MP2) and M06-2X density functional theory calculations are used to predict the interaction

energetics and free energies as a function of size, which correlate well with available mass spectrometric data. Taken together, these three types of systems variously exhibit competition and cooperation between ionic forces, hydrogen bonds, bond energies, and dipole-dipole interactions in an interesting, size-dependent manner. In particular, three different types of hydrogen bonds are predicted in ammonium fluoride clusters.



MARM 367

Water in dopamine receptors: Using solvation thermodynamics to modify a lead compound for specificity

Satish Gadhiya[1,5], Sudharshan Madapa[1], Thomas P. Kurtzman[3,5], Ian L. Alberts[6], ***Steven Ramsey**[2,4]*, *vpsramsey@gmail.com, Nagavara-Kishore Pillarsetty[7], Teja Kalidindi[7], Wayne W. Harding[1,5]. (1) Chemistry, Hunter College, CUNY, New York, New York, United States (2) Chemistry, Lehman College, Bronx, New York, United States (3) Chemistry, Lehman College, CUNY, New York, New York, United States (4) Biochemistry, CUNY Graduate Center, New York, New York, United States (5) Chemistry, CUNY Graduate Center, New York, New York, United States (6) Natural Sciences, LaGuardia Community College, New York, New York, United States (7) Radiology, Memorial Sloan Kettering Cancer Center, New York, New York, United States*

Dopamine receptors play an integral role in numerous neurological pathways, notably related to emotions and mental stability. Traditionally drugs have been targeted at this family of GPCR's with the intent of suppressing or modifying Schizophrenic tendencies as well as the treatment of Parkinsons Disease. By targeting D3 and minimizing affinity for D2 a drug like compound may be devised for the treatment of addictive behavior, also found to be influenced by Dopamine. In this study we discuss that rational lead modification of a known binder Stepholidine relying heavily on solvent thermodynamics, where we aim to add affinity and in particular, specificity to Dopamine receptor D3 while minimizing D2 affinity. Here we display the characteristics of solvent properties that were considered when guiding rational lead modification as well discuss modifications that have been synthesized by our collaborators at Hunter Colllege and, in particular, the computational validation performed on these derivatives.

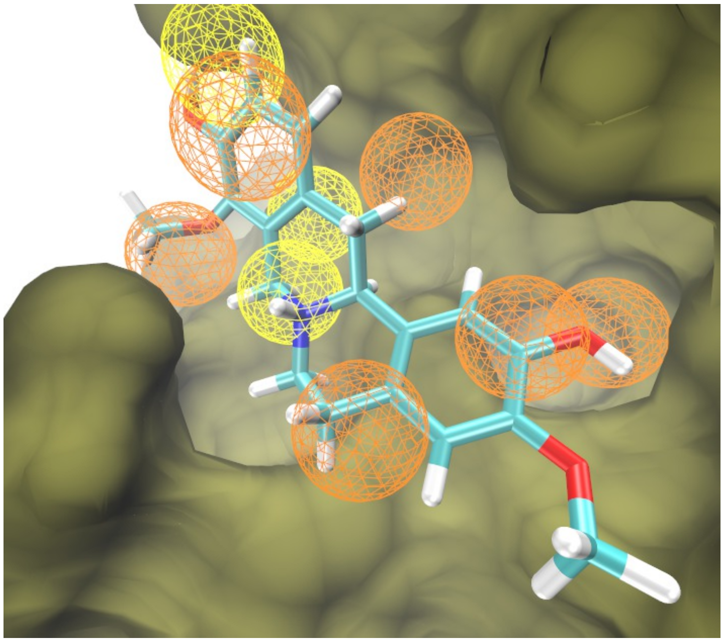


Figure 1. Lead molecule Stepholidine bound to Dopamine receptor D3. Sites of high occupancy water with unfavorable free energy are shown in orange and unfavorable entropy in yellow. These sites can be utilized to predict ligand binding behavior.

MARM 368

The isotropic local Wigner-Seitz model: An accurate theoretical model for the quasi-free electron energy in fluids

Cherice M. Evans[1,3], *cherice.evans@qc.cuny.edu, Gary L. Findley*[2]. *(1) Chemistry and Biochemistry, Queens College CUNY, Flushing, New York, United States (2) University of Louisiana at Monroe, Monroe, Louisiana, United States (3) Chemistry, Graduate Center -- CUNY, New York, New York, United States*

The quasi-free electron energy $V_0(\rho)$ is important in understanding electron transport through a fluid, as well as for modeling electron attachment reactions in fluids. Our group has developed an isotropic local Wigner-Seitz model that allows one to successfully calculate the quasi-free electron energy for a variety of isotropic fluids from low density to the density of the triple point liquid with only a single adjustable parameter. This model, when coupled with the quasi-free electron energy data and the thermodynamic data for the fluids, can also yield optimized intermolecular potential parameters and the zero kinetic energy electron scattering length. In this poster, we give a review of the isotropic local Wigner-Seitz model in comparison to previous theoretical models for the quasi-free electron energy. *Acknowledgments: All measurements were performed at the University of Wisconsin Synchrotron Radiation Center, a facility that was primarily funded by the University of Wisconsin – Madison with supplemental support from facility Users and the University of Wisconsin – Milwaukee. This work was supported by a grants from the National Science Foundation (NSF CHE-0956719), the Petroleum Research Fund (45728-B6 and 5-*

24880), the Louisiana Board of Regents Support Fund (LEQSF(2006-09)-RD-A33), and the Professional Staff Congress – City University of New York.

MARM 369

Conjugate chains and bimolecular electron transfer

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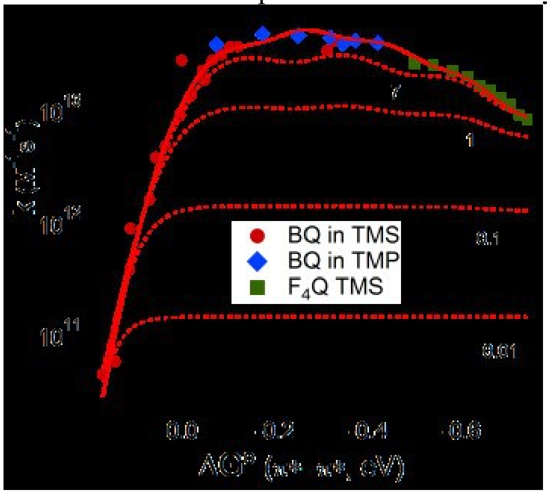
This talk will address two subjects. We would like to understand charge and exciton transport in long conjugated molecules, which are candidates to act as "molecular wires." Charges and excitons in these polymers are typically delocalized over a few nm, rather than highly delocalized as in some inorganic semiconductors. While this partial delocalization appears to help transport, we would like to probe what limits both delocalization and transport. Some recent results are the amazing behavior of triplet excitons, which traverse the entire lengths of conjugated polyfluorene chains up to >100 nm long in a time < 1 μs, and probably much faster. A surprising finding is that triplet excitons may move as fast or faster than singlets.(1) A related finding is the effect of large dihedral angles, which can act as barriers to transport, but more so for singlet excitions than for electrons, holes or triplets excitons.(2)

We also explore rates of bimolecular electron transfer in solution. The experiments of Rehm and Weller and more recent experiments did not find the decrease of electron transfer rates predicted by the Marcus theory to occur at high driving forces. The talk will describe experiments in which the electron donor is a high-mobility electron in a non-polar liquid. These reactions have two important features: 1) The electrons move so fast that the reaction rates are not constrained by the diffusion-controlled limit, and 2) The energy of the electrons and hence the thermodynamic driving force, -ΔG°, can be adjusted continuously over a range of nearly 300 meV by changing the pressure. Results at right show the we can observe a three-decade increase with driving force, the "normal region," and a small inverted region.(3) These reactions form products in electronically excited states.



The data also contain evidence for a much larger inverted region for electron transfer to form ground state products.

MARM 370

Obtaining redox potentials without any electrolyte by studying one electron charge transfer equilibria with pulse radiolysi

Matthew Bird[1]*, mbird@bnl.gov, Matthew Pearson*[2,1]*, John R. Miller*[1]*. (1) Chemistry, Brookhaven National Laboratory, Shoreham, New York, United States (2) Chemistry, Brown University, Providence, Rhode Island, United States*

Redox potentials are typically measured with cyclic voltammetry in polar solvents, yet the applications where we may wish to know the energy of charge states often occur in low polarity environments without electrolyte (organic photovoltaics, photosynthesis, solid state dye sensitized solar cells). By measuring one electron charge transfer equilibria with pulse radiolysis, as a function of electrolyte concentration, we are able to connect redox values measured from cyclic voltammetry in THF (ε=7.6) to their values in the absence of electrolyte. In a low polarity solvent such as THF it turns out that the majority of the shifts in redox potentials with electrolyte are caused by single ion pairing. These shifts are sensitive to the degree of delocalization of charge on the radical anion involved. Other smaller factors affecting redox potentials due to the presence of electrolyte including long-range Coulomb interactions and triple ions will be discussed and quantified. This work provides a pathway to obtaining redox values that truly reflect the energetics of ions in the environments where we would wish to know them.

MARM 371

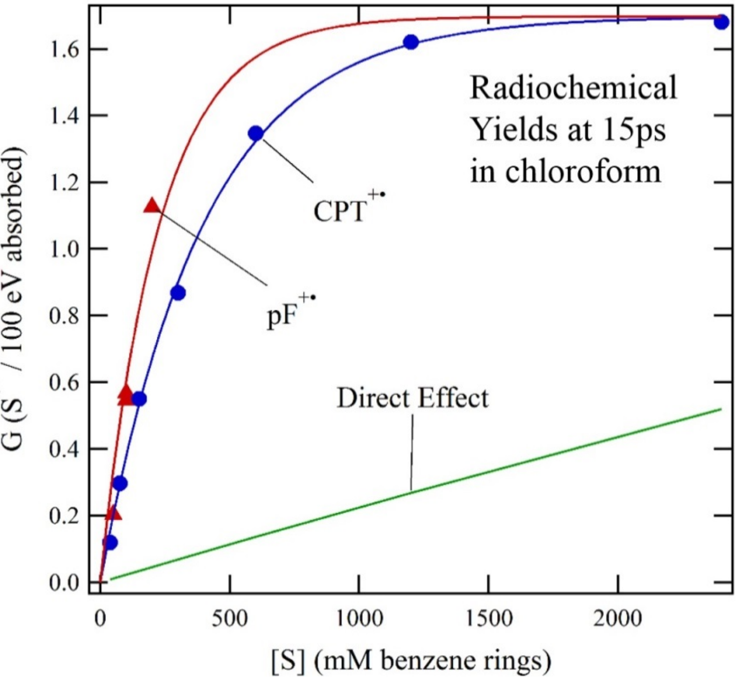
Exceptionally rapid capture of radical cations formed by pulse radiolysis

Andrew R. Cook*, acook@bnl.gov, Matthew Bird, John R. Miller. Chemistry, Brookhaven National Laboratory, Upton, New York, United States*

Ionization followed by capture of resulting electrons and radical cations are primary processes that define all chemistry occurring after radiolysis. Electrons ejected from solvent molecules are well known to be captured by solutes rapidly, having high mobility in many liquids. Before they are relaxed and solvated in the liquid, they are far more mobile and can attach efficiently at much higher rates to many solutes. The associated radical cations are expected to be solvent molecular ions which are captured by solutes at normal diffusion controlled rates; far more slowly than capture of electrons and in most cases in lower yield. Experiments at Brookhaven National Laboratory's LEAF facility surprisingly find otherwise. At 200mM of terphenyl(CPT) in chloroform, one might expect ~10% of solute radical cations to be captured fast; we find instead nearly all cations formed are captured in under 15 ps (see figure). Not only is capture exceptionally rapid, but it occurs in very high yield, rivaling that for capture of electrons. This is the first observation of this phenomena.

The mechanism of capture is not known. The data follow a similar form to that for capture of electrons prior to solvation, suggesting that radical cations in these experiments are also captured before solvation. Current efforts to understand this phenomena will be described. Experiments are finding substantial yields of solute radical cation production in a variety of media, suggesting that this process is a fundamentally important one that has been missed in the past, with significant consequences. One in particular is that it appears to provide a route to produce solute radical cations rapidly and unexpectedly in media not known

to make cations under normal conditions, important in many areas, including processing of nuclear fuel and waste.



MARM 372

Photochemical and pulse radiolysis studies of intermediates involved in CO_2 reduction

***David C. Grills**[1], dcgrills@bnl.gov, Jonathan J. Rochford[2], Ken T. Ngo[2], Sergei V. Lymar[1], James F. Wishart[1]. (1) Chemistry, Brookhaven National Laboratory, Upton, New York, United States (2) Chemistry, University of Massachusetts Boston, Boston, Massachusetts, United States*

The goal of our research is to gain a fundamental understanding of the processes involved in the capture and chemical conversion of solar energy, typically using transition metal complexes as catalysts. These processes involve multiple redox states, many of which are transient in nature. Gaining a detailed kinetic and mechanistic knowledge of catalytic cycles is crucial for understanding and developing more efficient photoconversion systems. To this end, we make use of time-resolved spectroscopic detection methods coupled with either laser flash photolysis (LFP) or pulse radiolysis (PR). Although we often make use of transient absorption (TA) detection in the UV/visible/near-IR regions, a particular emphasis is placed on time-resolved mid-IR (TRIR) detection techniques, which target improved characterization of transient intermediates due to the structural specificity of mid-IR spectroscopy. We recently implemented, for the first time, nanosecond TRIR detection for PR using high-power quantum cascade lasers (QCLs) as the IR source. This has opened up many new opportunities for mechanistic investigations of redox-active species that can be directly prepared by the short electron pulse in a PR experiment.

We previously reported[1] the use of PR-TRIR to unravel the kinetics and mechanism of formation of the one-electron reduced Mn-based CO_2 reduction catalyst, $[Mn(^tBu_2\text{-bpy})(CO)_3]_2$ ($^tBu_2$-bpy = 4,4'-$^tBu_2$-2,2'-bipyridine) from the precatalyst, *fac*-$Mn(OC(O)H)(^tBu_2\text{-bpy})(CO)_3$. The use of TRIR allowed all intermediate species to be directly observed and characterized, and the rate constant for dimerization, $2k_{\text{dim}} = 1.2\text{x}10^9\ M^{-1}s^{-1}$, to be determined. However, to probe the reactivity with CO_2 we require access to the two-electron reduced intermediate, [Mn(^{t}Bu$_2$-bpy)(CO)$_3$]$^-$. In this talk we will discuss the use of large dose electron pulses with a related Mn catalyst that possesses bulky mesityl groups in the 6,6’ positions of the bpy ligand (MnBr(mes$_2$-bpy)(CO)$_3$), in which case we can access the key two-electron reduced intermediate, [Mn(mes$_2$-bpy)(CO)$_3$]$^-$ via a disproportionation mechanism. Our efforts to identify and monitor subsequent Mn-CO$_2$ intermediates by TRIR will also be discussed. Related LFP and PR-TRIR studies on cobalt-based macrocyclic CO$_2$ reduction catalysts will also be described.

1. Grills, D. C.; Farrington, J. A.; Layne, B. H.; Lymar, S. V.; Mello, B. A.; Preses, J. M.; Wishart, J. F. *J. Am. Chem. Soc.*, **2014**, *136*, 5563-5566.

MARM 373

From epigenetic structural mechanism to targeted therapy

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Gene expression of the human genome in response to physiological and environmental stimuli is dictated by chemical modifications of the DNA and the DNA-packing histones, as well as transcription factors that work in concert to direct gene activation or silencing in an ordered fashion. This highly complex biological system that operates with a large number and different combinations of such chemical modifications in chromatin has defied a full investigation of its basic regulatory mechanisms. In this talk, I will present our latest structural and mechanistic study of protein-protein interactions involving master transcription factors and core histones that play an important role in epigenetic control of gene transcription lineage-specific cell differentiation. I will discuss the functional implications of our new findings of the basic principles that govern the molecular interactions and regulation in gene expression, as well as a strategy to develop new targeted epigenetic therapy in the fight against human diseases including cancer and inflammation.

MARM 374

Discovery of selective inhibitors for histone methyltransferases

Jian Jin, *jian.jin@mssm.edu. Icahn School of Medicine at Mount Sinai, New York, New York, United States*

Mounting evidence suggests that post-translational modifications of histones play critical roles in diverse biological processes. Among the “writers”, “readers”, and “erasers” involved in chromatin regulation, histone methyltransferases (HMTs) have received great attention as a new class of potential therapeutic targets. HMTs (also known as protein methyltransferases) are divided into two categories: protein lysine methyltransferases (PKMTs) and protein arginine methyltransferases (PRMTs). High quality selective inhibitors of PKMTs and PRMTs will permit biological and disease hypotheses concerning these enzymes to be tested with high confidence in cell-based and/or animal models. In this talk, I will present our recent progress on discovering substrate-competitive, allosteric and cofactor-competitive inhibitors of PKMTs and PRMTs.

MARM 375

Chemical interrogation of protein methyltransferases

Minkui Luo*, luom@mskcc.org. Box 248, Memorial Sloan-Kettering Cancer Center, New York, New York, United States*

Protein methyltransferases (PMTs) play essential roles in many biological processes through methylation of histones and diverse nonhistone substrates. Dysregulation of these enzymes has been implicated in many diseases including cancers. It is challenging to dissect the methylomes of individual PMTs in an unambiguous manner because Lys/Arg methylation unlike other posttranslational modifications doesn't significantly alter the physical property of the substrates. Pharmacological perturbation of these PMTs also requires high-quality inhibitors with distinct modes of action. To address these needs, we developed a set of cofactor-based chemical tools for PMTs. Our cofactor surrogates can be utilized wild-type and engineered PMTs for target labeling. This approach allows the identification of proteome-wide PMT substrates in an unbiased manner. Upon examining the catalytic mechanism of PMT-involved methylation reaction, we noticed the existence of dynamic configurations of PMTs, we were able to target these configurations and develop SAM-competitive or covalent inhibitors against certain PMTs. Under these contexts, several ongoing projects in the Luo laboratory will be present.

MARM 376

Ubiquitin-like modifications as targets for developing cancer therapeutics

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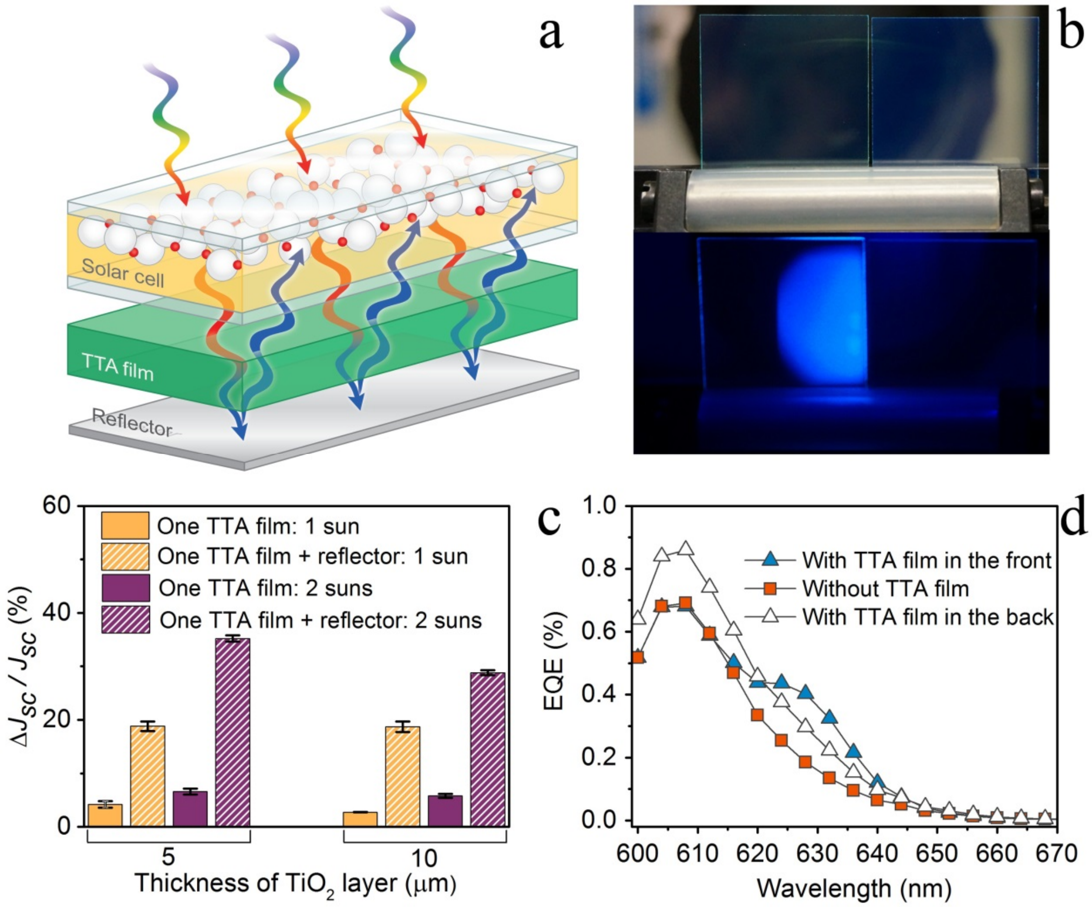
Ubiquitin-like modifications are potential targets for the development of novel therapies for life-threatening human diseases that lack a cure. Recent findings indicate that the key oncogenic pathways driven by Myc and KRas are dependent on, or addicted to, post-translational modifications by the Small Ubiquitin-like Modifiers (SUMO). Genome-wide siRNA knockdown identified the gene encoding the catalytic subunit of the SUMO activating enzyme (SAE), SAE2, as having the strongest synthetic lethal interaction with Myc hyperactivation. Similarly, genes encoding the SUMOylation enzymes were found to be critical for KRas-dependent tumorigenesis. These findings suggest that SAE is a novel target for developing anti-cancer therapeutics for cancers that are Myc-and KRas-dependent. We discovered an allosteric inhibitory mechanism to inhibit the SAE, and a chemotype of inhibitors that confer such inhibitory effects. Using the inhibitor and other biochemical methods, we have investigated the molecular mechanisms underlying the synthetic lethality of SUMOylation with Myc hyperactivation and KRas mutations. Validation of SAE as a novel target could potentially improve treatment of many cancers, as overexpression of Myc is estimated to contribute to 70% of all human cancers, and KRas is also frequently mutated in human cancers, but have proven difficult to inhibit pharmacologically.

MARM 377

Photocurrent enhancement from solid-state triplet-triplet annihilation upconversion of low-intensity, low-energy photons

Christopher Koenigsmann[1,2]*, koenigsmannc@yahoo.com, Chuanhao Li*[3]*, Fan Deng*[3]*, Anna L. Hagstrom*[3]*, Charles A. Schmuttenmaer*[2]*, Jaehong Kim*[3]*. (1) Chemistry, Fordham University, Bronx, New York, United States (2) Chemistry and Yale Energy Sciences Institute, Yale University, New Haven, Connecticut, United States (3) Chemical and Environmental Engineering, Yale University, New Haven, Connecticut, United States*

We present a red-to-blue upconversion system based on triplet-triplet annihilation (TTA) in a solid-state film configuration that significantly enhances the photocurrent of a model solar cell device. The film is robust against oxygen-quenching, and can be readily tailored to existing solar cell architectures. The photovoltaic performance of upconversion-assisted dye-sensitized photoelectrochemical cells was measured under both high-power coherent laser as well as low-power incoherent light irradiation (light emitting diode and simulated AM1.5G sunlight). By utilizing low-energy photons that would otherwise be wasted, the photocurrent is enhanced by as much as 35% under one-sun light intensity when a model solar cell device is coupled with a TTA film and a reflector.



A schematic illustration (a) of TTA film-assisted absorption of photons with energies below the HOMO-LUMO gap of the chromophore sensitizer in a dye sensitized photoelectrochemical cell. Photographs (b, top) of films (Left: TTA film, right: control film without the TTA sensitizer). The same films (b, bottom) are shown but under 2-sun-equivalent illumination by a solar simulator passed through a 600 nm long-pass filter. TTA-UC-induced J_{sc} enhancement (c) using simulated AM1.5G light as the light source. EQE spectra (d) of solar cells with and without integrated TTA films under two-sun illumination.

MARM 378

Design and manufacture of ICE test module to save gasoline with oxyhydrogen gas produced in alkaline electrolyzers

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Internal combustion engine vehicles are an important pollution source. Several research groups are implementing systems to reduce the hydrocarbon use. In the first stage, the gasoline enrichment with alternative fuels such as ethanol, hydrogen, and others ones have been considered. This paper investigated the effect of hydrogen-oxygen blends (oxyhydrogen gas) added to save gasoline in an internal combustion engine (ICE). Test module was adapted from a modified ICE, which was equipped with a hydrogen and oxygen injection system and a hybrid electronic control unit was adopted to control the oxyhydrogen gas produced and gasoline fed, Figure 1. Oxyhydrogen gas was produced by two water alkaline electrolyzer (WAE) in parallel-series stack, which had energy consumption from 60 to 500 W with 50 to 65% of efficiency. The WAE used in the study were designed and in-home built by our research group. Hydrogen storage system was not required because of the in-situ gas generation. The engine was run at a typical city-driving speed range from 1000 to 2000 rpm. First, the test was performed with only gasoline. Second, it was added the standard oxyhydrogen volume, the fraction in total intake air flow was constant, 903 smL min^{-1}. Gasoline consumption was analyzed. The oxyhydrogen gas enrichment system allowed to save gasoline volume and contributed to the decreased CO_2 emissions, Table 1.

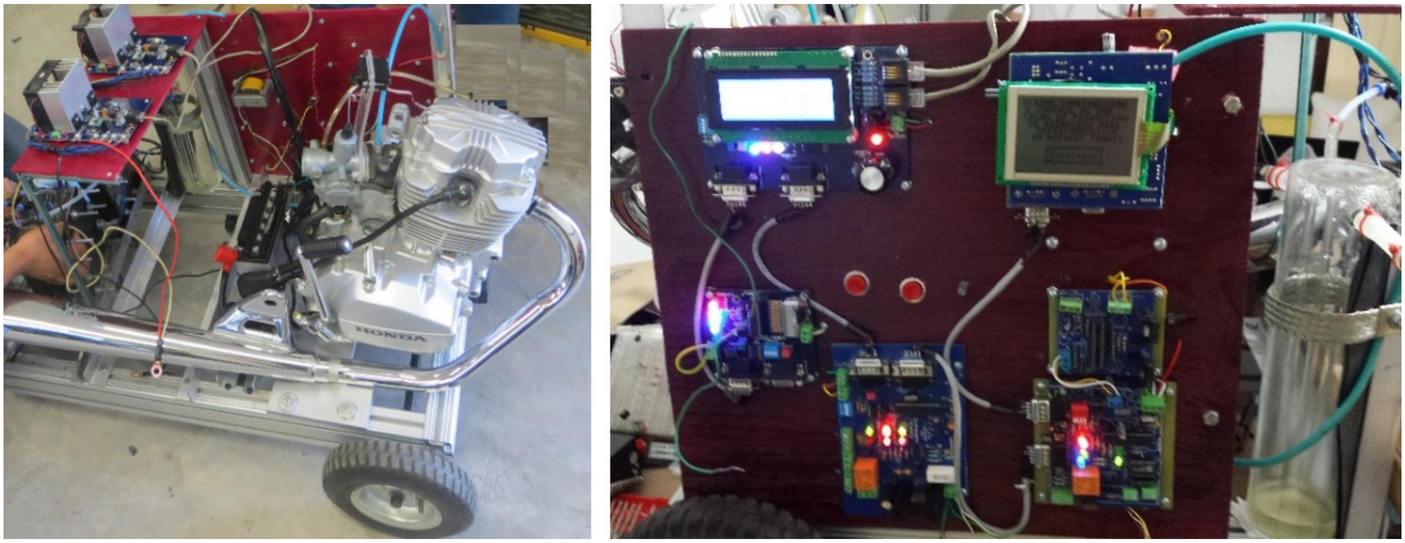

Figure 1. Test module and Control system

rpm	Gasoline volumetric flow real (mL min^{-1})	Gasoline volumetric flow with oxyhydrogen (mL min^{-1})	CO2 emission with gasoline (%)	CO2 emission with oxyhydrogen gas (%)
1000	2.4390	2.0270	---	---
1200	2.8142	2.2371	4.5	2.33
1400	2.9615	2.3640	5.79	3.31
1600	3.0510	2.4291	6.65	3.71
1800	3.2715	2.8818	7.6	4.2
2000	3.9113	3.1120	7.75	5.07

Table 1. Gasoline flow save with oxyhydrogen gas fed (at 20A and 11.36 V)

MARM 379

Bio-catalyzed regioselective synthesis in undergraduate organic laboratories: Multi-step synthesis of 2-arachidonoylglycerol

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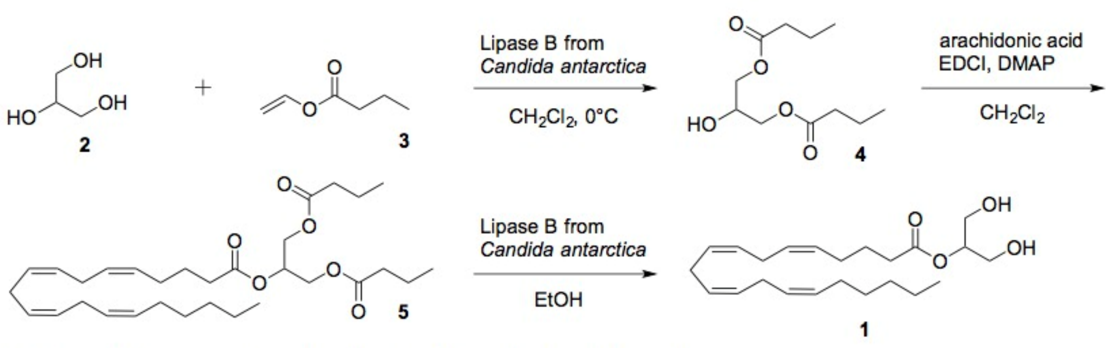
The use of biocatalysis in organic synthesis has been increasingly prevalent. Recent literature in the field of endocannabinoids has provided the impetus for adapting a novel synthetic strategy to a series of reactions applicable to the undergraduate organic chemistry laboratory. These publications explore the lipase-mediated synthesis of the cannabinergic ligand 2-arachidonoylglycerol (2-AG) (**1**). 2-AG is the predominant signaling molecule able to interact with the cannabinoid receptors (CB1 and CB2) in a similar fashion to Δ^9-tetrahydrocannabinol (THC), a classical cannabinoid isolated from the *Cannabis sativa* plant. Manipulating the concentration of these signaling molecules is an important area of investigation, as significant therapeutic benefits are anticipated. The synthesis of 2-AG is important to this area of research and has therefore, been actively pursued. The synthesis of signaling ligand 2-AG will increase student awareness of the significance and therapeutic potential of the endocannabinoid system. The outlined synthetic sequence (Scheme 1) exposes students to enzyme-mediated reactions, the challenges of multi-step synthesis, regioselectivity, and the strategy of utilizing protecting groups. This laboratory exercise also reinforces the importance of executing reactions under inert conditions, purification methods, and molecular characterization using thin layer chromatography (TLC) and ^{1}H nuclear magnetic resonance (NMR) spectroscopy.



Scheme 1: Lipase-mediated synthesis of 2-arachidonoylglycerol

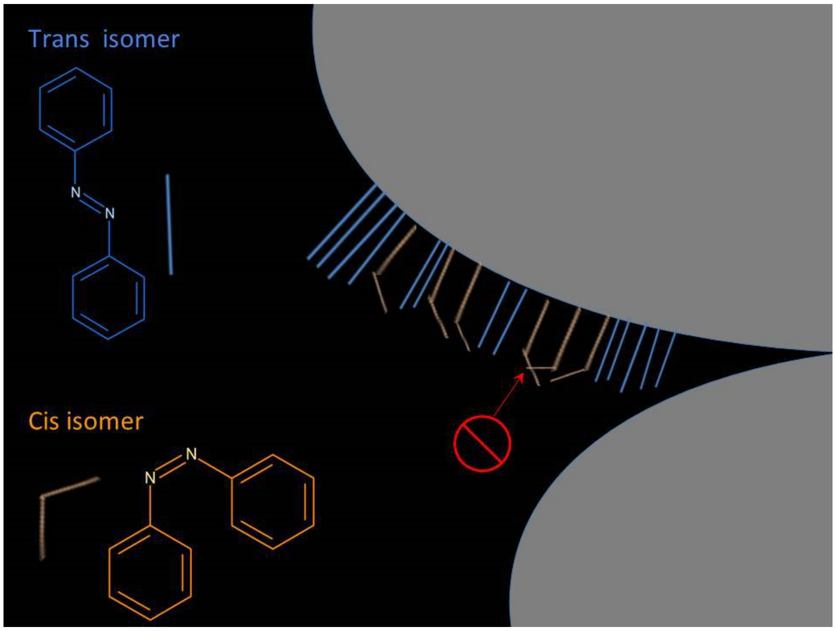
MARM 380

Analyzing the effect of ZrO_2 surface adsoportion on the intramolecular isomerization of azobenzene molecules

***Darren C. Achey**, achey@kutztown.edu, Craig Pointer, Argenis Williams, Kevin Singewald, Mallory Snook, Johnathan Alicea. Physical Sciences, Kutztown University, Alburtis, Pennsylvania, United States*

With the ever-increasing use of devices that anchor molecules to nanomaterial surfaces, there is much utility in understanding and, more importantly, predicting how reactions that surface-anchored molecules undergo are affected by attachment to the surface. This environment change could have various thermodynamics and kinetic effects on different types of reactions due to electrostatic changes at the surface, steric effects of the surface and other molecules, and by strange or uncommon molecular orientations at the surface, among many other possibilities. As such, thorough sets of experiments that quantify how various types of reactions change (or stay the same) in fluid solution and when attached to a surface, in this case nanocrystalline ZrO_2, are much needed to gain intuition as to how devices that utilize these interfacial molecular reactions can be best optimized.

Upon light irradiation, azobenzene molecules undergo well-known intramolecular isomer changes from *trans* to *cis* isomers. The *cis* isomer then thermally returns back to the *trans* isomer following a first order decay. This reaction can be monitored via UV-Visible spectroscopy due to the unique spectral signatures of the *cis* and *trans* isomers. Furthermore, analysis of this reaction at a range of temperatures allows for an activation energy to be calculated under both fluid solution and ZrO_2 adsorption conditions. Preliminary results suggest that the surface adsorbed molecules have smaller first order rate constants for this intramolecular reaction when compared to the molecules in fluid solution opening up the intriguing possibility of steric hindrance at the ZrO_2 surface factoring into the reaction rate.



MARM 381

Solar-hydrogen hybrid system integrated to a sustainable house in Mexico

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One of the most interesting developments of energy systems based on the utilization of hydrogen is their integration with renewable sources of energy. In fact, hydrogen can operate as a storage and carrying medium of these primary sources. An analytical model to size, analyze and assess the feasibility of a hybrid photovoltaic/hydrogen (PV/H_2) energy conversion system using real weather data is presented in this work, figure 1. The analysis considers an energy balance and electrical variables of the system components; it calculates the subsystems efficacy and proposes the improvements to increase the efficiency by the use of surplus energy produced by the hybrid system. We used solar radiation measurements from a meteorological monitoring station placed in the roof of the sustainable house located in the north side of Mexico City. The PV/H_2 system delivered electric power from a primary source (PV) to satisfy the electric load. Surplus energy is supplied to an electrolyzer in order to generate hydrogen. In energy deficit hours a PEMFC covers in part the electric demand. Therefore the hybrid system efficacy is calculated based on the level of energy stored, and the fulfillment of the electric load. Results shows that the highest PPV not always meet the highest efficacy of the hybrid system, figure 2, therefore the model allows determine the best subsystems configuration to avoid the oversizing or undersizing. The simulation data applied different scenarios show the h_M, around the 65 % at 1400 W of PPV, 4500 Wh of EHS, ~600 W of PFC and ~1000 W of PE.

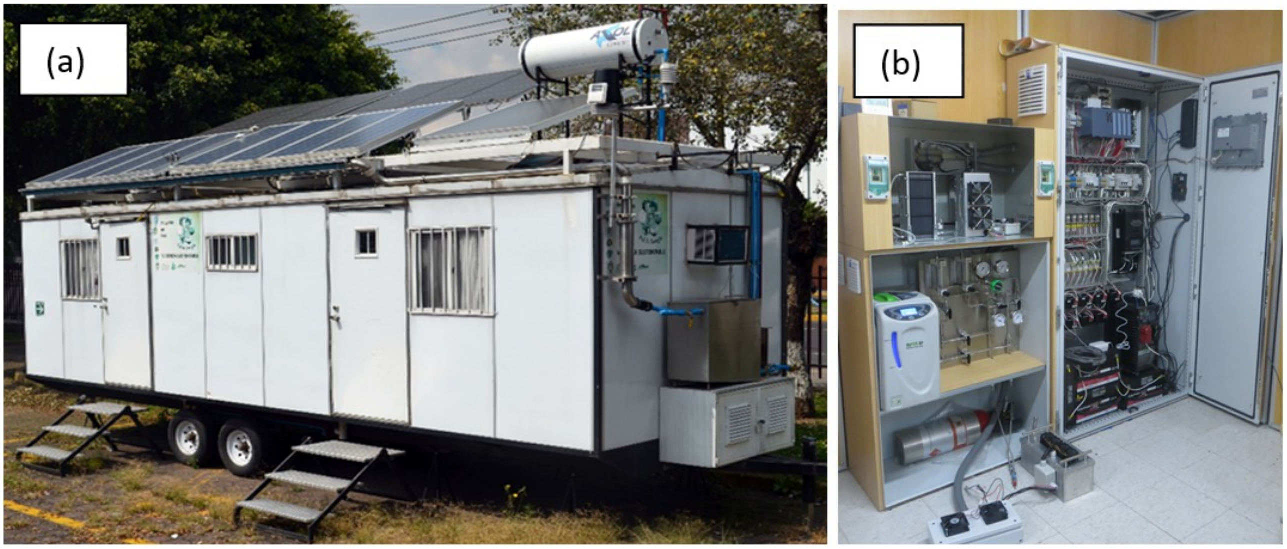

Figure 1 a) Sustainable House and b) Hydrogen system

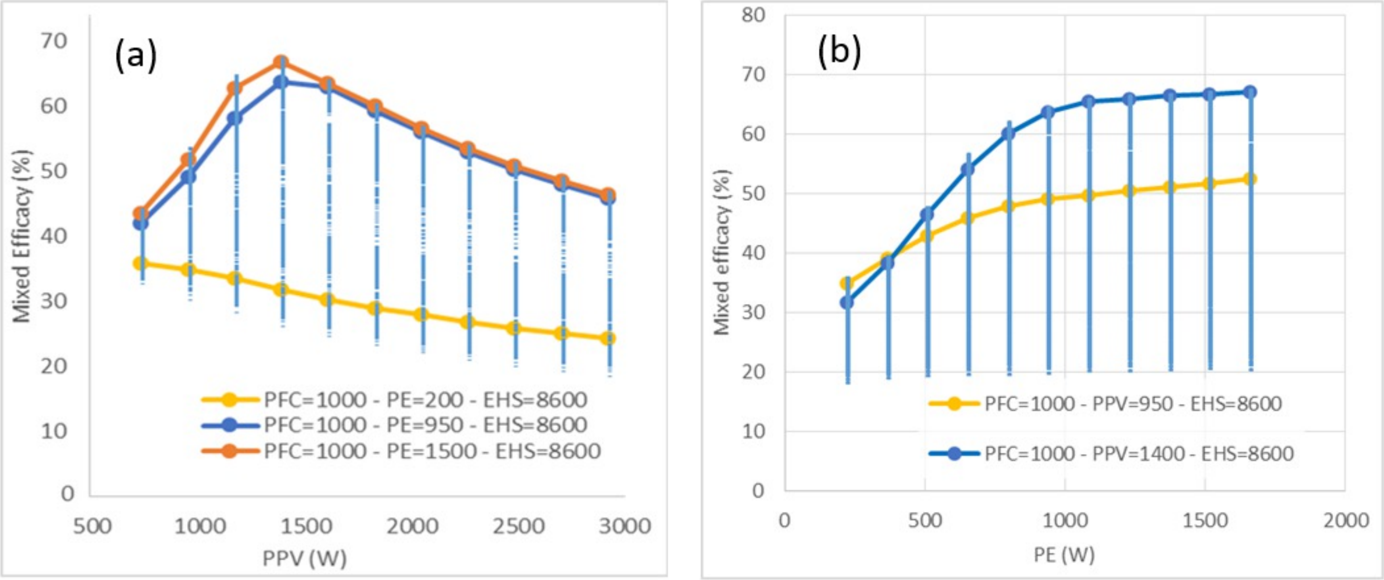

Figure 2 a) Performance for h_M versus PPV and b) h_M versus PE, with similar conditions to the installed subsystems

MARM 382

Stability of synthetic cathinones in preserved oral fluid samples

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Synthetic cathinones are new stimulants drugs derived from cathinone with powerful effects such as delusions, hallucinations and potentially dangerous behavior. We developed a method for the determination of 10 synthetic cathinones (cathinone, methcathinone, buphedrone, mephedrone, 4-

methylethcathinone (MEC), 3,4-methylenedioxypyrovalerone (MDPV), methylone, naphyrone, alpha-pyrrolidinovalerophenone (PVP) and N-ethylcathinone) in preserved oral fluid using liquid chromatography–tandem mass spectrometry, and assessed their stability at different storage conditions. Two mL of 1M Acetic Acid and 25µL internal standard solution were combined with 0.4 mL Quantisal sample (0.1 mL oral fluid and 0.3mL of buffer), and subjected to solid phase cation exchange extraction (Strata Drug-X B, Phenomenex). The chromatographic reverse-phase separation was achieved in gradient mode in 9 min. Compounds were identified and quantified by two transitions acquired in MRM mode. The analytical method was validated studying accuracy, precision, linearity, sensitivity, matrix effect, extraction and process efficiency, and stability. Oral fluid pools from 3 different donors were spiked at 3 ng/mL and 150 ng/mL concentrations, and were stored for 24h and one week at room temperature, at 4°C for one week, -20°C for one week, and submitted to 3 freeze-thaw cycles. The assay was linear from 1-250 ng/mL. Imprecision (n=15) was <20.7% and accuracy (n=15) was 84.0-115.3%. Extraction efficiency was 87.2-116.8% (n=6), process efficiency 30.9-103.7% (n=6), and matrix effect -65.1 to -6.2% (CV<15.1%, n=6). The synthetic cathinones were stable at 4°C and -20°C for one week and after 3 freeze-thaw cycles. Naphyrone, methylone, MDPV, and mephedrone, were not stable at room temperature for both 24h and one week with loses up to 44.7%. We developed a sensitive and specific method for the determination of 10 different synthetic cathinones in 0.4 mL preserved oral fluid. Synthetic cathinones were stable stored at 4 and -20°C in oral fluid samples in Quantisal buffer.

MARM 383

Short metal-metal separations in multimetallic Au(I), Ag(I) and Cu(I) complexes

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The attractive interaction between closed-shell late transition metals has received considerable attention. In particular, multinuclear complexes and coordination polymers having direct metal-metal interactions are of great interest because their conductivity, magnetic properties, and electrochemical behaviors are good candidates in the field of nano-scale or molecular scale electronics. Among the closed shell attractions, Au(I)-Au(I) interactions are the most studied, whereas the metallophilic attraction involving Cu(I) are less represented in the literature. However, many Cu(I) complexes with close metal-metal interactions are brightly luminescent even at room temperature.

Earlier our group reported the application of the 2-picolyl substituted NHC ligand toward stabilizing Ag(I)-Ag(I) interactions. The simple reaction of the NHC ligand precursor 1,3-bis(2-pyridinylmethyl)-1H-imidazolium tetrafluoroborate, $[H(pyCH_2)_2im]BF_4$ with silver oxide in acetonitrile produces the unusual triangulo-Ag_3 cluster, $[Ag_3((pyCH_2)_2im)_3](BF_4)_3$, with unusually short Ag-Ag separations (2.72 to 2.78 Å). We have now extended this chemistry to explore the electronic alteration of the ligand on the metal-metal separation. Additionally, we were able to produce mixed metal systems, and copper triangulo-Cu_3 clusters.

MARM 384

Fumed silica-based edible organogels and bigels

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The basic building blocks which are recently being explored as structurants for edible oil gelation include crystalline particles (e.g. waxes), polymeric strands (e.g. cellulose derivatives) and crystalline fibres (e.g.

12 hydroxy stearic acid etc.).[1-3]

In this work, we report for the first time, the use of colloidal inorganic particles, SiO_2 (a food-grade additive, E 551) as new structurants to fabricate clear gels in sunflower oil. Organogels with high gel strength ($G' > 10{,}000$ Pa), high resistance to flow ($\sigma_Y > 100$ Pa), temperature stability and a good thixotropic recovery (> 70 %) were obtained at 10-15 %wt of SiO_2. Cryo-SEM (along with energy-dispersive X-ray spectroscopy) revealed an interesting 'chain-like' arrangement of SiO_2 aggregates which is responsible for creating a structural framework. The fact that the positive results were only seen with hydrophilic SiO_2 (and not with functionalized hydrophobic SiO_2) strongly suggests that hydrogen bonds among surface silanol groups (Si-OH) contributed to the network formation of colloidal particles. Moreover, water phase (structured using food hydrocolloids) was added to organogel in different proportions to obtain stable 'bigels' with interesting microstructures (as seen under cryo-SEM and confocal microscope) and excellent rheological properties.

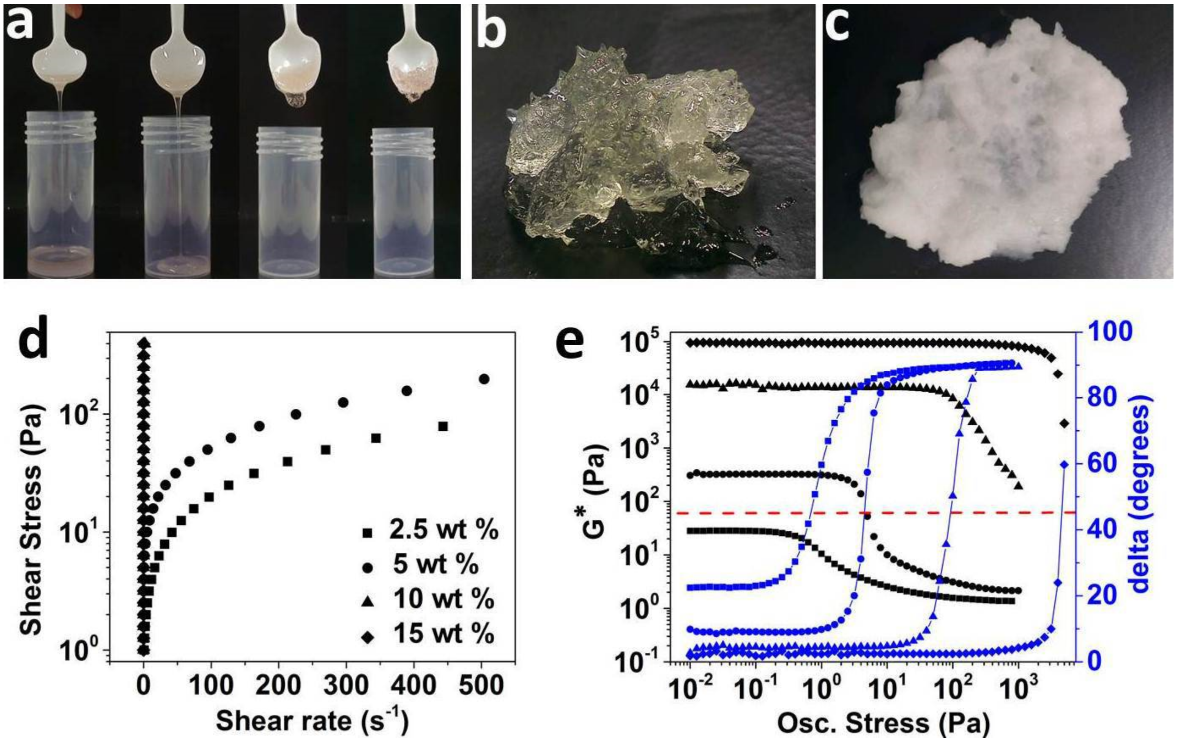

Fig 1. a) Photograph showing the flow behaviour of sunflower oil dispersions containing from left to right 2.5, 5, 10 and 15 wt% of A150; b) & c) Photographs of an organogel (sunflower oil with 15 wt% A 150) and a bigel (O:W ratio of 9:1) respectively; d) & e) Comparative curves from stress ramp and amplitude sweeps for sunflower oil dispersions containing 2.5, 5, 10 and 15 wt% of A150.

MARM 385

Synthesis, screening, and sensing applications of a novel fluorescent probe based on C-glycoside

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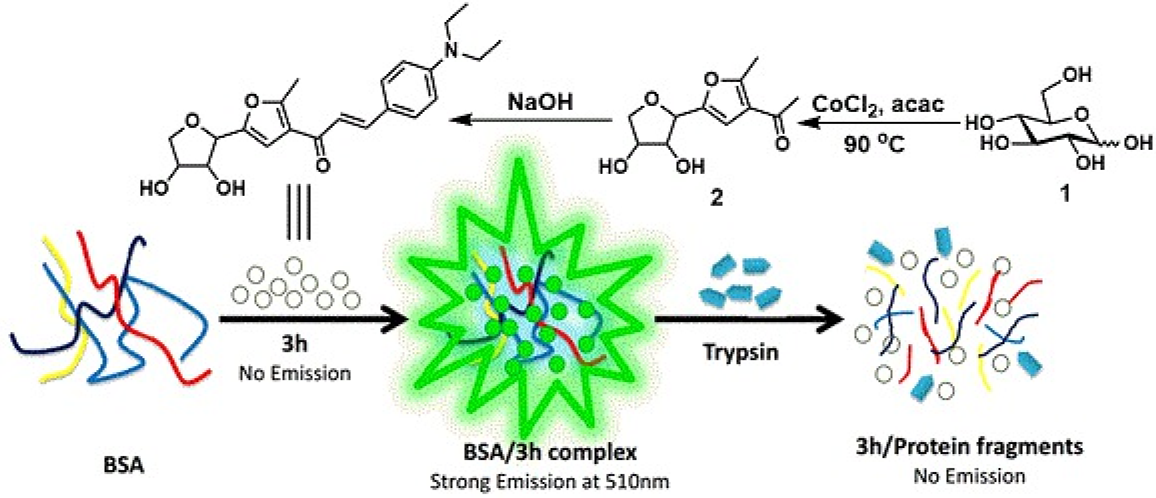
A novel water soluble fluorescent probe based on C-glycoside with aromatic aldehyde unit has been synthesized and its UV/Vis and fluorescence spectra, aggregation and disaggregation with bovine serum albumin were studied. To furnish the products, it calls for only two steps with high total yield. First, the condensation of glucose with acetylacetone in the presence of Lewis acid in ethanol afforded compound **2** in 87% yields. Second, compound **2** was subjected to aldol reaction with aromatic aldehyde by using NaOH as base catalyst in over 80% yields. Besides, the comparison between carbohydrate-derived probe and none-carbohydrate-derived probe indicated that neutral probes with carbohydrate moiety showed excellent hydrophily and biocompatibility. The absorption and emission max wavelength of the dye in different solvents were in the range 402-437 and 479-549 nm respectively. Fluorescence spectroscopic studies showed that the as-prepared dye could be used in the labeling of BSA protein and monitoring trypsin hydrolysis as it displayed a “turn-on” mechanism when the dye was incubated with protein in water. Compared to traditional probes, this neutral fluorescent probe has the advantages of being water soluble, easily synthesized and suitable for a wide range of applications involving biomolecules.



MARM 386

Structural study of the membrane-anchored protein, hippocalcin, using reverse micelles

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Hippocalcin is a membrane-anchored calcium binding protein that is speculated to be associated with long-term depression and several neurodegenerative diseases such as Alzheimer’s and Huntington’s. It has a Ca^{2+}/Myristol switch and three EF hands, only two of which bind to calcium. Structural analysis of such proteins in their membrane-anchored state has been challenging, but encapsulation of these proteins in the aqueous core of reverse micelles facilitates their study by providing a membrane mimetic environment. Reverse micelles and fluorescence spectroscopy are used here to optimize conditions for study of this membrane anchored protein using NMR. Supported by funding from Rowan University, the New Jersey Health Foundation, and the Osteopathic Heritage Foundation.

MARM 387

Electron paramagnetic resonance investigation of radiation damage and healing in Kapton

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There is a need for lightweight and durable materials in space missions that can withstand the challenging environments in the upper atmosphere and in space. Kapton is a lightweight polymer used for structural support and insulation that is stable over a wide range of temperatures. Kapton is largely insensitive to ionizing radiation characteristic of high altitude and space environments. However, a more thorough understanding of Kapton's ability to stabilize after exposure to radiation will shed further insight on its abilities and limitations in space flight. Radiation creates free radicals (atoms or molecules with unpaired electrons) by breaking chemical bonds. Free radicals cause a material to be more reactive and electrically conductive which is undesirable for its intended missions. Our aim is to measure the concentration of these free radicals produced by radiation; the time it takes Kapton to recover from these changes; and if heating Kapton reverses its recovery. We use Electron Paramagnetic Resonance (EPR) - a technique that directly detects unpaired electron spins in a magnetic field- to measure the effects of radiation in Kapton samples over time. In collaboration with Dr. Ryan Hoffman of the U.S. Air Force Research Laboratory at Kirtland Air Force Base, NM, we conduct measurements on electron-irradiated samples of Kapton. Our results indicate that Kapton heals quickly from irradiation; however we have also observed that heating a healed sample can partially reverse recovery. These results offer a more detailed understanding of how irradiation may compromise Kapton's stability through a wide range of environmental conditions.

MARM 388

Development of botulin-based small molecules as potential anti-cancer agents

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Betulin and betulinic acid are pentacyclic triterpene natural products isolated in from the bark of birch trees. Betulinic acid was found to be preferentially cytotoxic to cancer cells and this has led to an interest in developing betulin derivatives as therapeutic agents. One of the challenges in progressing further has been the limited aqueous solubility of these molecules. We have been working on the synthesis of betulin derivatives with increased water solubility and in this regard, we have employed multicomponent coupling reactions such as Passerini reaction, Ugi reaction, Click chemistry, Baylis-Hillman reaction, reductive amination, etc. Our synthetic efforts as well as the biological evaluation data will be presented.

MARM 389

Design and synthesis of functionalized benzoboroxoles as therapeutic agents

Suman Pathi, Drew Morgan, Md. A. Rahman, Justin Seay, Alexander Colfer, ***Subash C. Jonnalagadda****, jonnalagadda@rowan.edu. Chemistry and Biochemistry, Rowan University, Glassboro, New Jersey, United States*

Benzoboroxoles are cyclic boronic acid hemi esters and they are found to exhibit remarkable biological properties. Tavaborole (a fluorinated benzoboxorole) was recently approved for the treatment of onychomycosis (toe-nail fungal infection). Several other analogs of benzoboroxoles also enhibit anti-fungal, anti-bacterial, and anti-cancer acvitities. We have been working in the area of benzoboroxoles for some time and we have synthesized several densely functionalized benzoboroxoles employing reactions such as Baylis-Hillman reaction, Passerini reaction, reductive amination, aldol condensation, etc. Some of our molecules have shown good activity against pancreatic and triple negative breast cancer cell lines. Another series of benzoboroxoles have also exhibited activity against mycobacterium smegmatis. Our recent developments in this project will be presented.

MARM 390

Synthesis & spectroscopic characterization of standard long chain acyl carnitine derivatives for clinical diagnosis of fatty acid β-oxidation disorder

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β-Oxidation of acyl-CoAs in mitochondria produces various acylcarnitines that appear in blood and are excreted into urine. Acylcarnitine profiles have been used as biomarker for the diagnoses specific inherited metabolic diseases, such as medium-chain acyl- CoAdehydrogenase deficiency (MCAD), and long-chain hydroxyacyl-CoA dehydrogenase deficiency (LCHAD) by using tandem mass spectrometry. Carnitine acyltransferace enzymes reversibly interconvert acyl-CoA and, acylcarnitine derivatives, thereby it catalyze the translocation of the fatty acyl moiety across the mitochondrial membrane. The identification of the carnitine ester has not been fully recognized by tandem mass spectrometry. We have established a method for the synthesis of Long chain acyl carntines based on O-Acylation of carnitine chloride, and /or replacement of the acid chloride by equimolecular amount of thionyl chloride followed by the addition of carnitine chloride. We have synthesized of a series of Acyl-carnitine derivatives such as Cis-9- , and Trans-9 Tetradecenoyl carnitine carnitine, Cis 9 , and trans 9 Octadecenoyl carntines and Trans -2-Tetradecenoyl carnitine, among other long chain acyl carnitines. The synthesized carnitine derivatives was fully characterized by NMR, GC/EI-MS, LC/MS. The isolation of the C14:1 acylcarnitine from human urine, will be transesterified to form ester derivative, and characterized, these results will be compared to the synthesized standard acyl carnitines. The standards will then spiked in urine, and detected by HPLC/MS, and LC/MS. Based on the data that we expect from the analyses we can develop an assay for the detection of long chain acyl carnitine. Following the same methodology we will synthesis several substrates of acyl carnitine derivatives and develop a general chromatographic based assay for detection of small , Medium, long and very long chains Acyl carnitine in urine.

MARM 391

Development of radiofluorinated analogs of abiraterone

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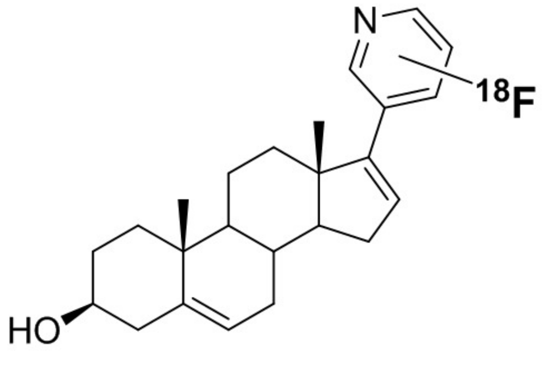
Pharmacology and Chemistry, Sloan Kettering Institute, New York, New York, United States (4) Medicine, Memorial Sloan Kettering Cancer Center, New York, New York, United States (5) Genitourinary Oncology Service, Memorial Sloan Kettering Cancer Center, New York, New York, United States

Abiraterone (Abi) is a molecularly targeted therapeutic for metastatic castration resistant prostate cancer (mCRPC). It disrupts the androgen synthetic apparatus in both normal and prostate cancer tissues by inhibiting a key steroid biosynthetic enzyme, CYP17A1. Determining which patients with mCRPC will respond to Abi treatment is complex and time-critical. Positron emission tomography (PET) imaging with an F-18 labeled analog of Abi would be non-invasive, quick, and could provide information about the patient's CYP17A1 status on a per-lesion basis, as is done in next-generation precision medicine. To this end, we designed and synthesized two F-18 labeled (and respective non-radioactive) analogs of Abi at the synthetically convenient 2' and 6' pyridyl sites. [^{18}F] 2'-FAbi and [^{18}F] 6'-FAbi were synthesized with 16.1±12.0% (n=4) and 14.5±7.5% (n=12) d.c.y, respectively from their chloropyridyl precursors. Abi, 2'-FAbi and 6'-FAbi weakly displaced the androgen receptor (AR) radioligand [^{18}F] FDHT (16β-fluorodihydrotestosterone) in AR-expressing cells (5-7μM IC_{50}). Neither [^{18}F] 2'-FAbi nor [^{18}F] 6'-FAbi could be displaced by abiraterone or by themselves in cells. In a liver microsome functional assay, 6'-FAbi inhibited androgen synthesis, while 2'-FAbi did not. Biodistribution studies were performed in murine xenograft models of prostate cancer (LNCaP, VCaP, and MDAPCa2b); both radiotracers distributed rapidly and were cleared primarily via the hepatobiliary route. No toxicity was observed. In vivo, [^{18}F] 2'-FAbi was moderately unstable and bone uptake was observed, presumably due to defluorination. [^{18}F] 6'-FAbi was stable over the course of experimentation; moderate uptake was observed in tumor xenografts and significant uptake was observed in the andrenal glands, a site of significant androgen biosynthesis. Looking forward, we anticipate that PET imaging with [^{18}F] 6'-FAbi has potential to clarify mechanistic details of abiraterone pharmacology, aid in dose stratification and complements existing PET radiotracers to further delineate mCRPC molecular target profile.



MARM 392

Hydroxypyridinones: Targeting HIV-1

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Hydroxypyridinones are an interesting class of compounds that exhibit promising novel and structure-dependent antiretroviral activity in HIV-infected cell cultures and in patients. Our structure-activity relationship evaluations indicate that a cyclohexyl moiety at the nitrogen of 3,4-hydroxypyridinones most effectively inhibits HIV protein synthesis (p24) at lower concentrations (35-40 μM). We have also found analogs of 1,2- and 3,4-hydroxypyridinones that have no effect on HIV. Our studies provide a foundation for the knowledge-guided development of novel antiretrovirals with HIV-ablating activity.

MARM 393

Effect of a physical classroom demonstration on understanding of chemical equilibrium

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Undergraduate students often have difficulty understanding some concepts of chemical equilibrium: namely, 1) that reactions do not stop at equilibrium (rather, they continue, with their rates equal) and 2) that the concentrations of the products and reactants are not equal at equilibrium (rather, they are unchanging). A physical demonstration of chemical equilibrium that reinforces these concepts was performed in a classroom, and its effect on understanding was evaluated. The demonstration involved two clear tanks, one initially half-full of colored water, with the volume of water in one tank representing the concentration of the reactants and, in the other tank, the products. Two students simultaneously scooped water out of each tank and poured it into the other tank, representing the forward and reverse reaction. Because the forward-reaction's scoop was larger than the reverse reaction's, the rates were unequal and the volume in the reactants' tank declined. However, as the volume became smaller, the big scoop was not able to fill completely, so the forward reaction rate declined and became equal to the reverse rate. At this point, equilibrium was reached. The students in the class could clearly, physically see that the reactions had not stopped (the people continued scooping) and that the concentrations were not equal (i.e., different volumes in the tanks). The effect of the demonstration was examined by comparing the class's percentage of correct answers about equilibrium with a class that did not see the demonstration. The students who saw the demonstration were also asked to what degree the demonstration was helpful in creating understanding about equilibrium.

MARM 394

Exploring polymers through experiments in the undergraduate laboratory

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The American Chemical Society recommends that ACS approved programs cover polymers in their course work. Polymers impact our lives and society in numerous ways including clothing, food packaging, automobiles, medical devices, research and toys. We have designed a series of experiments to explore and teach synthetic polymers at the undergraduate level. We are incorporating an understanding of polymers into our first and second year course, starting with some 'warm-ups' in General Chemistry to introduce the basic concepts of polymers. In our second year Organic Chemistry series, we are exploring more in depth experiments with polymers such as recycling, plasticizers, self-healing polymers and bio-based polymers.

MARM 395

Interaction energy of He with H_2S

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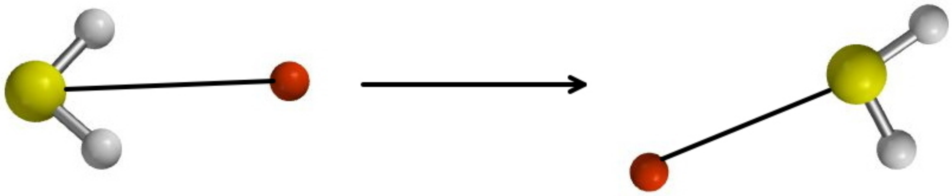
A three dimensional *ab initio* potential energy surface for the He-H_2S van der Waals complex has been constructed using the coupled cluster singles and doubles with perturbative [CCSD(T)] level of electronic structure theory. Various size basis sets were used to check for convergence and basis set superposition error was corrected by the full counterpoise method. There are two equilibrium structures that have been identified and the minimum energy path that connects these two structures will also be reported. The resultant potential energies at the various nuclear configurations have been fit to a polynomial expression so that vibrational eigenvalues and eigenvectors can be calculated.



MARM 396

Water oxidation catalysis with Ru carboxamide complexes

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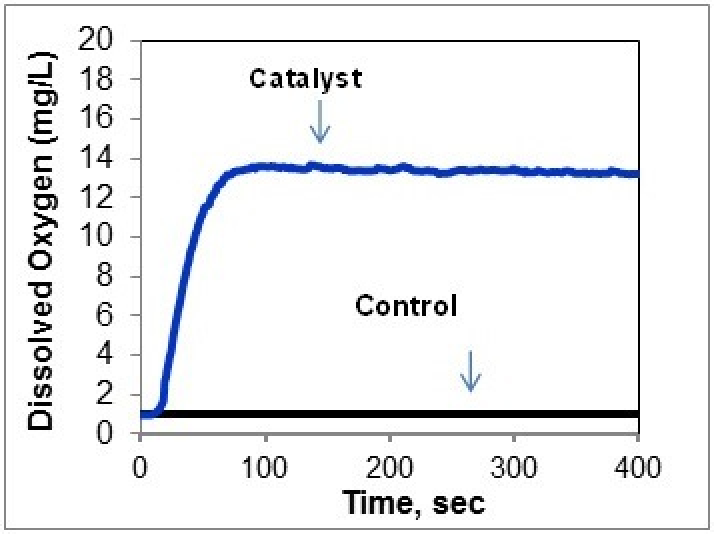
The pursuit for active water oxidation catalysts is crucial to advance solar fuel technology. The use of homogenous catalysts with molecular complexes allows the rationale design of redox active metal centers and provides mechanistic insight into their structure-activity-stability relationships. Herein we present a new class of mononuclear Ru(II) complex bearing an anionic amide ligand that exhibited high activity in cerium(IV) catalyzed water oxidation. The electrochemistry and kinetics of oxygen evolution in H_2O oxidation will be discussed and compared with other known ruthenium(II) water oxidation catalysts. In this work, we also demonstrate a new method using an optical probe to directly measure the concentration of dissolved oxygen in chemically-driven water oxidation which will aid in the rapid screening of effective catalysts for solar energy conversion.



MARM 397

Microwave-assisted synthesis of imidazolium-based ionic liquids for $LiFePO_4$ crystal engineering

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$LiFePO_4$, a cathode material for lithium-ion batteries, is typically synthesized using high temperature ceramic methods. This strategy is energy intensive and offers no control over particle morphology. Ionothermal syntheses, which utilize ionic liquids as both solvents and structure directing agents, have recently generated interest as low-temperature alternatives to previous methods. The flexibility in the choice of cations and anions presents opportunities to direct the nucleation and growth of $LiFePO_4$. To understand the role of the ionic liquid in the synthesis of $LiFePO_4$, imidazolium-based ionic liquids containing hydroxyl-terminated alkyl chains of various lengths are used to prepare $LiFePO_4$ from salt precursors. Powder X-ray diffraction, solid state nuclear magnetic resonance spectroscopy, and scanning electron microscopy were used to characterize the $LiFePO_4$ samples synthesized in several ionic liquids.

MARM 398

Hydrothermal synthesis and characterization of lithium mixed-transition-metal phosphates

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Lithium metal phosphates ($LiMPO_4$, M= Fe, Mn, Co, Ni) are attractive cathode materials for next-generation lithium ion batteries. The iron and manganese versions have relatively low production costs, low toxicity, and are environmentally safe. Lithium metal phosphates are usually synthesized using high temperature or hydrothermal methods. The hydrothermal methods are less energy intensive, and allow for more control over the size and morphology of the particles, but can lead to products with a relatively higher degree of structural disorder. Here, a series of lithium mixed-transition-metal phosphates are synthesized using hydrothermal methods and characterized using a combination of powder X-ray diffraction, solid state nuclear magnetic resonance spectroscopy, and scanning electron microscopy, to elucidate how synthetic conditions affect the local and long-range structure of the materials.

MARM 399

Synthesis and biological evaluation of siderophore derivatives as potential antibacterial agents

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Gram-negative pathogens such as *Pseudomonas aeruginosa, Burkholderia* and *E. coli* strains are responsible for numerous life threatening infections in hospital settings as well as through food contamination. These bacteria are resistant to majority of clinically used antibiotics, because their outer membrane (OM) acts as a permeability barrier. One of the novel approaches to target such pathogens involves development of siderophore analogs as targeted antibiotics. Siderophores, such as pyochelin and enterobactin are small molecule iron chelators produced by bacteria. They are biosynthesized via a multi-enzyme pathway, and transported through specific OM receptors. Since siderophores are essential for growth and pathogenicity, inhibition of their production and transport provides a unique opportunity to develop novel antibiotics. Halogenated analogs of enterobactin have been reported to have antibiotic activity. Based on these findings, we have initiated a research program to synthesize analogs of pyochelin (**1**) and azotochelin (**2**) as potential covalent or non-covalent inhibitors. We have synthesized the natural siderophores, and a library of their analogs (**3 - 10**). The non-covalent analogs have halogen atoms attached to the aryl ring. The halogenation strategy allows us to readily diversify the siderophore structure via metal-catalyzed cross-coupling approaches. The covalent analogs are designed to have electrophilic motifs, including acrylate. We plan to evaluate the antibacterial activity of these analogs against a panel of both Gram-positive and Gram-negative bacteria. Based on the initial bioactivity results, a subsequent generation of analogs will be designed and synthesized. Furthermore, we plan to synthesize siderophore-antibiotic conjugates as targeted-drug delivery systems to overcome the OM barrier. This second approach can be an effective approach to repurpose currently used antibiotics against drug-resistant infections.

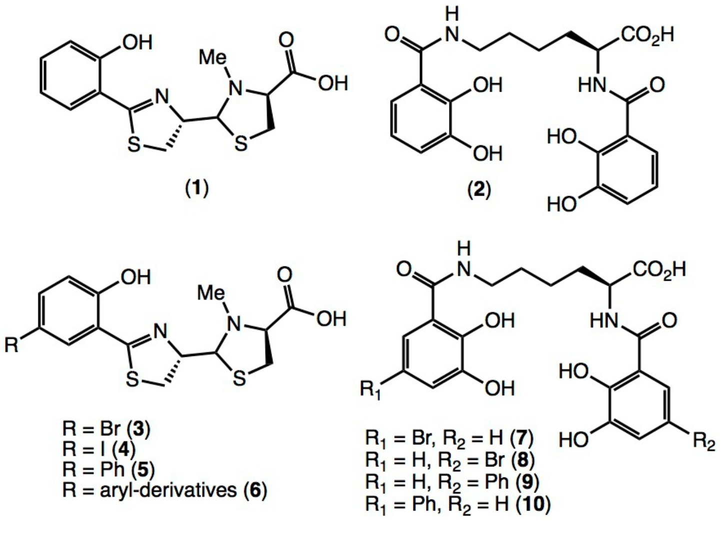

Figure 1. Structures of natural siderophores and their synthetic derivatives.

MARM 400

Differentiation of car paint chips

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Classification and identification of paints is used in the investigation of hit and run accidents with pigments and resins as important ingredients in paints. In this study, ATR-FTIR, GC-MS and Raman spectroscopic analyses were used to characterize organic binders as well as inorganic fillers and pigments found in automobile paint chips. Infrared spectroscopy was used for the identification of polymers and to help discriminate between them identifying indicative peaks. The fingerprint region contains useful information for the analysis of organic compounds. However, its complicated series of absorptions do not always allow for accurate interpretation. Therefore, the IR spectra in this study were tentatively interpreted. The indicative peaks distinguishing each polymer can be used to easily analyze the IR spectrum. Therefore, coatings could be discriminated and divided into different types of paint such as acrylic resin (1150 cm^{-1},1720 cm^{-1}), alkyd (1000cm^{-1}), and epoxy (825 cm^{-1}). Although IR Spectroscopy is not a particularly specific technique for indicating the presence of minor constituents of paint, it can be very useful for paint analysis.

MARM 401

Feasibility of remote sensing for comprehensive assessment of water quality of inland lakes in New York

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New York, as well as other states, devote great effort to assess the quality of its inland lakes. However, the costs of conventional water sampling and analysis are too large to permit a comprehensive spatial and temporal assessment of such waters. Remote-sensing (RS) methods, though, enable comprehensive monitoring because of their low cost, large spatial extent and detailed spatial resolution. Despite being fairly well developed, the methods are not widely applied by assessment agencies. Methods for using satellite images to assess clarity and chlorophyll a of lakes have been employed since the 1970s. Landsat images are a popular data source, although AVHRR have also been employed. The water quality parameters most often assessed included water clarity and chlorophyll (both important indicators of eutrophication), as well as turbidity, total suspended solids, colored dissolved organic matter and temperature. The feasibility of a large-scale, long-term RS-based approach was demonstrated in Minnesota by assessing water clarity in >10,000 lakes across Minnesota for 20 years using Landsat images. We are working to demonstrate the feasibility of such methods to assess water clarity and chlorophyll a in New York's inland lakes. The method will be calibrated and validated using the copious data collected by environmental agencies (eg, USGS, NYDEC) as well as volunteer, lake monitoring groups.

MARM 402

Catalytic cleavage of methylchlorosilane high boiling residue with methylimidazole: Alkyl phosphonium chloride compositions

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Methylchlorosilanes are manufactured via the Rochow-Müller Direct Reaction of methyl chloride with copper-activated silicon. The fraction of the crude product with normal boiling point greater than 72 °C is called Direct Product Residue (DPR). This higher boiling stream comprises methylchlorodisilanes ($Me_{6-x}Si_2Cl_x$, x=0 – 6, Me = CH_3), carbosilanes ($Me_wCl_ySi\text{-}CH_2\text{-}SiCl_nMe_z$, w+y =3; n+z = 3), siloxanes and hydrocarbons. Conventionally, DPR is subjected to tertiary-amine catalyzed hydrochlorination, whereby the $MeCl_2SiSiCl_2Me$ and $Me_2ClSiSiCl_2Me$ are cleaved to produce primarily $MeSiHCl_2$, Me_2SiCl_2 and $MeSiCl_3$. Carbosilanes and the disilanes with x = 0, 1 or 2 are not cleaved and are sent to waste disposal. We have now found(1) (2) that combinations of tetraalkyl phosphonium chlorides and N-Methylimidazole or 2-Methylimidazole catalyze the cleavage of all methylchlorodisilanes and carbosilanes to the monomers, $MeSiHCl_2$, Me_2SiCl_2 and $MeSiCl_3$, with a concomitant reduction in waste. The poster will present our results.

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MARM 403

Novel ionophoric polyphenols display potent antioxidant and anti-amyloidogenic properties, and are non-toxic towards *Tetrahymena thermophila*

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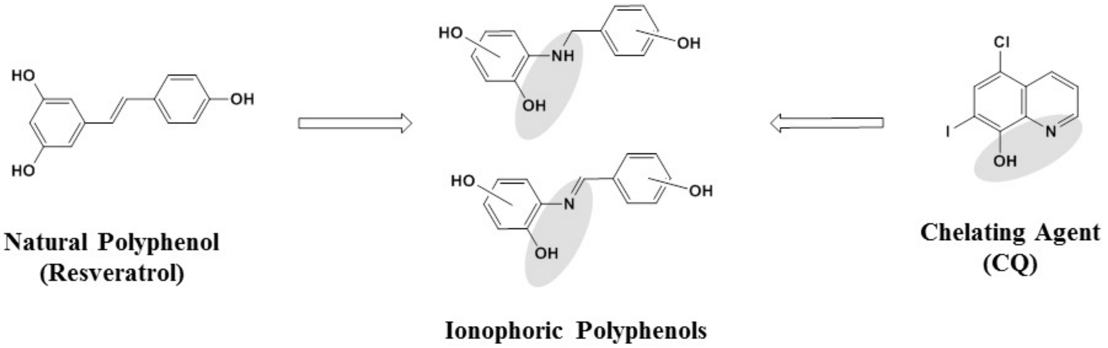
Alzheimer’s disease (AD) is the most common form of dementia affecting more than 28 million people in the world. Only symptomatic treatments are currently available. Anticipated tri-fold increase of AD incidence in the next 50 years has established the need to explore new possible treatments. The accumulation of extracellular amyloid-b (Ab) plaques, intracellular tangles in the brain, and formation of reactive oxygen species (ROS) are the major hallmarks of the disease that lead to an uncontrolled neuronal death. The active role of some metal ions, especially Cu^{2+}, in promoting both Ab aggregation and reactive oxygen species formation has rendered ionophoric drugs as a promising treatment strategy. In this work, a series of 5 disease-modifying and multi-target ionophoric polyphenols (**1-5**), inspired on the structure of natural resveratrol, have been synthesized and characterized. All compounds bind Cu^{2+} selectively over other biologically relevant metal ions. They form 2:1 (compound:Cu^{2+}) complexes with association constants $\log K_a$12-14 depending on the molecular design. Our results indicate that compounds **1-5** possess excellent antioxidant properties: they inhibit the Cu^{2+}-catalyzed reactive oxygen species production between 47% and 100%, and they scavenge DPPH and AAPH free radicals in general better than clioquinol, resveratrol and ascorbic acid. In addition, compounds **1-5** interact with Ab peptides and inhibit both the Cu^{2+}-catalyzed aggregation and the self-assembly of Ab(1-40) up to a ~92% extent. Interestingly, **1-5** are also able to disaggregate up to ~91% of pre-formed Ab(1-40) aggregates. In addition, cytotoxic studies show remarkably low toxicity of **1-5** toward *Tetrahymena thermophila* with LD_{50} values higher than 150 mM, comparable to non-toxic natural resveratrol. Therefore, this family of compounds represents a promising alternative as a potential treatment for AD.



Rational design of novel ionophoric polyphenols combining properties of natural polyphenols and ionophoric agents

MARM 404

A novel way to create a crime scene for forensic chemistry

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One usual activity for forensic science courses is to create a crime scene and have students identify the evidence, take photos, complete a log, and in some cases package the physical evidence. We have done this for several years, but it requires dedicating an office or lab as the crime scene and a lot of time for individual groups to visit the scene. An alternative is to create a variety of small scenes using doll house furniture. This type of crime scene was (or will be) used for criminal justice majors, for science majors with a concentration in forensic science, for a high school forensic science course, and even for Girl Scouts completing a forensic science badge.

MARM 405

Novel heterocyclic methodology for natural products synthesis

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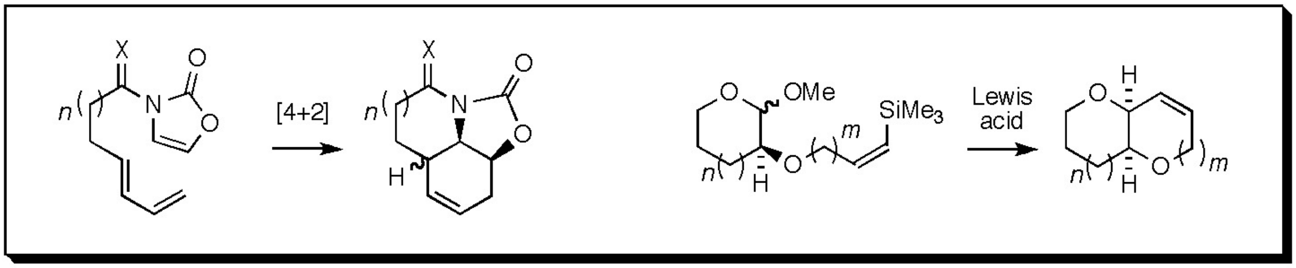
Our group's research focuses on the development of new heterocyclic methodology for the synthesis of bioactive natural products. Specific efforts include:

- Investigation and use of oxazolone as a useful heterocyclic scaffold for alkaloid synthesis – chiefly, intramolecular Diels-Alder reactions with oxazolone as the dienophilic species. Application in the synthesis of several alkaloid targets is currently underway.
- Novel organosilane chemistry for approaches to bioactive ether targets – a rapid synthesis of cis-fused bicyclic ether arrays in which oxocarbeniums undergo nucleophilic attack by vinylsilanes via a novel intramolecular annulation process. A wide variety of ether natural product motifs are thus accessible.



MARM 406

Assessing the fluoro-stabilization effect using *in vivo* unnatural amino acid incorporation

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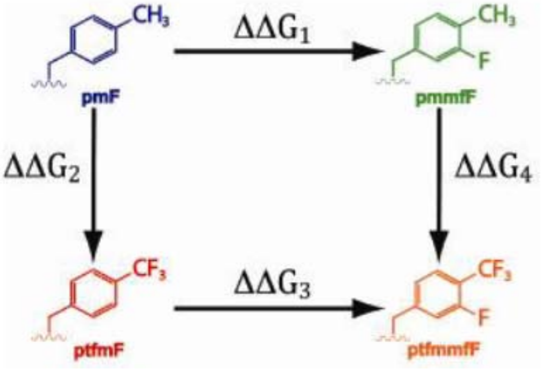
In vivo unnatural amino acid (UAA) incorporation extends the allowable range of chemical functionalities that can be used to probe site-specific structure-function relationships; one set of compounds includes fluorinated UAAs (F-UAAs). F-UAA incorporation may be a useful strategy in protein design given fluorine's unusual physicochemical properties, minimal structural perturbation and enhanced polypeptide stability upon F-UAA substitution. Understanding the thermodynamic basis of the "fluoro-stabilization effect" is currently an active field of research. While most studies have used F-UAA-containing polypeptides generated by solid-phase peptide synthesis (< 60 residues), we have developed a systematic study to examine the magnitude and molecular basis of fluoro-stabilization using an array of *in vivo* translated F-UAA-containing single-site superfolder green fluorescent protein (sfGFP) variants. Interestingly, denaturant equilibrium unfolding experiments suggest that fluorocarbon bond substitution *de*stabilizes sfGFP in a position-dependent manner. This atypical result may have intriguing implications for the denatured state of fluorinated sfGFP variants, as spectroscopic evidence suggests that F-UAA substitution at either solvent-exposed incorporation site does not affect native sfGFP secondary or tertiary structure.



MARM 407

Copper binding properties and antioxidant ability of multi-target compounds: Implications in the treatment of Alzheimer's disease

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Alzheimer's disease (AD) is an irreversible and progressive brain disorder that eventually leads to the loss of ability to carry out even the simplest tasks. This form of dementia, that affects more than 5 million Americans and 28 million people worldwide, is characterized by the formation of Amyloid-b (Ab) plaques and reactive oxygen species (ROS). Current treatments are symptomatic and none of them interdicts the underlying cause of AD. Therefore, there is an urgent need for viable chemotherapies that target the root of the onset and progression of the disease. Metal ions, specifically Cu^{2+}, are thought to be involved in the advancement of AD in several ways. They promote the aggregation of Ab into toxic forms of the peptide, and their presence is needed to catalyze the production of ROS. In our work we have assessed the Cu^{2+} binding properties (stoichiometry and binding affinity) and the total antioxidant ability of two multi-target compounds, AM49 and EE229, by means of UV-visible spectrophotometric titrations and the DPPH assay, respectively. AM49 and EE229 belong to a family of compounds that are designed to chelate toxic concentrations of Cu^{2+} ions, to inhibit both ROS formation and Ab aggregation, and to interact with enzymes that are relevant to the progression of AD. In our experiments it was found that AM49 and EE229 form 2:1 (compound:Cu^{2+}) complexes with Cu^{2+} and display binding affinities around logKa~15, suitable to allow competition with Ab peptides but not with needed metalloenzymes. It was also found that AM49 and EE229 can scavenge the DPPH radical. Based on these results compounds AM49 and EE229 show promising potential in the search for disease-modifying therapies against AD.

MARM 408

Use of multicomponent coupling reactions for the design and synthesis of azaheterocyclic compounds as anti-cancer agents

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Azaheterocyclic compounds play an important role in medicinal chemistry. Motifs such as imidazoles, piperazines, pyrazines, pyridines, triazoles, etc. are routinely observed in several compounds of pharmacological interest. Several natural products also contain these motifs in them. We have undertaken a library synthesis of heterocyclic molecules driven by the interest of the local pharmaceutical industry employing green chemistry techniques. We have synthesized a collection of >200 compounds employing Debus-Radziszewski reaction, Passerini reaction, and Baylis-Hillman reaction and tested them for their biological efficacy as anti-cancer agents. Some of the most potent derivatives showed IC_{50} values ranging between 70-200 nM against triple negative breast cancer and prostate cacer cell lines. Our detailed efforts towards structure activity relationship determination studies as well as the bioligical evaluation studies will be discussed.

MARM 409

Detection of anthropogenic influences on nutrient enrichment in New York City parks

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Over 80% of the US population lives in an urban environment. Urbanization has taken a toll on local ponds and lakes. In this study, the physico-chemical parameters in water samples from two lakes of New York City with different environmental settings were analyzed to ascertain the influences of human activities on constraining water quality. Obtained data were compared between freshwater lakes/ponds located in Queens (Corona Meadows Park, an intense recreational park and Kissena Park. An YSI (Yellow Spring Instruments, Inc) was used to measure the real-time water quality data. The results showed some variations as follows: pH 7.81-8.98, electrical conductivity 522-21867 µS/cm, temperature 23.5-29.3°C, total dissolved solute 0.33-13.31 g/L and oxidation reduction potential 79-129 mV. Chemical parameters of water including nitrate, nitrite, phosphate, ammonia and sulfate were investigated using CHEMetrics Vacu-vial kits and spectrophotometer. The distribution of nutrients are obtained consistently different between two lakes such as nitrate (0.11 and 0.09 mg/L), ammonia (3.47 and 0.41 mg/L), phosphate (0.42 and 0.18 mg/L) and sulfate (461.5 and 12.2 mg/L) in Corona Meadow Park lake and Kissena Lake respectively. The Metrohm Tiamo Titration instrument (model 888) was used to determine the alkalinity in terms of $CaCO_3$ (13.1-34.6mg/L). The soils were collected from different depths using GeoTech Environmental Soil sampler device and preserved them in the core at 4°C temperature until analyses are done by Lamotte soil test kit for nitrate, phosphate, potassium, pH. For further study, attempts will be made to use the Lachat 8500 series II Flow Injection Analyzer (FIA) for nutrients analysis and Dionex ICS-2100 for major anions and cations analysis to better monitor and re-evaluate the water quality data.

MARM 410

Electrochemical oxidation of methanol and ethanol catalyzed by copper (I) oxide in pursuit of alcohol-based fuel cells

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Both methanol and ethanol (a bionewable fuel), hold potential for the development of alcohol-oxygen fuel cells, in which the alcohol is electrochemically oxidized to carbon dioxide and water while oxygen is reduced to hydrogen peroxide or water, liberating electrical energy. Special requirements for implementation of practical,cost-effective fuel cells include identification of non-precious metal catalysts, development of robust electrodes, and discovery of conditions for high current density at high percent conversion. In the case of ethanol, it is also necessary to identify catalytic pathways for C-C bond breakage and complete conversion to carbon dioxide, rather than halting at intermediate products, such as acetic acid and acetaldehyde. Copper (I) oxide nanoparticles have been demonstrated by other workers to be effective for the electrolytic upconversion of carbon dioxide and water to methanol and oxygen. Consideration of microscopic reversibility suggests that the same or related catalysts may be effective for the reverse (methanol oxidation) pathway. In the current work, physically and chemically robust electrodes with low resistivity (<10 Ω cm-1) were fabricated from graphite core impregnated with metal oxides. These electrodes were used to oxidize methanol, ethanol, and intermediates compounds to high percent conversion at relatively high current density under basic aqueous conditions near room temperature and at voltages where water oxidation is minimal. For ethanol, conditions were found for

selectivity converting to acetaldehyde. A dual electrode system is therefore suggested for consecutive oxidation of ethanol to acetaldehyde and acetaldehyde to carbon dioxide. Cyclic voltammetry studies were used to probe the reaction mechanism.

MARM 411

Hybrid nanogels as recyclable catalysts

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Hybrid nanogels can be harnessed for tailored applications in the fields of catalysis, sensors, pharmaceuticals, and optoelectronics [1]. Our previous research has shown the successful copolymerization of silica-coated metallic nanoparticles and various functionalized silanes via the Si-OR moieties [2]. We are investigating these hybrid nanomaterials for many different purposes, including tailored nanocatalyts In addition, studies are underway for utilizing these materials for drug delivery applications because PEI is known to have a high transfection efficiency, which allows PEI-stabilized metallic nanoparticles the ability to permeate through the cell membrane for targeted drug delivery [3]. In this poster, we present the synthesis of a novel hybrid nanogels, using a previously described methodology, whereby we copolymerize silylated PEI metallic nanoparticles using various with various silanes, which then can be employed as a reusable, green, catalyst. Model catalytic reactions were used to determine the efficiency, reusability, and durability of the hybrid nanogel. The catalyst was then tested for recyclability purposed and analyzed to determine leaching and/or degradation effects on the metallic nanoparticles and the gel matrix. We will present a brief characterization of all the nanogels. In addition, a detailed comparison of the physical and chemical characteristics of the nanogel throughout the catalytic reaction will be presented via UV-Vis spectroscopy, FT-IR, TEM, and SEM/EDS.

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MARM 412

Pt/C and Pt-Ag/C nanostructured catalysts synthesized via ultrasonic irradiation for ORR: Acid and alkaline electrolyte effect

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Fuel cells are promising technologies due to their high energy density and low pollutant emission compared to conventional power sources. Recent advances in polymer anion exchange membranes have led to increasing studies of alkaline fuel cells (AFCs). AFCs have advantages over traditional proton exchange membrane fuel cell (PEMFCs) due to improved kinetics in the alkaline media where transitions metals that are cheaper than Pt can be used without a significant penalty in activity. Recently, a series of nanostructured Pt-Ag catalyst with different load of Pt and Ag are been investigated in order to improve the electrocatalytic activity. Nanoparticles of Pt, Ag and Pt-Ag were synthesized using ultrasonic irradiation at room temperature with no consecutive thermal treatment to catalyze the acidic and alkaline oxygen reduction reaction (ORR) at room temperature. The kinetic formation of the silver and platinum nanoparticles in solution was followed using UV-vis spectroscopy. The metal nanoparticles obtained were supported on Vulcan XC-72 carbon substrates. The materials synthesized (Pt/C, Ag/C and Pt-Ag/C) were characterized by XRD, TEM, and cyclic and lineal voltammetry techniques. An electrochemical study was performed using both acidic and alkaline electrolytes to analyze the mediums effect on their electrocatalytic properties. XRD results show the crystalline structure of metallic nanoparticles with <10nm in size. TEM confirmed the particle size in form of agglomerates. CVs curve of Pt-Ag in KOH electrolyte indicated more stability compared to the H_2SO_4electrolyte. Electrocatalytic results show that Pt-Ag nanoparticles have electrochemical activity for the ORR in both electrolytes and can be used as cathode in PEMFC as well as AFC.

MARM 413

Effects of Russian propolis metal free ethanol extracts on bacterial biofilms

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In this study, the antibacterial activity of Russian propolis ethanol extracts (RPEE) and Russian propolis metal-free ethanol extracts (RPMFEE) was evaluated. The activity of this antibacterial was tested on two biofilm-forming bacteria: penicillin resistant*Staphylococcus aureus* and *Escherichia coli*. The results of this study indicate that Russian Propolis Ethanol Extracts free of metals have almost identical antibacterial activity against both bacterial species. Complete biofilm inactivation was observed when biofilms were exposed for 40 hours. These findings indicate that the heavy metals present in propolis have antibacterial activity but do not have an essential role in the mechanism of action of propolis. Additionally, metal free samples caused significant damage to the cell membrane structures of both species, resulting in bacteriolysis. These findings suggest that the mechanism of action of Russian propolis ethanol extracts results from the organic compounds found in the antibacterial.

MARM 414

Developing self-assembled bio-organic matrices for targeted drug delivery into tumor cells

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Bio-organic matrices have been gaining importance in the development of scaffolds for drug delivery devices, tissue engineering and biosensors. In this work we have synthesized hybrid matrices that can specifically attach to and deliver chemotherapeutic drugs to tumorigenic cells such as mouse breast cancer cells. For the first set of matrices, we functionalized graphene oxide with specific peptides or polyphenols that are known to mitigate toxicity, scavenge free radicals and possess anticarcinogenic activity. In the second set we functionalized polymers such as polyethylene glycol which were functionalized with peptide sequences and further incorporated with folate, to specifically target over-expressed folate receptors on cancer cells. The formation of the nanoscale drug delivery vehicles developed was confirmed by various spectroscopic as well as electron microscopy analysis. The thermal properties were analyzed by differential scanning calorimetry. Cell proliferation assays, fluorescence microscopy studies were carried out to examine the interactions of cells with the formed constructs. In some cases, in addition to specifically targeting cancer cells, the materials were also found to display antioxidant activity.

MARM 415

Synthesis and anticonvulsant activity of 2’H,3H,5’H- spiro-(2-benzofuran-1,4’-imidazolidine)-2’,3,5’-triones

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Herein we report the synthesis and anticonvulsant activity of a library of nineteen new spirohydantoin compounds that are structural mimics of the clinically used antiepileptic drug, e.g. phenytoin. This class of compounds contain a N-1’,N-3’-disubstituted spirohydantoin scaffold, where the N-1’ and N-3’ positions are modified with an alkyl group or aryl group. Of the nineteen compounds synthesized and tested, three compounds that have a 4-nitro phenyl substituent at N-3’ position exhibited the best anticonvulsant activity. They were more effective than the positive control (phenytoin) when compared using the Racine’s score. Based on the structure activity relationship (SAR), we concluded that small alkyl groups (ethyl, propyl or cyclopropyl) at N-1’ position and 4-nitro phenyl group at N-3’ position are desirable.

MARM 416

Probing organic solute binding in serum albumins using solvatochromic π* indicators: Experimental and modeling studies

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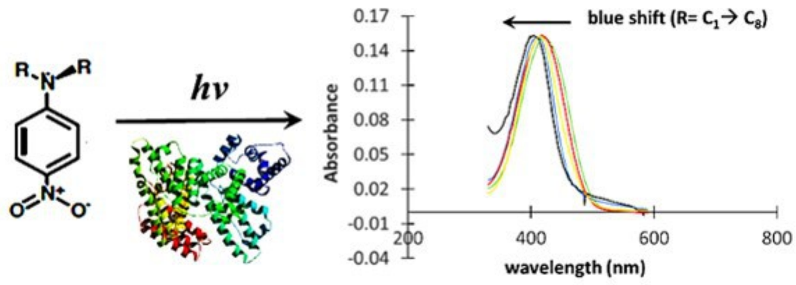
A homologous series of di-n-alkyl-*p*-nitroaniline solvatochromic π* indicators has been applied to the study of dipolarity/polarizability in binding sites of human and bovine serum albumins (HSA and BSA). The solvatochromic absorption band for individual indicators in both HSA and BSA shows increasing blue shift with increasing n-alkyl substitution on the probe. Circular dichroism (CD) spectra of bound and unbound HSA suggest that perturbation of the alpha helical structure of HSA as a result of individual partitioned probes is constant and independent of probe n-alkyl chain length. Results from measurements of the quenching of intrinsic HSA and BSA fluorescence on the part of partitioned probe dyes will be presented and integrated into our findings from CD and absorption spectroscopy experiments. The binding location(s) of the probe molecules on HSA which can be related (in part) to their solvation environments are being estimated using Autodock molecular docking tools.



MARM 417

Imidazolium ionic liquids bearing symmetrical and asymmetrical cations and anions

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Ionic Liquids (ILs) continue to attract interest from a broad audience owing to their attractive tunable physical properties. Their properties of high conductivity, low volatility, low flammability, high thermal stability and ability to be recycled make them attractive alternative solvents in a myriad of applications. Imidazolium ionic liquids have been widely studied and characterized. However, there is still a desire for improvements in their physical properties such as their high viscosity. In this work we explore the effect of adding asymmetrical side chains on the cations and anions of imidazolium ILs on their physical properties. The effect of side-chain length is also assessed. The ILs were prepared by first synthesizing the halide salt precursor, where 1-methylimidazole was reacted with an alkylhalide of the desired chain length on the bench top under reflux conditions. After purification, and structure confirmation, the halide salts were converted to ILs bearing the bis(trifluoromethylsulfonyl)amide (NTf_2) and other fluorosulfonyl anions. The structures of the ILs were confirmed using H-1 and C-13 NMR spectroscopy. The synthesis and preliminary physical characterization of this series of imidazolium ILs will be discussed.

MARM 418

Synthesis and properties of asymmetric dicationic ionic liquids

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A series of Ionic liquids (ILs) containing symmetrical and asymmetrical dications were synthesized in order to study the effect of structural asymmetry on their physical properties. Asymmetrical dicationic ILs bearing triphenylphosphonium and trimethylammonium cationic sites bridged to imidazolium, and pyrrolidinium cationic sites by a carbon chain, with the bis(trifluoromethylsulfonyl)imide $(NTf_2)^-$ anion were synthesized. The ILs were characterized using differential scanning calorimetry and thermal gravimetric analysis to determine their thermal properties including melting point, glass transition point, and degradation point. Further characterization included temperature dependent viscosity and conductivity measurements. Two of the ionic liquids synthesized were found to be room temperature liquids, while the triphenylphosphonium dicationic IL was a solid with a melting point of 70 °C**.** It was observed that ILs containing longer carbon chain bridges appear to have an inverse correlation with the melting point of the IL. Current efforts involve synthesizing ILs bearing triphenylphosphonium and quinolinium cation sites bridged by carbon chains of varying length.

MARM 419

Thio-and thio-bromo "click" approaches to carbohydrate functionalized thioglycosides

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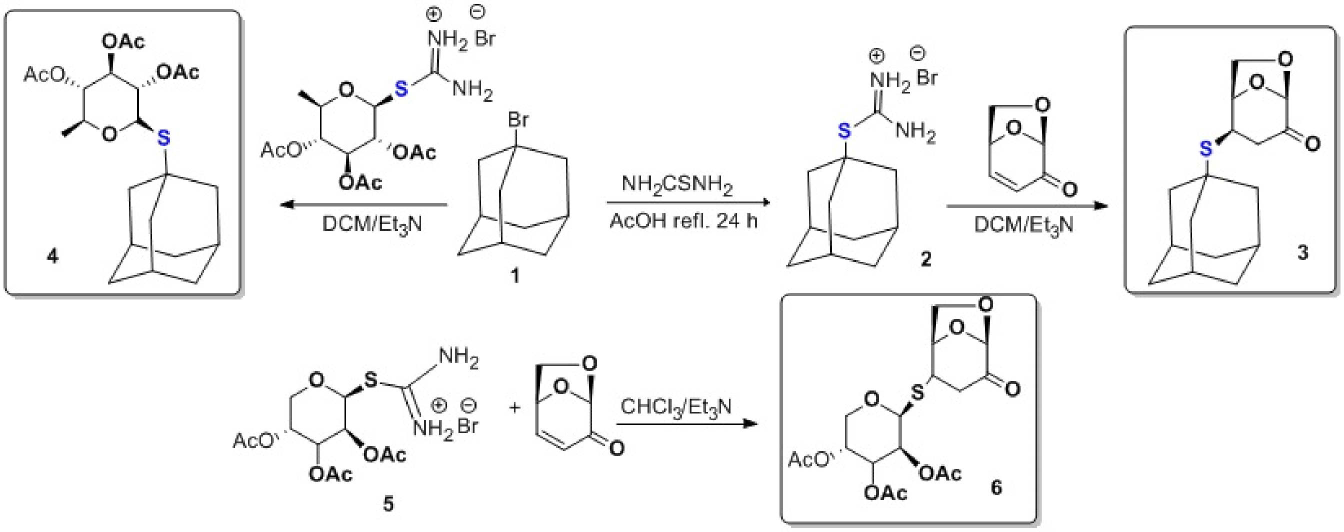
Thio-click chemistry became a well-accepted and useful compartment in the click reaction toolbox. In the area of carbohydrates this approach requires specifically modified chiral building blocks with sugar framework in the locked conformation of the pyranose ring. One of the ideal synthons fitting this category is levoglucosenone, a convenient template for thio-click strategy that was developed in our laboratory. The exceptional robustness of levoglucosenone in this context has been demonstrated by synthesizing a number of new chiral intermediates produced by thio-click addition as depicted below. In particular, the discussed strategy was applied to synthesizing novel adamantine derivatives, which exhibit interesting biological properties.
In this work we accomplished the synthesis of new thio-functionalized *S*-adamantane thioglycosides **3** and **4**, as products of base catalyzed 1,4-thio-click Michael addition of thiouronium adamantane **2** to levoglucosenone and thio-bromo-click of rhamnose thiouronium to 2-bromoadamantane **1**, in 78-82% yields Subsequent, 1,4-thio-click Michael addition of thiouronium L-arabinose **5** to levoglucosenone produced (1-4)-*S*-thiodisaccharide **6** in 79% yield. The structures of all products were confirmed by the proton and carbon NMR analysis. The tentative mechanism of formation of thio-functionalized *S*-adamantane thioglycosides will be discussed as well.



MARM 420

Preparation of starch-poly-glutamic acid graft copolymers by microwave irradiation and the characterization of their properties

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Graft copolymers of waxy maize starch and poly-γ-glutamic acid (PGA) were produced in an aqueous solution using microwave irradiation. The microwave reaction conditions were optimized with regard to temperature and pH. The temperature of 180°C and pH7.0 were the best reaction conditions resulting in a PGA graft of 0.45% based on nitrogen analysis. The average graft content and graft efficiency for the

starch-PGA graft copolymer prepared at 180ºC and pH7.0 were 4.20% and 2.73% respectively. Grafting was confirmed by FTIR spectroscopy. The starch-PGA graft copolymer produced at 180ºC and pH7.0 could absorb more than 20 times its own weight amount of water and form a gel. The preliminary rheology study revealed that the starch-PGA graft copolymer gel exhibited viscoelastic solid behavior while the control sample of waxy starch showed viscoelastic liquid behavior.

MARM 421

CMDwater: A tool for ranking crystallographic waters for displacement during ligand design

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Displacement of crystallographic waters is a commonly used strategy in rational drug design. However not all waters in protein-ligand complexes are easily displaceable. CMDwater is a computational physics-based tool for making decisions about displacing crystallographic waters with ligand groups during lead optimization. CMDwater makes its recommendations based on how much rotational entropy a water loses due to charge interactions. The greater the loss in rotational entropy, the harder it is to displace with ligand groups. CMDwater runs fast and it showed good accuracy for a set of crystallographic waters of known displaceability. Here we describe how the loss in entropy is calculated and show the results for a literature data set.

MARM 422

Testing of GMO foods for consumer purchase in Connecticut

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The information on the abundance of GMO foods in Connecticut is lacking, which is consistent with the rest of the United States. The public opinion on the use of GMOs,especially for human consumption, is mixed. In 2013, Connecticut was the first state in the country to enact a law requiring that foods be clearly labeled on the retail package as to whether they contain GMOs. However, the CT law was written so that it would not go into effect until a certain number of states passed similar legislations. This seems to have catalyzed a reaction over the past years, since recently Vermont and Maine have also passed similar mandatory labeling laws. The current research tested the abundance of GMOs available for consumer purchase in CT and therefore added to the body of scientific data on the abundance of GMOs in consumer products in CT and beyond.

MARM 423

The strengthening of polysaccharide-polyamine hybrid hydrogels by incorporating alginate

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Recently we reported a facile modular approach to rapidly prepare pH-responsive hydrogels by crosslinking polysaccharides with polyamines. Hybrid polysaccharide-polyamine hydrogels are prepared by first reacting the less reactive polysaccharides with the crosslinker epichlorohydrin and completed by the addition of polyamines. The crosslinking of polysaccharides with polyamines provides a facile method for incorporating functionality into polysaccharide based hydrogels. These hydrogels however showed poor toughness which would be a hindrance to their utility. To improve their strength we incorporated sodium alginate, chondroitin sulfate and xanthan gum and crosslinked them with Ca^{2+} to prepare interpenetrating networks (IPN). The hydrogels were characterized by FTIR, swelling and yield strength studies. Hydrogels with Ca^{2+} crosslinking showed lower swelling ratios and improved strength, confirming the creation of the IPN.

MARM 424

Development of an organic laboratory experiment to introduce undergraduate students to olefin metathesis

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Olefin metathesis, though common in organic synthesis and materials chemistry, is not typically discussed in an undergraduate organic course. This procedure uses the synthesis of trans-stilbene from styrene with the Hoveyda-Grubbs catalyst to introduce students to Nobel Prize winning topic of olefin metathesis. The neat liquid reactant can be stirred in the presence of the catalyst to afford the solid stilbene product. The synthesis and characterization process was designed to be completed within a typical undergraduate lab period. This laboratory experiment was tailored for chemistry programs in smaller colleges and universities that may not have access to sophisticated equipment; the solid product can be characterized by simple techniques such as thin layer chromatography and melting point comparison. The solvent-less catalytic conditions, as well as the potential to re-use the styrene as a starting material in a multi-day lab sequence, also presents an opportunity to incorporate green chemistry principles.

MARM 425

The relationship between osteoblast-osteoclast interaction and interleukin 6/STAT3 and sphingosine 1 phosphate signaling pathway

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Normal bone development is maintained by osteoblasts and osteoclasts. The balance between osteoblasts which lay down bone matrix and osteoclasts which resorb bone suggests that a coordinate regulation between these cells in normal homeostasis. Indeed, osteoblasts have been reported to secrete RANKL which is an important cytokine regulating osteoclast development and functions. However, the function of osteoclasts regulating osteoblasts is begun to emerge. Recent studies have shown that the chemokine Sphingosine-1 Phosphate (S1P) produced by osteoclast may be involved in the osteoblast recruitment. We have recently shown that the transcriptional factor, STAT3 a downstream of IL6 signaling, can upregulate the expression of sphingonise-1 phosphate kinase 1 and kinase 2, the enzymes that convert sphingosine to S1P. Using the mesenchymal stem cells (MSCs, precursors to osteoblasts), we demonstrated that MSC migration is affected by conditioned media from osteoclast cultures. We are currently examining the function of STAT3 as a downstream intracellular signaling partner of RANKL and to investigate the mechanism by which MSC recruitment is dependent on STAT 3 signaling in osteoclasts.

MARM 426

Facile fabrication of droplet patterned hierarchical microstructures by condensation of high-boiling liquids onto structured surfaces

***Brian M. Jun**, bjun2@ncsu.edu. BMJ Technologies, Fairfax, Virginia, United States*

In this poster presentation, we present the usage of high-boiling liquids in the formation of droplet patterns on solid surfaces via condensation, and molding the patterned surfaces with uncured polymer mixtures or polymer-solvent blends to fabricate hierarchically patterned structures with porous surfaces. While breath figure formation methods have been successful in creating patterns on polymer surfaces, their disadvantages include the difficulty in applying the droplet patterns on microstructured surfaces to create hierarchical structures. We have investigated the evaporation and condensation of two high-boiling liquids, glycerol and petrolatum, on microstructured surfaces based on polystyrene and epoxy respectively. We have then successfully molded the droplet-patterned surfaces with polydimethylsiloxane (PDMS) or a viscous solution of polyvinyl alcohol (PVA) and water respectively to create hierarchically structured templates. The advantages of using high-boiling liquids to pattern the surfaces include easier control of the process and versatility. We hope that this novel method will provide routes to facile and readily accessible methods of hierarchical microstructure fabrication.

MARM 427

Determination of pesticides in fruits, vegetables, and grains via the Luke method

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The classical procedural methods used to determine residual pesticide levels in food generally tend to be labor intensive, require significant volumes of organic solvents and result in the production of large quantities of hazardous waste. The Luke method, which was introduced in 1981, uses an extraction procedure that is performed three times for maximum pesticide recovery. Minimal amount of solvents are used with low production levels of hazardous waste. The method is comprised of two groups – Section 302 and C6: SAX/PSA Cartridge Cleanup. Section 302 involves extraction with acetone, liquid-liquid partitioning with petroleum ether and dichloromethane solvents. C6 provides improved cleanup required for data analysis and recovery on polar and nonpolar residues. Lastly, mass spectrometry reveals the structures of all pesticides present in the food in question (analyte). The data from mass spectrometry will be cross-referenced with pesticide tolerance levels set forth by the U. S. Environmental Protection Agency (EPA) to determine whether or not a particular food, local or imported, is safe to consume by the American people. Application of this method in case studies will be presented.

MARM 428

Morphological characterization of supragranular neurons in the primary somatosensory cortex

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The cerebral cortex is the outer covering of gray matter in the mammalian brain. It is involved in various functions, including motor functions and touch sensation. We are conducting a morphological analysis of supragranular neurons in the barrel cortex of the mouse which receives sensory input from the whiskers. Our purpose is to determine the morphological characteristics that differentiate different groups of neurons and if those correspond to particular roles within the cortical circuit. Slices from the mouse barrel cortex are processed with DiOlistics to reveal the morphology of individual neurons. *In vivo* injections of fluorescent beads in other cortical areas (ipsilateral M1 and S2, contralateral barrel cortex) label the neurons that project from the barrel cortex. Computerized three-dimensional reconstructions of neurons are created, and morphological parameters are measured. Principal component analysis and cluster analysis are applied to the measurements to determine morphological classes of neurons. Previous work from our lab has defined six morphological classes. Additional cells are being added to the database and the identification of neurons based on the circuit labeling with fluorescent beads will be completed. Finally, sensory deprivation is being used to determine if neuronal activity affects neuronal morphology.

MARM 429

Synthesis of a new α-substituted [13]-macrodilactone

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Macrocycles are a versatile platform for organizing functional groups that can bind a biomolecular target with a well-defined geometry. Examples of macrocycles as important ligands of proteins and nucleic acids can be found in natural products and designed compounds. The design and synthesis of new macrocycles is therefore a promising area of medicinal chemistry. Macrocycles are cyclic compounds containing nine or more atoms with physical properties that are in between small molecules and (bio)polymers. They are conformationally restricted, which increases their rigidity and therefore gives them higher selectivity when binding to proteins and other biomolecules. Our group is interested in synthesizing and analyzing [13]-membered macrocyclic rings in attempt to discover and build a library of potential biologically active molecules. Here we report on the design and synthesis of a new member of our family of [13]-macrodilactones. The new macrocycle contains a hydroxymethyl group a- to one of the carbonyl carbons. An important aspect of the synthesis was the development of a sequence for alkylating and then functionalizing a g-lactone. Synthesis of this hydroxymethyl functionalized [13]-macrodilactone sets the foundation for the preparation of derivatives that vary groups at the a- position of the macrocycle.

MARM 430

Selenium: A potentially powerful tool to design potent anticancer molecules

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Selenium (Se) is an essential micronutrient whose deficiency has been linked to the cause of several diseases including cancer. The halt of SELECT trial that concluded the Se and Vitamin E, taken alone or

together did not prevent prostate cancer, however, placed a question mark on the use of Se molecules as chemopreventive agents in humans. Our studies and literature evidence have shown that, the position of the Se atom as well as other structural features of a molecule dictate the overall properties of a compound and therefore the failure of selenomethionine is not the failure of all Se molecules. This is particularly true in terms of their application as therapeutic agents, because several new Se molecules have shown promising therapeutic efficacy in preclinical cancer models. Over the past few years our laboratory has been involved in developing novel Se compounds as cancer preventive and therapeutic agents. A notable example of this strategy is the development of ISC-4, an PI3K/Akt pathway inhibitor designed by the optimization of structures of naturally occurring isothiocyanates. ISC-4 was shown to effectively reduce tumor growth in melanoma and colon cancer xeongrafts, and inhibit lung tumorigenesis. In addition, the potency of temozolomide (TMZ), first-line drug for treating gliomas, was substantially enhanced by incorporating Se moiety into the molecule. We showed that Se-TMZ retained the oral bioavailability and ability to cross the blood–brain barrier, showed a superior cytotoxicity to that of TMZ in human glioma and melanoma cells and a more potent tumor-inhibiting activity than TMZ in mouse glioma and melanoma xenograft models, and was also effective against a TMZ-resistant glioma cell line. More recently, through extensive SAR studies based on NSAIDs structures, we have identified two novel aspirin derived Se hybrid molecules, which were >100 times more potent than aspirin in inhibiting the viability of various cancer cells. We found these Se-NSAID compounds to be effective against a variety of cancer cells with an IC_{50} in the range of 1 to 2.5 μM, while being non-toxic to normal human dermal fibroblasts (nHDFs), effectively induced apoptosis in various cancer cells via activation of caspase 3/7 and PARP cleavage, and were also more potent than the clinically used chemotherapeutics such as 5-FU, gemcitabine etc. Our studies clearly demonstrate that Se containing small molecules could be a valid avenue to design future cancer drugs.

MARM 431

Mechanistic investigation of hydrogen generation by new bio-inspired Ir complexes for dehydrogenation of formic acid in water

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Dihydrogen (H_2) has many desirable features as a solar fuel and an energy carrier. However, the physical properties of H_2 lead to safety issues and transportation problems. An attractive solution is the storage of H_2 using liquid phase chemicals, e.g., formic acid, which possess favorable stability and storage properties. Himeda and co-workers reported a series of Ir(III) based molecular catalysts with proton responsive ligands that provide reversible storage of H_2 in the form of formic acid (or formate) using CO_2 in aqueous solutions at ambient conditions.[1,2] The pH of the medium was shown to have a determining role in the catalysts' function: at moderately low pH, dehydrogenation of formic acid generates H_2 and CO_2, whereas at slightly high pH, the reverse reaction, hydrogenation of CO_2 to formate, proceeds.

In this contribution, we will describe the experimental and theoretical mechanistic investigations of bio-inspired complexes with ligand combinations of azole and hydroxypyridine or dihydroxypyrimidine (Chart), which produce H_2 by formic acid dehydrogenation efficiently and robustly. The proposed mechanisms based on density functional theory (DFT) calculations provide insight on the observed dependence of the activity profile and kinetic isotope effects (KIEs) on the pH of the medium, and offer new principles for the design of effective homogeneous organometallic catalysts for H_2 generation from formic acid.

(1) Hull, et al. *Nat. Chem.* **2012**, 4, 383.

(2) Suna, et al. *Organometallics*, **2014**, 33, 6519.

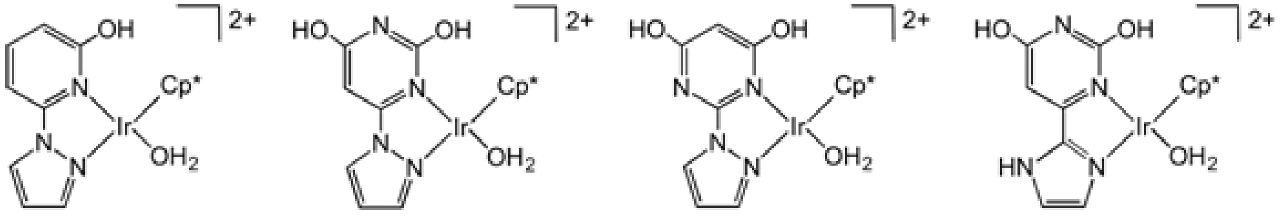

Chart. Novel biomimetic complexes for formic acid dehydrogenation in aqueous solution.

MARM 432

Use of first-row transition-metal hydrides as hydorgen atom donors in radical reactions

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Radical cyclizations have been employed extensively in small-scale synthesis, however concerns on the use of stoichiometric H atom donors (such as SnBu3H) have limited the applicability of radical reactions on industrial scale. We have used transition metal complexes (e.g. CpCr(CO)3H, HV(CO)4dppe, $Co(dmgBF_2)_2(THF)_2$) as replacements for traditional H atom donors, sometimes observing enhanced reactivity due to reduced M–H bond strengths. Furthermore, some of the complexes can be utilized catalytically under H_2. We explore the use of M–H bond strength as a determining factor in understanding observed reactivity, addressing the reformation of the M–H bond under H_2 and the utility of such complexes in organic transformations.

MARM 433

Polynuclear copper hydrides as catalysts for electron transfer from hydrogen

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We have found that $(Ph_3P)_6Cu_6H_6$ is a potent one-electron reductant ($E_{1/2}$ is –1.01 V vs Fc/Fc^+), and it can be easily prepared from H_2 with base (for example, from $Cu_4(O^tBu)_4$ with PPh_3, H_2). So we believe copper hydrides are promising molecular catalysts for H_2oxidation, and are likely to have less overpotential than previous catalysts. Currently, our research focuses on the electron transfer reactions of $L_6Cu_6H_6$ and the regeneration of copper hydride with H_2.

Previously we have reported a single-electron transfer step as an initial step in the reaction of a net hydride transfer, by treating copper hydride clusters ($[(Ph_3P)CuH]_6$) with certain substrates (such as pyridinium cation). The one-electron oxidation product, the radical cation $[H_6Cu_6(PPh_3)_6]^{+\bullet}$, was observed in a stopped-flow apparatus. We further investigated the fate of this radical cation $[H_6Cu_6(PPh_3)_6]^{+\bullet}$. The cation radical ($[(PPh_3)_6Cu_6H_6]^{+\bullet}$) slowly evolves H_2 and forms other hydride complexes, one of

which is a heptanuclear cation $[H_6Cu_7L_7]^+$ with the structure shown below. One face of the original hexamer has become capped by a $[(PPh_3)Cu]^+$. Another major hydride complexe is a hexanuclear pentahydride cation $[H_5Cu_6L_6]^+$, which is synthesized separately with MeOTf. These copper hydrides are potentially important intermediates in copper-catalyzed hydrogenation reactions and copper-catalyzed H_2 oxidation reactions.
We have also found a reliable synthesis of the previously reported $H_5Cu_5(PPh_3)_5$[1], and characterized it by NMR. It is *not* formed from $[H_6Cu_6(PPh_3)_6]^{+\bullet}$, and does not rearrange to $H_6Cu_6(PPh_3)_6$.

1. Albert CF, Healy PC, Kildea JD, Raston CL, Skelton BW, White AH (1989) Lewis-base adducts of Group 11 metal(I) compounds. 49. Structural characterization of hexameric and pentameric (triphenylphosphine)copper(I) hydrides. Inorganic Chemistry 28 (7):1300-1306. doi:10.1021/ic00306a019

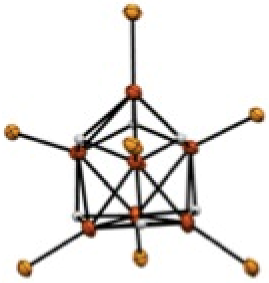

Figure 1. Structure of $H_6Cu_7(PPh_3)_7^+$

MARM 434

Catalytic carbon monoxide oxidation at ambient condition in basic solution

*Daniel Shlian, Jack Alboucai, Michael Khaloo, Avraham Benhaim, Miriam Stock, Jonathan Lewis, **Jianfeng Jiang**, jiang@yu.edu. Chemistry, Yeshiva University, Fort Lee, New Jersey, United States*

Carbon monoxide is a good reducing agent. However, the oxidation of carbon monoxide at ambient condition is very slow due to high activation energy. Our recent study has shown that carbon monoxide can be oxidized to carbonate in basic solution in the presence of nickel, cobalt or copper salts, especially in the presence of cyanide. Nickel and cobalt cyano carbonyls are the reactive intermediates and they are structurally characterized. The oxidation kinetics of carbon monoxide by oxygen gas at room temperature and atmospheric pressure was studied. A crude carbon monoxide powered fuel cell was built to demonstrate the direct conversion to electrical energy.

MARM 435

Mechanistic considerations in water oxidation catalysis by ruthenium bipyridine-dicarboxylate and ruthenium bipyridine-phosphonate-carboxylate complexes

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Reported here is a detailed kinetic study of ruthenium water oxidation catalysts with substituted bipyridine-dicarboxylate (bda) ligands and a new set of hybrid catalysts utilizing a tetradentate bipyridine-phosphonate-carboxylate (bpc) ligand. The rate-limiting step in water oxidation by (bda)Ru(L)$_2$ (L = pyridine-type ligand) catalysts is found to vary with concentration, with an oxidation being limiting at higher catalyst concentrations and a bimolecular coupling being limiting at lower catalyst concentrations. Kinetic isotope experiments show that both steps involve proton transfer, which is inconsistent with oxo-oxo coupling mechanisms proposed in the literature. It is notable that the rate-determining step is different at concentrations typical for electrochemical experiments (~10^{-3} M) and those typical for stopped-flow absorption experiments (~10^{-6} M), which could account for some discrepancies observed in the literature. Installing electron-withdrawing substituents onto the bda ligand has opposite effects on the two possible rate-determining steps, highlighting the importance of prudent catalyst design.

New single-site water oxidation catalysts based on a hybrid tetradentate bipyridine- phosphonate-carboxylate (bpc) ligand improve upon their bda and bipyridine-diphosphonate (bpa) counterparts in that each oxidation from ruthenium(II) to ruthenium(V) is a proton-coupled electron transfer step, which moderates the oxidation potentials. The ruthenium(III/II) couple is accompanied by proton loss from the phosphonate group. The binding of water at the ruthenium(III) state (in contrast to the bpa catalysts) allows for all subsequent oxidations to be proton-coupled. In contrast to (bda)Ru(L)$_2$, the (bpc)Ru(L)$_2$ catalysts proceed through a single-site water nucleophilic attack mechanism, with the phosphonate group acting as a pendant base to facilitate the atom-proton transfer step involving concurrent O-O bond-formation and deprotonation of the incoming water molecule. Stopped flow kinetics find the rate-determining step to be a proton-coupled oxidation of the catalyst. The rate constant for the rate-limiting oxidation step is significantly larger than that for both the bda and bpa complexes. Fast single-site catalysts like these avoid obstacles presented in surface-attached systems by catalysts requiring a bimolecular coupling step (like the bda catalysts).

MARM 436

Synthesis and reactivity of a molecular titanium nitride

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Our research involved synthesis of a titanium nitride complex with a highly polarized Ti-N bond that could serve as a nucleophilic N-atom in transfer reactions. We previously reported the β-diketiminate supported titanium nitride dimer, $[\mu_2\text{-K}]_2[(^{tBu}\text{nacnac})\text{Ti}{\equiv}\text{N}(\text{Ntolyl}_2)]_2$ ($^{tBu}\text{nacnac}^- = [\text{ArNC}^t\text{Bu}]_2\text{CH}$; Ar = 2,6-$^i\text{Pr}_2\text{C}_6\text{H}_3$), but detailed reactivity studies were hindered by the propensity of the nitride functionality to undergo intramolecular cross metathesis reactions with the ligand. In order to eliminate this problem we chose to use a potentially more robust ligand, the monoanionic, chelating ligand PN (PN^- = (N-(2-(diisopropylphosphino)-4-methylphenyl)-2,4,6-trimethylanilide).

With the complex Ti(PN)$_2$Cl in hand, our efforts towards a titanium nitride species focused on reduction of the complex in the presence of N_2. The reduction of Ti(PN)$_2$Cl with KC_8 leads to activation of N_2, forming $(\text{PN})_2\text{Ti}(\mu\text{-N}_2)\text{Ti}(\text{PN})_2$. Complete reduction and cleavage of the N≡N bond does not occur, even with photolysis, heating or the presence of excess strong reductants.

We therefore sought to use N_3^- as the source of nitrogen. Reaction of Ti(PN)$_2$Cl with NaN_3, results in formation of a Ti(III) azido complex. Reduction of the azide complex with KC_8 results in clean formation

of the titanium nitride dimer, $[\mu_2\text{-K}]_2[(PN)_2Ti{\equiv}N]_2$. Addition of 18-crown-6 breaks the apart the dimer, and addition of 2,2,2-Kryptofix yields a terminally bound nitride species. The structures of the three titanium nitride complexes were confirmed by crystallographic and spectroscopic methods, and the $Ti{-}N_{nitride}$ bonding was studied theoretically by DFT-based methods.
As expected, the nitride ligand is a strong nucleophile, participating in salt elimination reactions and N-atom transfer reactions with a variety of electrophiles. We also explored the redox chemistry of the titanium nitride species, to gain insight into the potential formation and stability of a nitridyl radical species, Ti≡N●. Such species have been proposed in a number of H-atom transfer and decomposition reactions. Oxidation of $[\mu_2\text{-K}]_2[(PN)_2Ti{\equiv}N]_2$ results in oxidation of one of the PN ligands to form a dianionic phosphinimide-anilide ligand. This species likely forms via a nitridyl or iodonitrene species, which then oxidizes the phosphorous atom of the PN ligand.

MARM 437

Human serum albumin-heme with proximal tyrosine ligand exhibits nitrite reductase activity

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Members of the heme enzyme family are uniquely diverse in structure particularly with respect to the ligand proximal to the heme, but can share similar functionality. For example, heme enzymes that have proximal histidine (e.g. hemoglobin, myoglobin, neuroglobin) and cysteine (e.g. Cyt P450s) can generate nitric oxide (NO) via nitrite reduction, and have therefore been perceived as nitrite reductases (NiRs). However, no known pentacoordinated heme complex with a proximal tyrosine ligand has displayed NiR activity because of its low redox potential. This is attributed to the basicity of the phenolate ligand thereby making it a challenge to reduce the heme Fe center (e.g. catalase). In this work, we utilize human serum albumin (HSA) reconstituted with heme *b* (referred to as HSA-heme), which forms a pentacoordinated complex via Tyr161 and has a reduction potential of -228 mV vs Ag/AgCl. Spectral absorption analysis of the product formed between Fe^{II} and nitrite confirms the formation of NO under anaerobic conditions. This is further verified by a fluorimetric assay involving the N-nitrosation of 2,3-diaminonaphthalene, which converts to the fluorescent compound 2,3-naphthotriazole in the presence of nitrite.

MARM 438

Towards development of a mass spectrometric database for the rapid identification of plant drugs of abuse by ambient ionization mass spectrometry

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The use of new psychoactive substances and in particular, plant-based psychotropics, has increased due to the marketing of these products as safe and “legal” alternatives to common drugs of abuse. Currently, there are few standard operating protocols (SOPs) available to characterize and identify these complex plant matrices. Furthermore, the constantly changing landscape in the variety of abused plant products makes method development and validation for each new drug unrealistic, particularly when relying on conventional methodologies. An added dimension to the problem of identifying psychoactive plant products is the lack of statistical analysis in forensic science reporting, as highlighted in the 2009 National Academy of Sciences report.

Direct analysis in real time-high resolution mass spectrometry (DART-HRMS) provides an opportunity to circumvent some of the disadvantages of current drug testing methodologies. Plant material was tested directly without the need for complex sample preparation steps. *Datura* spp. seeds, Kratom powder, Kava powder, *Salvia divinorum* leaves, Kanna crushed leaf material, *Mimosa hostilis*, *Banasteriopsis caapi* and Morning Glory seeds were analyzed in their native forms using DART-HRMS under soft ionization conditions. Psychoactive brews made from mixtures of plants could also be identified. Furthermore, characteristic biomarkers contained within the complex matrices could be identified through in-source collision-induced dissociation experiments.

The complete mass spectral profile of the psychotropic plant materials provided a diagnostic chemical fingerprint which was unique enough to enable species identification and classification through the application of multivariate statistical analysis methods, including linear discriminant analysis (LDA), hierarchical clustering analysis (HCA), and partial least squares-discriminant analysis (PLS-DA). The application of statistical analysis methodologies enabled species-level identification of plant-based drugs of abuse with a defined level of confidence. The results serve as a foundation upon which a database of abused plants can be created to aid in their rapid identification in a forensics context.

MARM 439

Deducing the structures of amphetamine and cathinone unknowns from chemometrically processed ambient ionization mass spectral datasets of known synthetic amphetamine and cathinone structures

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The exponential rise in the abuse of synthetic cathinones in recent years continues to present unique challenges to the law-enforcement community. The ease with which their molecular scaffolds can be modified has led to the rapid availability of numerous novel structural variants. This influx of structurally modified chemotypes makes the identification of new “unknowns” extremely difficult. Here, we show using in-source collision induced dissociation (CID) by direct analysis in real time mass spectrometry (DART-MS), that cathinones exhibit characteristic neutral mass losses that correspond to diagnostic structural features. A dataset of forty one cathinones was subjected to unsupervised statistical analysis by hierarchical clustering of the neutral loss data. The resulting dendrogram revealed diagnostic relationships between structurally similar cathinones based on their proximity to one another in the observed clades. Using these clustering relationships provided by unsupervised analysis, inferences regarding the structural features of an unknown cathinone could be made. Kernel discriminant analysis (KDA), a supervised statistical method, was performed on the neutral mass loss data of a small subset of cathinones as well. The subset contained three structurally different groups of cathinones including ethcathinones, pyrrolidine ring containing cathinones, and cathinones with a methylene dioxy moiety. Using 18 feature masses, distinct clusters of each group of cathinones were observed. Within each cluster, the individual cathinones of which they were comprised could be distinguished from one another. Futhermore, KDA could be used to discriminate between cathinones and non-cathinones, including the common cutting agents lidocaine, benzocaine and caffeine.

MARM 440

Screening of drugs of abuse using DART-MS and in-source CID reverse library search

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Routine screenings for drugs of abuse in many laboratories generally involve presumptive techniques such as color tests and immunoassays or confirmatory techniques such as GC-MS and LC-MS. Although these techniques still represent the gold standard for routine analysis and identification of drugs of abuse, presumptive tests lack the desired selectivity and are designed to identify the presence of a set of possible drugs whereas chromatography- based methods are time-consuming. Direct analysis in real time – mass spectrometry (DART-MS) has been shown as a capable method for rapid, real time detection and identification of drugs of abuse. In an effort to improve selectivity and the level of confidence for drug identification, the utility of in-source CID and reverse library search was investigated. A DART source was interfaced to a single quadrupole mass spectrometer as a means of providing an economical platform with the capability of in-source fragmentation. Standards of each drug were analyzed individually for the creation of the library. The voltage applied to the mass spectrometer sample cone was varied to induce fragmentation. A reverse search library that is modeled after the NIST DART Forensic library was created. The library consisted of four entries, one from each of four cone voltages, with the most characteristic precursor and fragment ions for each drug. Ten drugs of abuse with different chemical properties, such as volatility, polarity, molecular weight, etc., were first evaluated to determine four voltages that will be employed for library. We have shown that +15V, +30V, +50V and +70V provided sufficient molecular ion and fragmentation data required for identifying and differentiating 23 drug compounds. Drugs of abuse cut with adulterants and diluents that represent typical, street quality, controlled substances submitted for forensic analysis were employed to evaluate the performance of the library and algorithm. A 100% positive identification (probability match of greater than 0.95) was achieved for individual components with concentrations as low as 0.5 ppm. The library was then expanded to include 156 compounds from various classes of drugs of abuse and validated using both single component samples and multi-component mixtures consisting of varying ratios and isomers as well as “real world” case samples. The results show a promising cost-efficient approach for drug screening that is more selective than conventional approaches.

MARM 441

An overview of ambient ionization mass spectrometry efforts at NIST-STCAG

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This presentation will provide an overview of some of the forensic related work currently being pursued in the Surface and Trace Chemical Analysis Group (STCAG) at the National Institute of Standards and Technology (NIST). The focus of our group is on the development of new, and evaluation of existing, ambient ionization sources for forensic and trace contraband detection applications. In addition traditional source characterization, we use a suite of visualization and measurement tools to better understand and optimize individual sources for specific applications. We also concentrate on creating realistic yet reproducible standards for the validation and cross-comparison of these techniques. This talk will provide examples on potential applcations of ambient ionization mass spectrometry for the detection of explosives, narcotics, lotion and lubricants, latent fingerprints, and bodily fluids. Also, the concept of useful yield and production of inkjet printed test materials will be discussed as they pertain to ambient ionization sources.

MARM 442

Time flies: Species identification of blow flies by direct analysis in real-time, high-resolution mass spectrometry (DART-HRMS) for postmortem interval estimations

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Several species of blow flies are of importance in forensic entomology. Their life cycles are highly predictable and this fact, along with blow fly colonization patterns and insect succession order enable them to be used as biological clocks to determine the postmortem interval (PMI). This assessment requires that the species of colonizing flies be known. Conventional methods for fly species determination are often difficult and time-consuming, and typically require the rearing of juvenile flies to maturation in order for an entomologist to make an identification. This task can be even more challenging if flies cannot be reared because the entomological evidence is not viable. Here we show through analysis by direct analysis in real time-high resolution mass spectrometry (DART-HRMS) that fly species eggs exhibit distinct chemical fingerprints. Processing of these profiles using multivariate statistical analysis tools enabled species-level identification of blow flies. The method requires no sample preparation, and eggs can be analyzed in their preserved form after retrieval from a crime scene. Six species of eggs, namely *Calliphora vicina, Lucilia sericata, Lucilia coeruleiviridis, Phormia regina, Phoridae* and *Sarcophagidae*, were analyzed by DART-HRMS. Their chemical profiles displayed interspecies differences as well as intraspecies similarities. Linear discriminant analysis was performed using a training set of 90 mass spectra and nine feature masses. Three principal components accounted for 96% of the variance and the leave-one-out cross validation (LOOCV) was 80%. Tight clustering was observed and each species was well resolved from the others. The results demonstrate that species-level identification is possible through chemometric processing of chemical fingerprints acquired by DART-HRMS analysis of blow fly eggs.

MARM 443

DART-TOF-MS analysis of personal lubricants

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Sexual assaults are an unfortunate reality in modern society. A recent survey conducted by the National Center for Injury Prevention and Control revealed that roughly 1 in 5 women and 1 in 71 men will encounter a sexual assault in their lifetime. While this statistic is concerning, condom usage in sexual assaults has gradually increased over recent years, as assailants attempt to mitigate the transfer of biological evidence. In the absence of biological evidence, sexual lubricants may be the only actionable information available to investigators.

Silicone-based, water-based and condom lubricants were analyzed to identify discriminating class features that can be used to characterize unknown lubricants recovered from victims. Previous research have focused mostly on assigning unknown personal lubricants to one of the major four lubricant types: silicone-based, water-based, petroleum-based, and organic-edible based. Characterization features within lubricant groups have not been explored. In this research, over one hundred individual lubricants were characterized by direct analysis in real time - time-of-flight mass spectroscopy (DART-TOFMS). DART-TOFMS is a high resolution-accurate mass ambient ionization technique that is capable of rapidly analyzing every component in a lubricant mixture, while requiring little to no sample preparation.

Ultimately, this capability has greater potential of characterizing lubricants over conventional instrumental techniques, e.g. infrared spectroscopy. The resultant mass spectral data was evaluated using principal component analysis and linear discriminant analysis to identify potential classes. Statistical analysis revealed that it was possible to easily differentiate between the silicone-based and water-based personal lubricants, as well as the spermicidal condoms which contained nonoxynol-9. Furthermore, sub-groupings were identified within the main lubricant classes based upon the lubricant's oligomeric range or the presence and/or absence of additive components. Identifying unique features within each lubricant group will aid in identifying the specific class and sub-class of unknown lubricants, when only a questioned sample is available.

MARM 444

Using APCI-MS for the screening of arson samples for the presence of accelerants

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An APCI-MS/MS method has been developed to screen arson samples common accelerants. The samples were placed in paints cans with a carbon strip and heated overnight at approximately 80°C. The carbon stips were then extracted with 2 mL of carbon disulfide which was slowly injected into the MS/MS using a flow injection technique at 20 uL/min. The MS/MS, an ABI Sciex 3200 QTRAP triple quadrupole mass spectrometer, utilized an APCI source in positive-ion mode. Dimethly sulfoxide was also evaluted as a potential extraction solvent and the use of anisole as a dopant was also tested but carbon disulfide gave the bet overall sensitivity with the least amount of ino source fragmentation. For each sample 30 scans were acquired using the peak hopping scan mode with a step size of 1 amu and the intensities were summed for each mass. A Q1 scan and 2 precursor scans (91 and 128 amu) were also run for each accelerant sample under these conditions.

Accelerants such as gasoline, diesel, lighter fluid, mineral spirits, turpentine, paint thinner, WD-40, and kerosene were sampled. Prominent peaks in the Q1 and precursor ion scans presented a different profile for each accelerant. To allow for Principle Component Analyses, the masses were then summed in 10 amu bins and the bins were normalized to the largest bin value. To evaluate the reducibility of the method over time both a gasoline sample and a diesel sample were run multiple times over a 4 month period. To evaluate the reproducibility within a type of accelerant, 5 different brand of diesel, 6 different brands of gasoline and 20 different samples of kerosene were all run and compared against each other . In every case the profiles in the 3 types of scans were reproducible enough that the samples could be correctly grouped. The results of these reproducibility studies will be presented along with the PCA results.

MARM 445

Using bioinformatics to elucidate the evolutionary dynamics of rhomboid proteases in *Streptomycetes*

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Proteolytic enzymes are ubiquitous and active in a myriad of biochemical pathways. One type, the rhomboids are intramembrane serine proteases that release their products extracellularly. These proteases are present in all forms of life and their function is not fully understood, although some evidence suggests they participate in cell signaling. *Streptomycetes* are prolific soil bacteria with diverse physiological and metabolic properties that respond to signals from other cells and from the environment. This present study uses bioinformatics to characterize five evolutionarily distinct rhomboid families found in the genomes of these bactiera and compares them to those of other prokaryotes and eukaryotes. Additional research using knock out (KO) mutants is being conducted to fully understand the role these enzymes play.

MARM 446

Using template-based modeling and bioinformatics to gain insight into the function of various protein domains/proteins

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The long-term research goal of our lab is to apply computer modeling to gain insight into cellular signal transduction pathways, specifically to provide deeper insight into both the normal and aberrant subcellular targeting and functioning of domains contained in proteins which are part of macromolecular complexes and function in various biological processes. The focus of our work is on understanding the molecular basis of interactions of specialized protein domains with lipid, ligands, and protein partners that contribute to their subcellular localization and function. The protein/membrane and protein/protein complexes that function in signaling pathways are often not amenable to traditional structure determination. The integration of bioinformatics and structure determination tools to analyze genomic data with detailed computer calculations of the physical interactions can provide novel insights into the molecular basis of the formation and regulation of these macromolecular complexes and, thus, allow the suggestion of rational and experimentally testable predictions as to their function. This approach can be successfully extended to a protein family or genome-wide level, allowing for the analysis of emerging families of specialized protein domains with multiple roles at the whole genome level. Using examples from various membrane targeting domains, proteins/domains with novel folds, and well-established folds such as catalytic domains, we demonstrate the strength and wide applicability of our approach.

MARM 447

The evolutionary dynamics of LINE transposable elements in the vertebrate genome

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LINEs (Long Interspersed Nuclear Elements) constitute the dominant class of autonomously replicating retroelements in the vertebrate genome. These elements have been a significant source of evolutionary novelties and have substantially affected the size and structure of vertebrate genomes. In mammals, L1 copies make up an estimated 20% of studied genomes, exerting large genomic loads onto their hosts. The impact LINEs have on the evolution of their host depends on their abundance and diversity which result from the interactions between the rate of replication, the intensity of selection against new inserts and the demographic history of populations. To decipher between these different processes, we performed a comprehensive evolutionary analysis of the LINEs in the genome of 12 vertebrate species representative of all major vertebrate lineages (mammals, reptiles, amphibians, fish). Two distinct patterns emerged. First, there is a clear difference between mammal and non-mammalian vertebrates: LINEs in mammalian genomes have comparatively low diversity between families but are represented by extremely large copy numbers whereas non-mammalian vertebrates have large diversity between families, each represented by small copy numbers. This suggests a fundamental difference in the way mammalian and non-mammalian

genomes interact with their intra-genomic parasites. Second, we have observed that, in vertebrates, the diversification of LINEs is primarily driven by the acquisition of novel promoter sequences, suggesting that new lineages emerge and amplify only when they do not compete with other lineages for host-encoded transcription factors.

MARM 448

Evolutionary interpretations of mycobacteriophage biodiversity and host-range through the analysis of codon usage bias

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As part of an evolutionary genomics course sponsored by the Howard Hughes Medical Institute, students across the world have isolated and sequenced the genomes of more than 1,125 mycobacteriophages, making it the largest database of sequenced viruses able to infect a single host, *Mycobacterium smegmatis,* a common soil bacterium. Genomic analysis suggests that these mycobacteriophages can be grouped into 26 different clusters based on genetic similarity. Furthermore, these clusters span a continuum of genetic diversity, with extensive genomic mosaicism among phages in different clusters. However, little is known regarding the standard hosts of these mycobacteriophages in their natural habitats, nor of their broader host ranges. As such, it is possible that the primary host of many newly isolated mycobacteriophages is not *M. smegmatis.* Rather these mycobacteriophages may infect unknown, but closely related, bacterial species. This alternative is not easy to test experimentally because of the difficulties associated with mycobacterial cultivability, pathogenicity and growth. Another way to gain insight into mycobacteriophage host range and ecology is through bioinformatic analysis of their genomic sequences. To this end, we examined the correlations between the codon usage biases of 199 different mycobacteriophages and those of several fully sequenced mycobacterial species as means to gain insight into the natural host range of these mycobacteriophages. We find that UPGMA clustering tends to match, but not consistently, clustering by shared nucleotide sequence identify. In addition, analysis of GC content, tRNA utilization and correlations between mycobacteriophage and mycobacterial codon usage bias suggests that the primary host of most clustered mycobacteriophages is not *M. smegmatis*, but instead other members of the mycobacteria complex.

MARM 449

Ancestors in our genome: The new science of human evolution

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Two of the biggest scientific breakthroughs in paleoanthropology occurred in 2010. Not only had we determined a draft genome of an extinct Neandertal from bones that lay in the Earth for tens of thousands of years, but the genome from another heretofore unknown ancient human relative, dubbed the Denisovans, was also announced. An over one-hundred year old conundrum was finally answered: did we mate with Neandertals? It was now undeniable that modern humans, with all our modern features had met and mated with**both** of these extinct human-like beings. The questions are now: what are the consequences of archaic DNA in our genomes?
These breakthroughs open a window of fresh air onto the field of anthropology after many decades of speculation. We are also making base-by-base comparisons of our genome with our primate cousins and finding some of the genomic bases of our unique features – our large and complex brains, our complex

cognition and spoken language. Simultaneously, we are learning more about the continuum existing between us and other primates. Darwin presciently wrote "the difference in mind between man and the higher animals, great as it is, certainly is one of degree and not of kind." Today, we are realizing Darwin's dream.

Genomes allow us to probe how human populations adapted to hot and cold climates, high altitudes, different diets, and to myriad pathogens we encountered in our world-colonization. Already well-underway, is a large project collecting thousands of genomes of peoples from around the world. By comparing them, we are discovering ancient footprints left by natural selection. Surprisingly, pathogens appear to have left some of the largest footprints in our genome.

The genomic highway has an unchecked speed limit. We are unlocking fascinating secrets about our ancestry at an exhilarating pace. This talk will give an overview of how full genomes from living humans, our primate relatives and our extinct archaic cousins are reinventing the science of human evolution.

MARM 450

Lead-free ammunition

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Environmentally friendly, or lead-free ammunition is becoming more popular in the shooting community. This is a result of an increased awareness of the health and environmental hazards inherent in traditional lead-based ammunition. Traditional ammunition can contain lead in the bullet, the primer compound, or both. Ammunition manufacturers are now designing bullets with some innovative alternative compositions to address concerns about lead. Lead-free bullet alternatives include the use of other alloys, compressed metal powders and metal spheres held together with adhesive resins. This research examines the construction and ballistics of several examples of lead-free ammunition as compared to traditional lead bullets.

MARM 451

The chemical methods of gunshot residue analysis

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The chemical analysis of gunshot residues will be presented. Upon introduction of the chemistry associated with ammunition and the discharge of a firearm, the methods and historical development of the chemical detection of gunshot residues in forensic investigations will be described. Chemical detection methods currently employed in crime laboratories, including microchemical crystal tests and color tests, will be discussed with respect to their role in muzzle-to-target distance determinations and shooting reconstructions. In addition, the role of gunshot residue detection and analysis for the determination of whether or not a person recently fired a weapon will be explained. Finally, this presentation will introduce the instrumental methods used for the analysis of gunshot residue. Case studies from the presenter's experience as a Criminalist in the Trace Evidence Analysis Unit of the NYPD Forensic Investigations Division will be used to enhance the analytical approaches to gunshot residue throughout the presentation.

MARM 452

Instrumental methods for the detection of gunshot residues

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The determination of the fact that an individual has recently discharged a weapon has long been an elusive goal of Criminalists (Forensic Scientists) The methodologies employed progressed from functional group color tests, through micro-crystal tests, chemical instrumental analysis using various spectrometer methods to the currently use of micro particle analysis by Scanning Electron Microscopy and Energy Dispersive X-ray Spectrometry (SEM-EDS). This presentation will take the audience through the instrumental analysis methods utilized, discussing the advantages and shortcomings of each. In addition, what valid conclusions the expert can testify to in court will be presented.

MARM 453

Health effects of asbestos: What issues are current?

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Asbestos is a group of six commercial minerals (actinolite, amosite, anthophyllite, crocidolite, tremolite and chrysotile) recognized as human carcinogens by the International Agency for Research on Cancer. US regulatory agencies have set the same permissible exposure limit (PEL) for all the asbestos types, starting with the first Occupational Safety and Health Administration (OSHA) PEL of 12f/mL in 1971 (currently the PEL is 0.1f/mL). To control occupational exposure to asbestos the US limits the airborne concentration of fibers 5 microns in length or greater (with length to width of 3:1 or greater). Anthophyllite in 1977, amosite in 1992 and crocidolite in 1997 stopped being mined while actinolite asbestos and tremolite asbestos were rarely used commercially. The only type of asbestos remaining in commerce worldwide is chrysotile with production steady at about 2 million tons per year (about 1,000 tons continues to be used each year in the US). However, exposures to chrysotile continue in the non-occupational environment which are of current interest. A recently completed study of the potential for health hazard from recreational riding of motorcycle on soils containing chrysotile. The exposures to airborne asbestos from this activity have been quantified by activity based air sampling. The risk of developing asbestos-related cancer from these cumulative exposures were calculated using the current EPA Asbestos Health Update and compared to other risks from recreational activities.

MARM 454

Talc and ovarian cancer

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The mineral talc is a naturally-occurring magnesium silicate hydrate that has found its way into many hundreds of industrial applications and consumer products. It is mined from open pits and underground workings and milled and beneficiated for physical and chemical properties intended for its specific end-use. Consumer application for talc has included pharmaceuticals, foodstuffs and cosmetics. The use of talc in body powders has recently gained media and legal attention with the allegation that those women who have used body talcum suffer an increased of risk of death from ovarian cancer.

Talc mineral, in its natural state, may co-exist and be co-mixed with other minerals depending on the nature of its host rock and the conditions under which talc formed. This variation in geologic conditions of formation has resulted in talcum products that contain the amphibole minerals tremolite and anthophyllite (as well as other amphiboles), serpentine minerals (including chrysotile asbestos), and quartz. The issue concerning the alleged carcinogenic properties of talc appears to focus on the habit of crystallization of the associated amphiboles, whether their end-points have formed amphibole asbestos or not.

Inhalation of talc dust in mining, milling and the industrial environment has been shown to be associated with a pneumoconiosis called talcosis. The International Agency for Research on Cancer (IARC) classifies talc with asbestiform fibers as a human carcinogen but not talc. A central issue is the mineral complexity of talc deposits and whether or not amphibole asbestos is present. Some epidemiology studies show an excess of ovarian cancer in women who use body talcum while other studies do not. Experimental animal studies have shown talc itself lacks carcinogenic properties. The Food and Drug Administration (FDA) of the United States has listed consumer talc in their GRAS Document as “generally regarded as safe.” The strength of the scientific studies addressing the question of body talcum as a cause of ovarian cancer will be presented. Another central issue is if the scientific evidence is sufficient to require that the users of body talcum be warned of an increased risk of ovarian cancer from the use of this product.

MARM 455

Ion chromatography tandem mass spectrometry for ultra-trace analysis of hexavalent chromium

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The reliable analysis of highly toxic hexavalent chromium, Cr(VI) at safe environmental levels remains challenging, given its easy conversion to non-toxic trivalent chromium. This work demonstrates a novel analytical method to quantify Cr(VI) at low ng L^{-1}concentration levels in environmental water samples by using speciated isotope dilution (SID) analysis. Ion chromatography tandem mass spectrometry (IC-MS/MS) was used for the analysis of Cr(VI) as $HCrO_4^- \rightarrow CrO_3^-$. Whereas a classical linear multipoint calibration curve approach obtained a method detection limit (MDL) of 7 ng L^{-1} Cr(VI), the SID-MS method adapted from U.S. EPA 6800 allowed for the quantification of Cr(VI) with an MDL of 2 ng L^{-1} and provided results corrected for Cr(VI) loss occurring after sample collection. The method was applied for the analysis of environmental surface and ground water samples in the Ring of Fire region in Northern Ontario. Preservation at pH values > 8.5 was required for all ground waters and acidic samples and caused little to no oxidation of environmental Cr(III). The SID-MS approach proved to yield more precise results than the classical linear multipoint calibration curve method and allowed for compensation of Cr(VI) reduction during sample transportation and storage.

MARM 456

Chemical characterization of urban soil in New York City

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This research aims to study the chemical dynamics in NYC parks to understand their soil quality. This study reports the spatial variability of chemical contaminants in NYC park environment that was obtained from three months summer research in 2015. The study was conducted in two of the city parks: 1) Corona Meadows Park, an intense recreational park in Queens and 2) Kissena Park in Queens. A wide range of elements including RCRA (Resource Conservation and Recovery Act) toxic metals and fecal indicative bacteria (FIBs) in soils were studied. The spatial distribution of fecal indicative bacteria (FIBs) including total coliforms, E. coli and enterococcus was also investigated in these two study areas to understand the microbial fate and transport in the lake environment. The soils were collected from different depths using GeoTech Environmental Soil sampler device and preserved them in the core at 4^{o}C temperature until analysis done for the microbiology. Nitan handheld XRF (X-ray Fluorescence Spectrometry) was used to detect the array of elements in dried soil samples. The data were generated for bulk samples and also for the fine fraction <0.25 mm). The standard reference materials (NIST) were run to maintain the QA/QC of the data. The preliminary data obtained from bulk samples showed elevated level of several RCRA toxic elements in NYC park soils. Higher occurrences of FIBs in soil are very consistent with the elevated level of FIBs in adjacent water bodies.

Left: Locations of soil cores in Corona Meadow Park,
Middile: Study Areas
Right: Locations of coils cores in Kissena Park

MARM 457

Bromination of soil organic particulates through abiotic mechanisms

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Enzymatic bromination is well established in the environment, but the importance of natural abiotic bromination has only recently been revealed, through several studies on seawater. We have investigated abiotic bromination in a very different system, forest soil, where both pH values and background Br concentrations are lower than in the marine environment. We hypothesized that soil conditions could lead to abiotic oxidation of inorganic bromide and consequent bromination of plant-derived organic substrates. Through a series of lab-based experiments on natural samples, we found that Br is readily incorporated into particulate organic matter at levels from tens to hundreds of mg/kg, even under mild, environmentally feasible conditions. Fresh plant material is more susceptible to bromination than decayed plant litter and soil humus. Bromination of fresh oak leaves and pine needles is limited primarily by bromide concentration and produces both aliphatic and aromatic forms of organobromine. Abiotic bromination of humified soil material requires oxidants such as hydrogen peroxide and/or ferric iron and produces mainly aromatic organobromine. This suggests the existence of a labile pool of aliphatic compounds in plant material that are transformed during early decay stages. These findings illuminate a novel environmental phenomenon: the role of bromide as a versatile electron donor in abiotic reactions that potentially contribute to the degradation and preservation of soil organic matter.

MARM 458

Sorption of dioctyl sodium sulfosuccinate to coastal Gulf of Mexico sediment

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Dioctyl sodium sulfosuccinate (DOSS) is a major ingredient in Corexit 9527 and 9500 dispersants used to mitigate some effects of the Deep-water Horizon oil spill. DOSS proved to be relatively persistent in seawater and was detected in water column and sediment samples. Sorption to suspended particles affects the distribution and fate of similarly hydrophobic anionic surfactants in saline nearshore environment. Better understanding of DOSS sorption is important for predicting fate in nearshore environments, and constrain interpretations or hypotheses related to the use of DOSS as a water mass tracer or the possible mechanisms responsible for levels of DOSS detected in some sedimentary regimes, including surprisingly high levels (2-9 µg/g) at one site. The sorption of DOSS to coastal marine sediments was determined to characterize the effects on sorption of solution properties, DOSS concentration (1- 17,000 µg/L), and sediment properties in order to improve predictive capabilities for DOSS speciation across a range of water compositions. Sorption onto 12 sediments with varying combinations of properties (e.g., organic carbon contents of 0.18 – 8.59 %) resulted in isotherms that were most often nearly linear at more environmentally relevant concentrations (1-200 µg/L). Total organic carbon content was also a surprisingly good predictor of sorption with carbon normalized sorption coefficients averaging 7500 ± 2500 L/Kg. These results suggest and even more important role of organic matter than determined for linear alkylbenzene sulfonates (LAS), potentially related to well document unique properties of DOSS at H_2O/oil interfaces. In regards to effects of solution properties, the dependence on pH was much less than described in prior studies of anionic surfactant sorption under low ionic strength conditions, and the increased sorption with salinity could be described empirically by a linear combination of the independently determined effects of Ca^{2+}, Mg^{2+}, and Na^+. While the importance of Ca^{2+} on sorption of organo-sulfonates is well recognized, the increasing importance of Na^+ with salinity at low surfactant concentrations presents questions about the mechanism responsible. The very important effects of Mg^{2+} (neglected in prior sorption studies with organic compounds) was a novel result, with implications for marine and freshwater systems, where the Mg^{2+}/Ca^{2+} is highly variable. The results obtained will be compared to mechanistic sorption models.

MARM 459

Perfluoroalkyl acid (PFAA) transport and remediation at an aqueous film forming foam (AFFF)-contaminated site

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Aqueous film forming foams (AFFF) have been used at firefighter training areas to extinguish liquid fuel fires and the repeated historic use of AFFF is associated with elevated perfluoroalkyl acid (PFAAs) concentrations in the subsurface. In this work, batch and 1-D flow-through column experiments were conducted to determine the effects of trichloroethylene (TCE), pH, and cation concentration on sorption of eleven PFAAs. In batch studies, both cation concentration and pH were determined to affect PFAA sorption to soil. PFAA sorption to soil increased with increasing aqueous cation concentration, and the effects increased with increasing chain length. Based on water-TCE two-phase batch studies, TCE non-aqueous phase liquid (NAPL) was determined to primarily absorb PFAAs, where partitioning was generally independent of water quality consideration (pH, polyatomic cations). In 1-D flow through column experiments, the presence of TCE was associated with retarded PFAA transport (i.e., decreased mobility). 1-D flow through column studies were also employed to assess PFAA fate and transport in saturated porous media; the effects of non-aqueous phase co-contaminants (e.g., trichloroethylene; TCE) and chemical oxidants as would be used in *in situ* chemical oxidation remediation approach (i.e., ISCO) were considered. Three chemical oxidants were tested: permanganate, persulfate activated with ferrous chloride and citric acid, and catalyzed hydrogen peroxide (CHP). Chemical oxidants were not found to transform PFAAs when applied to porous media-filled 1-D columns; however, PFAA mobility was substantially affected, and mobility changes were similar in the presence and absence of TCE. Permanganate and CHP application resulted in accelerated PFAA transport which was attributed to both geochemical and water quality changes. By contrast, persulfate application resulted in increased PFAA retardation (i.e., decreased mobility), which is likely at least in part due to changes in water quality.

MARM 460

Biochar ozonization and characterization with biochar water filtrate assays

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In this study, biochar materials were made from pinewood through pyrolysis at 300 and 400 C for comparative studies with ozonization. Biochars were treated with ozone for 0, 30, 60, and 90 minutes and analyzed through cation exchange capacity (CEC) assays, dissolved organic carbon (DOC) assays, metal adsorptive assays using ions of copper, calcium, cadmium, and lead within a pH range of 4.5 and 5.5. The CEC of ozone-treated biochars increased from 9.22±2.19 cmol/kg for untreated biochar to 26.52±6.29 cmol/kg for 30 minute biochar, to 30.65±2.96 cmol/kg for 60 minute biochar, and to 18.39±0.94 cmol/kg for 90 minute treated biochar. More oxygen-functional groups were found to be present in the 90 minute treatment times, than the 60, 30 or 0 minute treatment times, indicating cleaving of biochar. FTIR-ATR showed an increase in oxygen functionality as treatment time increased. Ozone-treated biochar showed much better adsorption capabilities than the non-treated biochars. Copper (II) cation adsorption increases beyond the saturation limit. Lead (II) ion adsorption was found to increase by a factor nearly 2 for the 30 minute and 60 minute ozone-treated biochars. Calcium and cadmium ion adsorption also increased. Furthermore, biochar filtrates were analyzed through toxicity assays with algae, excitation emission matrix spectroscopy, pH measurement, and FTIR-ATR. A simulated "biooil-contaminated biochar" sample was made by mixing biochar materials with 20% (w/w) of biooils to analyze the toxicity of biochar-adsorbed biooils. The DOC levels of "biooil-contaminated biochar" decreased with ozonization treatment. Excitation Emission Matrix Spectroscopy (EEMS) was used to analyze the humic acid-like groups in the filtrate of the non-contaminated biochar, which was deemed non-toxic.

MARM 461

Monitoring of aquifer geochemistry to understand the mobilization of arsenic and manganese in groundwater of Chittagong, a rapidly expanding coastal city in Bangladesh

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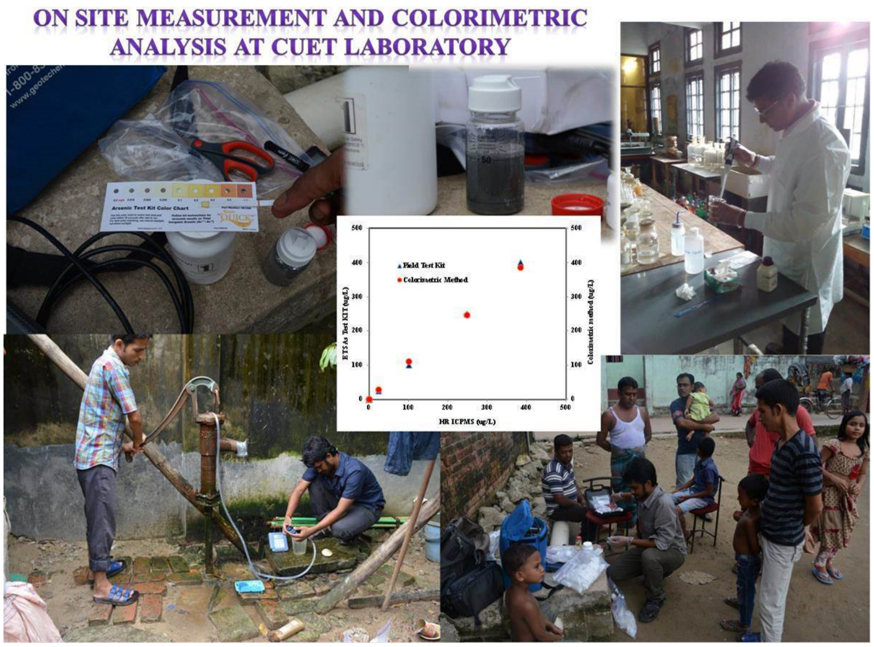
While serious health effects due to extensive consumption of groundwater elevated in arsenic (As) have been documented in several South Asian countries, the source and mechanisms responsible for As mobilization in aquifers remain poorly understood. This happens particularly, in coastal city Chittagong, Bangladesh where flood plain and coastal aquifer systems occurred in the sediments of Quaternary age. The study area has the complex groundwater system; the northern part of the city is a part of Anticline associated with Tertiary aquifer system and the southern part of the city is more or less plain land. The unique geological settings of Chittagong provides opportunities to understand the geochemical processes that fuel arsenic concentrations in both Quaternary and Tertiary aquifer systems. This is a globally significant environmental and public concern because similar type of aquifers supply the drinking water to billions of people throughout the world. Preliminary studies have reported the elevated arsenic and manganese in groundwater of flood plain and coastal aquifers of proposed study area. However, as to date, no hydro-geochemical study has been conducted to understand the geochemical processes that control the arsenic distribution in water and sediments. In light of this suggestion, this study aims to investigate the detailed geochemistry of As and other redox sensitive elements in groundwater and sediments collected from the Quaternary and Tertiary aquifer systems. An improved understanding of these processes has broad implications to assess the risks posed by the As-&Mn-enriched sites and to design the mitigation strategies.



Feild measurment at Borehole site of Chittagong, Bangladesh and Colorimetric measurement of arsenic in the laboratory of Chittagong University for Engineering and Technology.

MARM 462

Development of cell-active chemical tools to study cathepsin L function

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Cysteine cathepsins are important class of enzyme that belongs to papain class of cysteine proteases. There are eleven members of cysteine cathepsins (cathepsin B, C, F, H, K, L, O, S, V, X and W), conventionally regarded as lysosomal mediator of terminal protein degradation. Several recent studies have revealed their tissue-specific expression patterns suggesting that their functional roles are precise and context-dependent. Not surprisingly, their aberrant activities have often been associated with plethora of human diseases, including cancer and autoimmune disorders. Despite their intricate involvements in diseased physiology, their accurate functional assignments remain poorly understood. This work involves development of a new class of cell-active and small molecule inhibitor of cysteine cathepsin L, and its utilization for development of a highly selective activity-based probe. These chemical tools are then utilized to decipher the roles of cathepsin L in appropriate cellular contexts.

MARM 463

Mechanism and interactions of human pyruvate dehydrogenase complex with its kinase 1

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The human pyruvate dehydrogenase complex (PDC) consists of three principal catalytic components for its mission: E1, E2, and E3. The core of the complex is a strong subcomplex between E2 and an E3-binding protein (E3BP). The PDC is subject to regulation at E1 by serine phosphorylation by four kinases (PDK1−4), an inactivation reversed by the action of two phosphatases (PDP1 and 2). Specifically, the regulation of PDC via phosphorylation of E1 by PDK1 is the focus of these studies, as PDK1 has been strongly implicated as an overexpressed culprit in multiple cancer cells; hence inhibition of the interaction of PDK1 with the E1 or E2-E3BP, could provide novel targets for the design of anticancer agents. Since the PDKs reside on (have a stronger binding to) the E2-E3BP core of the entire complex, specific inhibition of the PDK1-E2-E3BP interaction provides a possible new approach to treatment of cancer. Recently, the Jordan group defined the interaction loci between PDK1 (PDK2) and the E2-E3BP core by two complementary methods, HD-exchange MS (HDX-MS) and NMR.[1] Interrogation of the sites on E2-E3BP identified to interact with PDK1 (PDK2) was accomplished by site-directed mutagenesis studies in order to validate the identified 'hot spots'. To date, there is evidence of the variants on the L1L2S region of E2 effecting inactivation of E1 via phosphorylation by PDK1. Further studies will be performed to identify the protein-protein interaction of these L1L2S variants with PDK1 and PDK2 using HDX-MS, isothermal titration calorimetry (ITC) and fluorescence titrations. These measurements will confirm whether the 'hot spots' interrogated indeed are important for the interaction of E2-E3BP with the PDK1, and whether it is specific to PDK1 by comparing such measurements with PDK2. These experiments will identify 'real' hot spots, against which rational drug design could be undertaken.

[1] Wang, J. et al. Biochemistry, 2015, 54 (1), 69-82.

MARM 464

Molecular docking and evaluation of small molecule inhibitors for matrix metalloproteinase-1 and 9

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Matrix Metalloproteinases (MMP) are a class of zinc enzymes that are responsible for the degradation of extracellular matrix components. MMP are copious throughout the body and play many roles that include breaking down damaged and worn out structural proteins. MMP enzymes are also important in maintaining healthy and youthful skin. Skin matrix is constantly being synthesized by fibroblasts and the role of MMP enzymes is to degrade the damaged matrix. Therefore, in healthy and youthful skin, there is a balance of synthesized and degraded matrix. However, MMP levels increase with age and causes this balance to be disturbed. This imbalance can be improved by either stimulating the synthesis of matrix or inhibiting its degradation. Also, MMP-9 has the strongest link to the development of cardiac dysfunction. Aging associates with increased MMP-9 expression in the left ventricle of the heart and reduced cardiac function. Our research focuses on the inhibition of MMPs. Here, small molecules from the NCI diversity set III database were screened against the active site of MMP-1 and MMP 9 using the docking program, AutoDockVina. This gave us many hit molecules with binding energies varying from -3.9 to -9 kcal/mole. Potential inhibitors were screened using the Synergy HT Multi-Mode Microplate Reader spectrophotometrically

MARM 465

Kinetic analysis and substrate binding studies of the *Escherichia coli* nitrile reductase QueF

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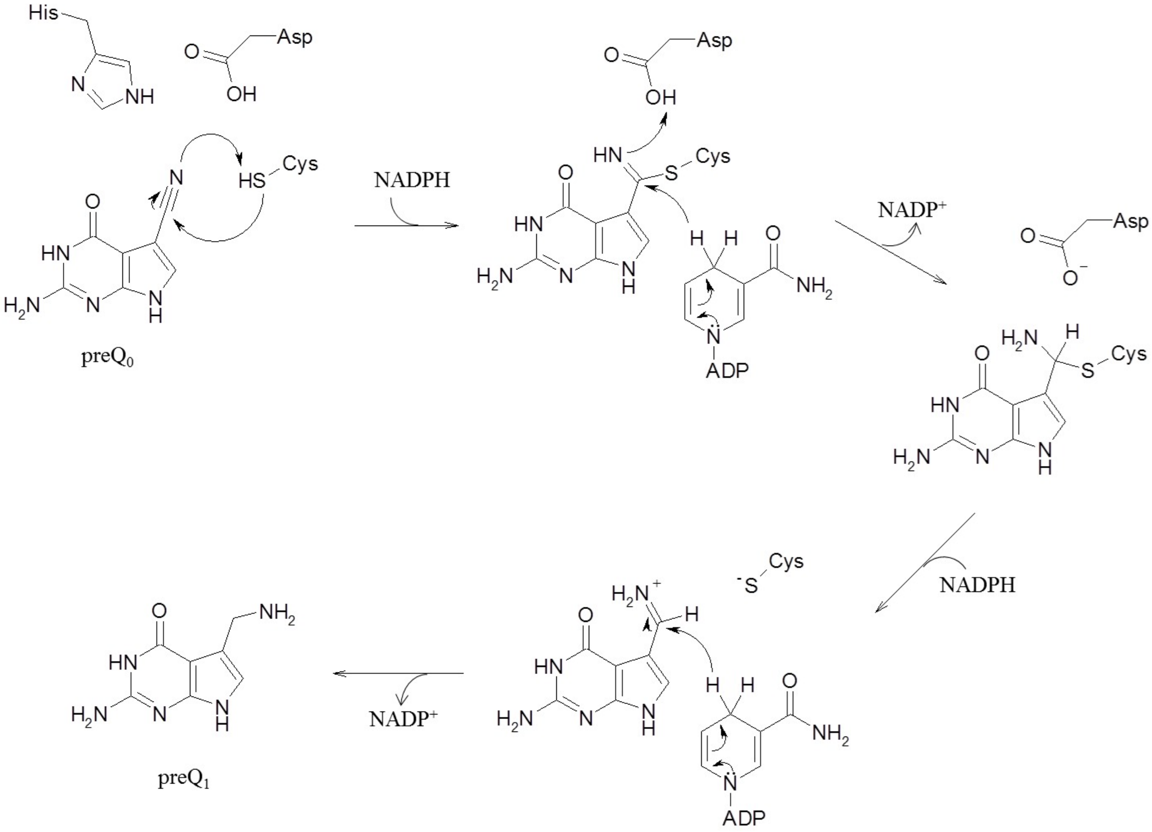
The enzyme QueF catalyzes the conversion of the nitrile group of 7-cyano-7-deazaguanine (preQ$_0$) to the amino group of 7-aminomethyl-7-deazaguanine (preQ$_1$), only known biocatalyst in biology. The mechanistic studies of the QueF have been required to design highly selective anti-bacterial drugs as well as to develop the engineered enzyme for commercial interesting nitrile-to-amine transformation. The enzymatic reduction process of preQ$_0$ consists of a covalent thioimide adduct formation between preQ$_0$ and a cysteine nucleophile in the enzyme, and subsequent two NADPH-dependent reduction to convert preQ$_1$. Here, we present that the *Escherichia coli* QueF binds preQ$_0$ in an induced-fit process. It was investigated by a comparison of biochemical and thermodynamic binding properties for preQ$_0$ with the corresponding results for substrate analogues thereof. Ensuing reduction steps were examined with 4*R*-[^{2}H]NADPH that a hydrogen (^{1}H) of dihydronicotinamide ring is substituted with a deuterium (^{2}H). High primary deuterium kinetic isotope effect (KIE) is observed on apparent catalytic efficiency (k_{cat}/K_{NADPH}). Transient- and steady-state kinetic analyses with simulation reveal that two chemical steps are mainly rate-limiting with a large KIE on the covalent thioimide reduction and a relatively smaller KIE on the imine reduction to preQ$_1$. A substrate binding process and a biocatalytic mechanism for the enzyme are proposed based on these data.



V.M. Chikwana et al., 2012, J. Biol. Chem., 287, 30560-30570

Figure 1. The proposed catalytic mechanism of the enzyme QueF

MARM 466

Substrate specificities of the Venezuelan equine encephalitis virus nonstructural protein 2 cysteine protease

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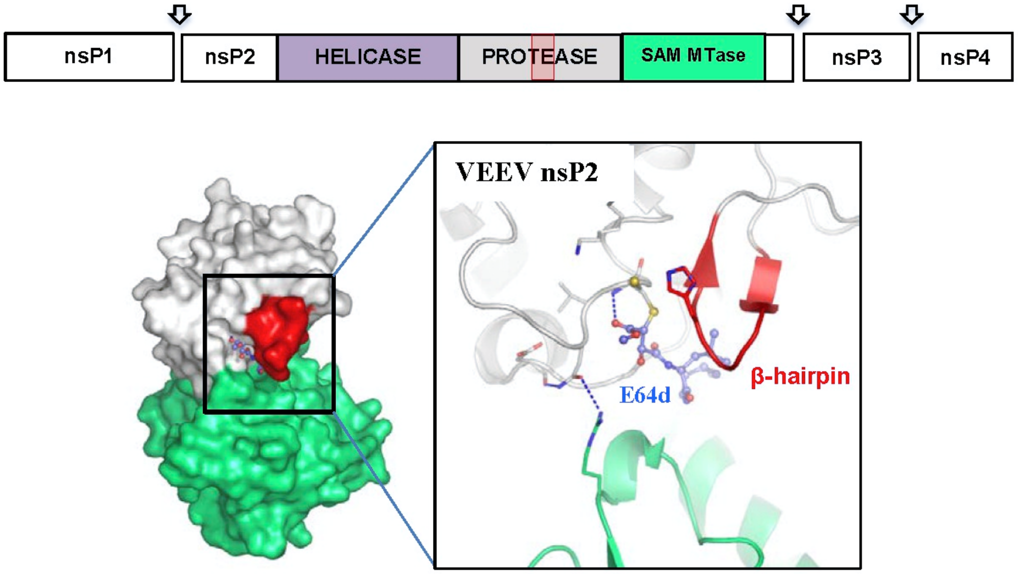
The Venezuelan equine encephalitis virus (VEEV) nonstructural protein 2 (nsP2) cysteine protease (EC 3.4.22.-) is essential for viral replication and is involved in the cytopathic effects (CPE) of the virus. The VEEV nsP2 protease is a member of MEROPS Clan CN and characteristically contains a papain-like protease linked to an S-adenosyl-L-methionine-dependent RNA methyltransferase (SAM MTase) domain. The protease contains an alternative active site motif, ^{475}**NV**<u>**C**</u>WA**K**^{480}, which differs from papain's (CGS<u>**C**</u>WAFS) and lacks a transition state (TS) stabilizing residue homologous to Q19 in papain. To identify active site residues a mechanism-based inhibitor, E64d, was co-crystallized (2.1 Å) with the enzyme and mutants were analyzed. The N475A mutation led to a 24-fold reduction in k_{cat}/K_m, however the orientation of the side-chain was not consistent with oxyanion stabilization. N475 forms the base of the P1 binding site and likely orients the substrate for nucleophilic attack or plays a role in product release. An Asn homologous to N475 is similarly found in coronaviral papain-like proteases (PLpro) of the Severe Acute Respiratory Syndrome (SARS) virus and Middle Eastern Respiratory virus (MERS). Last, we identified a new host protein substrate of the viral protease. Human TRIM14 is a component of the mitochondrial antiviral-signaling protein (MAVS) signalosome, a human protein which contains the viral P12 cleavage site. TRIM14 was cleaved by the VEEV nsP2 protease, but not by the nsP2 protease of the Old World Chikungunya alphavirus. Western analysis of VEEV-infected cell lysates confirmed the cleavage of TRIM14. The cleavage site in TRIM14 is notably absent from equine TRIM14 homologues. The proteolysis of the TRIM14 protein by the VEEV nsP2 protease suggests a possible mechanism of innate immune response evasion which may allow the virus to replicate during an acute viral infection.



MARM 467

Development of drug-like inhibitory agents of Nek2 kinase

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An effective treatment for the highly metastatic triple negative breast cancer (TNBC) subtype is currently unavailable. Nek2, a mitotic serine/threonine kinase, is overexpressed in multiple forms of highly metastatic breast cancers. High Nek2 levels are associated with drug resistance leading to poor prognosis, and has been proposed as a key therapeutic target for TNBC patients. In this work, a novel class of drug-like Nek2 kinase inhibitors have been developed and evaluated using a whole animal-based Nek2 overexpression model. It is anticipated that the acquired inhibitory agents will exhibit potent and effective anti-TNBC activities.

MARM 468

Cartilage: A tough biological gel

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Cartilage is a load-bearing tissue located at joint surfaces. It can be viewed as a fiber-reinforced, highly permeable composite gel filled with physiological salt solution. The unique properties of cartilage originate from the architecture and organization of its extracellular matrix (ECM). Cartilage ECM consists of a fibrous collagen network, which is prestressed by the osmotic swelling pressure exerted by negatively charged proteoglycan (PG) assemblies embedded in the collagen network. The major PG is the bottlebrush-shaped aggrecan, which, interacting with linear hyaluronic acid (HA) chains and a link protein forms large aggregates (size: > 1 mm) imbedded in the fibrous collagen network. The swelling of PG assemblies is constrained by the collagen network. At equilibrium the osmotic swelling pressure of the aggrecan–HA complexes is balanced by the elastic stress developed in the collagen matrix.
The quantitative characterization of the morphology and mechanical properties of biological tissues is essential for a better understanding of their behavior. We determine the interactions between the main macromolecular components of cartilage ECM using an array of experimental techniques (osmotic pressure measurements, small-angle X-ray scattering, small-angle neutron scattering, and dynamic light scattering) probing the structure and dynamics over a broad range of length and time scales. This knowledge is critically important to understand biological function and develop successful tissue engineering strategies for cartilage repair.

MARM 469

Supramolecular hydrogelators and hydrogels: From soft matter to molecular biomaterials

Xuewen Du, Jie Zhou, Jie Li, Huaimin Wang, Zhaoqianqi Feng, ***Bing Xu***, *bxu@brandeis.edu. Chemistry, Brandeis University, Waltham, Massachusetts, United States*

This talk will discuss the applications of supramolecular hydrogels/hydrogelators as molecular biomaterials. After a brief introduction of methods for generating supramolecular hydrogels, we discuss supramolecular hydrogelators based on small peptides, nucleobases, and saccharides. Following molecular design, we focus on various potential applications of supramolecular hydrogels as molecular biomaterials, classified by their applications in cell cultures, tissue engineering, cell behavior, imaging, and unique applications of hydrogelators. Particularly, we discuss the applications of supramolecular hydrogelators after they form supramolecular assemblies but prior to reaching the critical gelation concentration (CGC) because this subject is less explored but may hold equally great promises for helping address fundamental questions about the mechanisms or the consequences of the self-assembly of molecules, including low molecular weight ones. We will illustrate molecular biomaterials as a frontier of gel chemistry.

MARM 470

Hydrogel materials construction with peptide design and solution assembly

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Self-assembly of molecules is an attractive materials construction strategy due to its simplicity in application. By considering peptidic molecules in the bottom-up materials self-assembly design process, one can take advantage of inherently biomolecular attributes; intramolecular folding events, secondary structure, and electrostatic interactions; in addition to more traditional self-assembling molecular attributes such as amphiphilicty, to define hierarchical material structure and consequent properties. These self-assembled materials range from hydrogels for biomaterials to nanostructures with defined morphology and chemistry display for inorganic materials templating. The local nano- and overall network structure, and resultant viscoelastic and cell-level biological properties, of hydrogels that are formed via beta-hairpin self-assembly will be presented. Importantly, the hydrogels do not form until individual peptide molecules intramolecularly fold into a beta-hairpin conformation. Subsequently, specific, intermolecular assembly occurs into a branched nanofibrillar network. These peptide hydrogels are potentially excellent scaffolds for tissue repair and regeneration due to inherent cytocompatibility, porous morphology, and shear-thinning but instant recovery viscoelastic properties. Slight design variations of the peptide sequence allow for tunability of the self-assembly/hydrogelation kinetics as well as the tunability of the local peptide nanostructure and hierarchical network structure. In turn, by controlling hydrogel self-assembly kinetics, one dictates the ultimate stiffness of the resultant network and the kinetics through which gelation occurs. During assembly and gelation, desired components can be encapsulated within the hydrogel network such as drug compounds and/or living cells. The system can shear thin but immediately reheal to preshear stiffness on the cessation of the shear stress. Additionally, a new system comprised of coiled coil motifs designed theoretically to assemble into two-dimensional nanostructures not observed in nature will be introduced. The molecules and nanostructures are not natural sequences and provide opportunity for arbitrary nanostructure creation with peptides.

MARM 471

Experimental and theoretical aspects of hydrogel-based microcantilever sensors

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Stimuli-response hydrogels change volume in response to changes in ionic strength, solvent, stress, light intensity, electric field, magnetic fields, etc. The reversible swelling property of the hydrogels has also been used to develop chemical and biological sensors. This work tends to summarize hydrogel-based microcantilever chemical and biological sensors for a variety of species, such as H^+, CrO_4^{2-}, glucose, and F^-. The microcantilever undergoes reversible and reproducible bending deflection upon exposure to solutions containing various analyte concentrations due to swelling or shrinking of the hydrogels. I will describe the sensors for the measurement of analytes in terms of the theoretical behavior, as well as the experimentally-determined range, sensitivity, and stability.

MARM 472

Engineering shear-thinning supramolecular hydrogels for biomedical applications

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Hydrogels represent a class of biomaterials that have great promise for the repair of tissues, particularly due to our ability to engineer their biophysical and biochemical properties. Hydrogels can provide instructive signals through material properties alone (e.g., mechanics, degradation, structure) or through the delivery of therapeutics that can influence tissue morphogenesis and repair. Here, I will give examples of the design of hydrogels based on hyaluronic acid for use as injectable therapeutics or towards 3D bioprinting applications.

Towards cardiac repair, my laboratory is interested in designing materials that can influence the left ventricular remodeling process that occurs after myocardial infarction. To permit percutaneous delivery of hydrogels (e.g., via catheters), we have developed a class of shear-thinning and self-assembling hydrogels that can be used for the delivery of mechanical signals, as well as cells and therapeutics (e.g., protease inhibitors). These hydrogels assemble based on guest-host interactions and can be designed to degrade via matrix metalloproteinases or to become more stable through secondary crosslinking. These iterations on material design are teaching us what important signals are needed in these hydrogels towards the next generation of translatable therapeutics for cardiac repair.

Beyond injectability, these hydrogels are also useful for bioprinting in the area of additive manufacturing. Our approach involves the printing of a shear-thinning and self-healing hydrogel ink into another support hydrogel in 3D space. Shear forces disrupt the hydrogel structure for extrusion and also to receive the extruded material, with resolutions dependent on needle diameter, printing speed, and extrusion rate. This approach allows for the printing of cells, multiple inks into the support gel, and pockets of materials. Additionally, open and perfusable structures (e.g., channels) can be fabricated with secondary photocrosslinking of the support hydrogel and washing of the ink.

MARM 473

Nanocatalysis and the slurry-phase direct synthesis of methylchlorosilanes and alkoxysilanes

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Conventional fluidized-bed Direct Synthesis of methylchlorosilanes is typically run with 45 – 500 micron silicon and 1 – 5 micron copper and promoter sources (1). Preferential elutriation of the finer particles occurs due to the marked differences in the escape velocities of silicon, copper catalyst and promoters. Accordingly, there are increased raw material consumption and cost. In slurry-phase Direct Reactions of silicon, elutriation does not occur. Exploitation of this advantage has led to the use of nanosized copper and copper compounds with average particle sizes 0.1 – 600 nanometers (an average of 100 times smaller than the conventional) in the Direct Synthesis of methylchlorosilanes and trialkoxysilanes (2). Nanosized promoters have also been used advantageously in the Direct Synthesis of methylchlorosilanes. Data will be presented to show that nanosized materials afford high dispersion of catalytic sites on silicon and contribute to high reaction rates, high selectivity and high silicon conversion in the Direct Synthesis of methylchlorosilanes, trimethoxysilane and triethoxysilane. Nanosized catalyst effects are also used to explain the catalytic instability observed when the slurry phase Direct Synthesis of trimethoxysilane is done in alkylated benzenes, paraffins and cycloparaffins (3).

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MARM 474

Characterizing axial resolution while imaging $NaYF_4$:Yb,Tm nanoparticles

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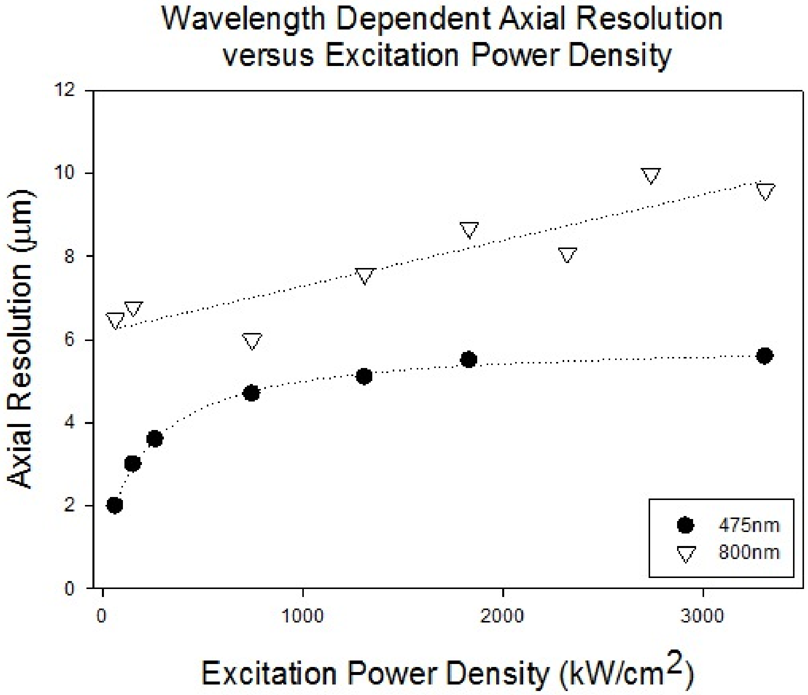
Upconverting lanthanide nanoparticles (UNPs) are a unique contrast agent that has developed over the last couple decades. A main focus of UNPs is their anti-stokes emission which minimizes auto-fluorescence noise in imaging. The ability to excite, and optionally collect emission, at near-infrared (NIR) wavelengths, within the biological window, at efficiencies several orders of magnitude greater than other two photon processes is especially appealing. However, these wonderful properties are accompanied by several challenges such long lifetimes which convolute 3D imaging and highly sensitive response to excitation properties. While iterative deconvolution techniques have been employed to minimize lifetime effects, excitation control remains a challenge in some regards. Traditional fluorophores have a linear relationship between excitation power density and resolution. UNPs are unique in that as the power density of excitation increases the axial resolution becomes poorer. To achieve best imaging resolution when using UNPs as a contrast agent with a pulsed laser excitation power densities less than 250kW/cm^2 should be used. Ultimately these response relationships for excitation power density and axial resolution show the uniquely counterintuitive property of UNPs and also help define imaging parameters for $NaYF_4$:Yb,Tm in consideration with other desired sample luminescence properties.



MARM 475

Improving healthcare and industry: Grafting cyclosiloxane stabilized metallic nanoparticles onto various substrates

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Nanomaterials are widely applicable in the healthcare industry [1]. Specifically, noble metal nanoparticles can be active therapeutics, biosensors, and antimicrobial agents [1,2]. Silver, a well-known antimicrobial, has been used as a treatment for bacterial infection. Unfortunately, some microbes have developed resistance and do not respond to such treatment. However, nanoparticles display different activity from their bulk counterparts and silver nanoparticles can possibly overcome bacterial drug resistance [2]. Recently, the deposition of nanoparticles onto various surfaces has been used to investigate potential applications. In our previous work, we presented the synthesis of silver nanoparticles that displayed nanoraspberry morphology [3]. Because silver nanoparticles have a tendency to agglomerate, this raspberry morphology is short-lived. This unique property propelled our desire to synthesize and immobilize these nanoraspberries onto the surfaces of various substrates. We specifically detail their deposition onto cotton fibers for potential wound dressing applications.

In this paper, we detail the successful synthesis of gold, palladium, platinum, and silver nanoparticles using cyclicsiloxane, 1,3,5,7 tetramethyltetracyclosiloxane (D_4^H). We will present a comparative analysis of the different morphologies synthesized as a product of the reduction of their corresponding metal salts. The mechanistic investigations related to the formation of metallic particles via a catalytic cycle in which the Si-H bonds undergo oxidative addition/reductive elimination process is also detailed. Furthermore, we will show our successful grafting of these novel nanostructures onto different substrates, including glass, cotton fibers, and charcoal. These substrates can be used in a variety of applications, including green catalysis, therapeutics, and medical imaging. The synthesis and conjugation onto these surfaces was confirmed via UV-Vis spectroscopy, FT-IR, TEM, and SEM.

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MARM 476

Microwave-assisted green synthesis of uniform ruthenium nanoparticles supported on non-functional single-walled carbon nanotube for Congo red dye degradation

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Studies have shown that single-walled carbon nanotubes offer superior electrical, mechanical and catalytic performance over multi-walled carbon nanotubes due to their smaller and more homogeneous diameter, higher surface area and less defect densities. Herein, non-functionalized single-walled carbon nanotubes reinforced with uniform distribution of ruthenium nanoparticles (~5 nm) were achieved by microwave irradiation in ethanol. The ruthenium nanoparticle-single-walled carbon nanotube composites were characterized by High Resolution Transmission Electron Microscopy (HR-TEM), Energy Dispersive X-ray Spectroscopy (EDS), and UV-Vis Spectroscopy. A comparative study of the catalytic degradation of Congo red dye by these novel synthesized ruthenium nanoparticle-single-walled carbon nanotube composites was also performed.

MARM 477

The catalytic behavior of an alkene incorporated metal nanoparticle supramolecular gels via alcoholysis

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Catalysts in the nanoscale regime are known to have excellent catalytic efficiency and recyclability properties, which are of high interest in many fields [1,2]. The physical characteristics and stability of nanoparticles are extremely dependent on the method of preparation; therefore, choosing stabilizing agents with different structures and properties can synthesize unique recyclable heterogeneous catalysts. A polymer like an aliphatic alkene can ideally provide enhanced and specialized catalytic properties due to its structural and chemical properties. In our previous research, we showed that the stereochemistry of aliphatic alkenes plays an important role in synthesizing and stabilizing nanogels [3] via the interaction of the alkene groups of polybutadiene and the Si-H moiety present in poly(methylhydrosiloxane) (PMHS). In addition, it was discovered that the isomer structure plays an important role in producing different nanomaterials depending on the metal salt, which can be further tailored for specific applications [4].
In this poster, we briefly introduce the synthesis of various metal-imbedded supramolecular hybrid gels. Silver, platinum, palladium, gold, and copper nanoparticles were synthesized via PMHS and were stabilized via cis-polybutadiene. We present NMR, FTIR, TEM, SEM, and XRD analyses of these supramolecular gels. Furthermore, we will detail a comparative analyses of the catalytic activity and specificity of these nanohybrid gels via the alcoholysis of PMHS and various alcohols. In addition, we will investigate the catalytic activity of these gels via NMR and FTIR and assess the gel composition after catalysis via TEM and SEM.

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MARM 478

Comparative study of formation of hydroxyapatite

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Hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$) (HA) is a common component of the human bones and teeth. On the other hand the main role of synthetic HA is to promote osteogenesis. The osteoblast cells (bone cells) grow on the surface of the HA, which makes this material very useful for bone tissue engineering and especially for bone regeneration.
In this study we prepared HA through two methods. First, we involved the sol-gel method for which used calcium nitrate hexahydrate ($Ca(NO_3)_2$ $6H_2O$) and phosphorous acid (H_3PO_3) in the presence of 200 proof ethanol. The second method, was a slurry method which involved calcium hydroxide ($CA(OH)_2$) and

phosphoric acid (H_3PO_4). The HA-1 prepared through sol-gel method required a second step of calcination at 575°C for 3 hours for crystallization of the HA-1. This temperature was established by thermogravimetric analysis coupled with differential thermal analysis (TG-DTA). At ~550°C an endothermic effect due to formation of HA was observed. The weight loss of HA-1 during the thermal treatment was ~38% while for the HA-2 prepared through the slurry method this was ~8%. The HA-2 sample shows a continue loosing of water and hydroxyl groups. The samples were structurally characterized by X-Ray diffraction and FT-IR spectroscopy. The crystallite size was calculated for both samples being 7.9 nm for HA-2 and 15.6 nm for HA-1. The BET surface area and the particle size distribution was also measured the investigated samples. The prepared hydroxyapatite were also incorporated into polysaccharide based hydrogels to demonstrate their utility in the bioengineering of bone.

MARM 479

Tuning of optical, magnetic and colloidal properties of nanoparticles by dendritic ligands

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A library of highly flexible, lipophilic dendritic ligands was designed and built to bind the surfaces of colloidal nanocrystals through ligand exchange. Inter-particular spacings in resulting hybrids are increased as a function of dendrimer generation and can be tuned from 2.2 to 6.3 nm. This is a range that is intermediate between commercial ligands and DNA-based ligands. Such precise tuning of inter-particle spacing allows the control of optical, magnetic and colloidal properties.
Dendritic organic shells also modify nanoparticle self-assembly behavior. Dual mixtures of dendronized hybrids result in an unprecedented binary superlattices (where both components have the same inorganic core, but different dendritic ligand) which are isostructural with $NaZn_{13}$ and $CaCu_5$ crystals.
The synthetic routes towards dendritic ligands as well as nanoparticle properties and self-assembly details will be discussed.

MARM 480

Diastereoselective cycloadditions for the synthesis of five-membered ring nitrogen-containing heterocycles

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Nitrogen-containing five-membered rings are highly conserved pharmacophores among blockbuster drugs and natural products. Thus, there is a continuous demand for the development of more efficient and systematic methods for their synthesis. Our laboratory has developed simple and inexpensive reaction conditions for the efficient synthesis of a wide variety of protected diaziridine scaffolds, which upon exposure to metal complexes undergo diastereoselective cycloadditions across the *N-N* or the *C-N* bonds to access a wide variety of stereochemically-dense heterocycles. These discoveries would allow for the efficient and continuous access to streochemically-dense heterocycles, which will facilitate the development of convergent approaches towards the synthesis of more complex heterocyclic pharmacophores.

MARM 481

1, 3-dipolar cycloadditions of nitrile oxide with acetylenic aldehydes

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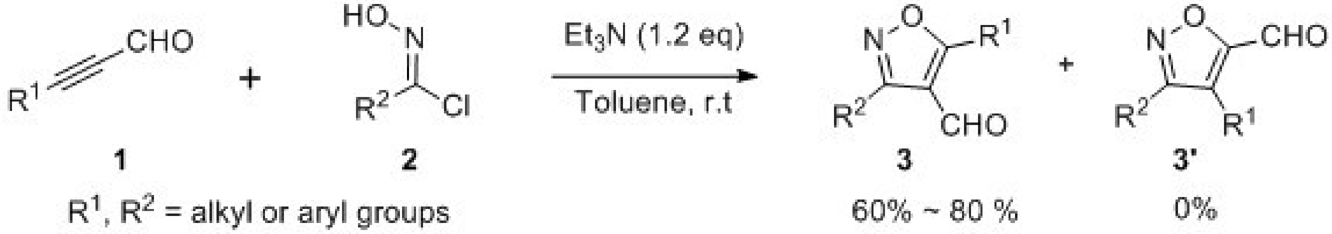
1,2-oxazol derivatives were prepared by a highly regioselective 1,3-dopolar cycloaddition of nitrile oxides and acetylenicaldehydes in good yield. Reactive nitrile oxides were generated in situ from stable chloro-oximes reagents and triethyl amime. The cycloaddition reaction showed broad substrate scopes and good functional group compatibility.



MARM 482

'Ene' reactions of singlet oxygen at the air-water interface

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The ene reaction of singlet oxygen at the air-water interface was investigated with prenylated surfactants $[(CH_3)_2C{=}CH(CH_3)(CH_2)_nSO_3^{-}\ Na^{+}\ (n = 4, 6, 8)]$. The reactions occur regioselectively with a preference for a secondary rather than tertiary surfactant hydroperoxide. At the air-water interface, the regioselectivity increases with the number of carbon atoms in the hydrophobic chain arguing for close packing and an orthogonal prenyl position in the longer chain on the liquid surface. This study highlights control of a synthetic reaction on a liquid support, where the oxidant (airborne $^1O_2$) is delivered as a gas for the efficient formation of hydroperoxides.

MARM 483

Oxazolone cycloadducts as versatile frameworks for alkaloid synthesis

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The intramolecular Diels-Alder reaction of N-substituted oxazolones provide a variety of heterocyclic frameworks with obvious potential for alkaloid synthesis. Two main strategies are currently under investigation -- either Direct Incorporation of the immediate cycloadduct scaffold itself, or Rearrangement to complementary patterns with further applications. Divergent synthesis of several distinct alkaloid classes from individual cycloadducts is currently underway.

MARM 484

Heterocycle synthesis from quinols

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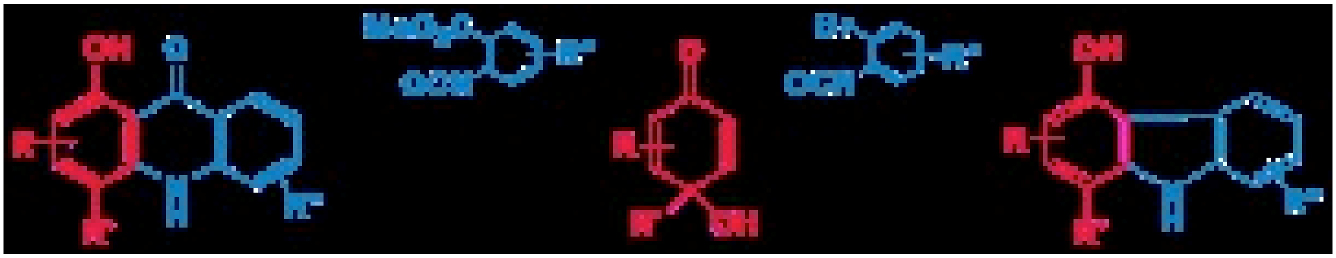
A variety of substituted 1-hydroxyacridones were synthesized in a one-pot carbamation/Michael addition/Claisen Condensation/decarboxylation cascade in two steps from commercial phenols in good to excellent yields (41-96%). Furthermore, synthesis of 4-hydoxycarbazoles from quinols was realized through a carbamation/Michael/enolate-aryl coupling/aromatization sequence. This methodology was also applied to a short total synthesis of carbazomycin B.



MARM 485

Instituting research at the community college level: Strategies that will secure the success of STEM students at the post-undergraduate level

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Since 2000 Queensborough Community College of the City University of New York has established undergraduate research opportunities for promising students as early as their first year of their college career. The results have led to multiple presentations at professional conferences as well as publications to peer-reviewed journals and valuable NSF-STEM REU experiences nationwide. Successful candidates have been accepted to post-undergraduate programs and eventual careers both in academia and industry. The systematic approach of this effort will be described with emphasis on the difficulties associated with the grooming of these students and the strategies that overcome them.

MARM 486

Queensborough MSEIP: Using a three-tiered model to engage, retain, and graduate STEM students at a community college

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Queensborough Community College has successfully engaged community college students in high-caliber undergraduate research for a long time. Our experience, institutional commitment, faculty and modern laboratories have positioned us for unprecedented success. With the help of US Department of Education Queensborough MSEIP (Minority Science and Engineering Improvement Program) grant, our main goal is to use Undergraduate Research as a tool to engage, retain and graduate Queensborough students. We intend to substantially expand the depth and breadth of research opportunities for students, particularly underrepresented females. Students are engaged in a three-tiered research program, allowing them to begin research projects early in their academic careers and supporting them for increasingly rigorous research that culminates in placements at partner four-year colleges. This has led to increased retention and graduation rates of our STEM students.

The program uses multiple prong approach 1) Providing intensive summer immersion experiences for at risk high school students 2) Expanding undergraduate research experience for QCC freshman by easing them in STEM field through seminars and workshops then pairing them with research mentors for long term research projects and 3) Launch comprehensive faculty development program to train new faculty mentors. The success of this multi-tiered model will be discussed in detail.

MARM 487

Engaging students in research

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Providing college and high school students with research opportunities has become a significant part of their education. It has also become a great opportunity to recruit and identify students into the challenging and rewarding fields of STEM research in general and chemistry in particular. Research engagement and programs involving high partnerships with high schools and colleges will be presented.

MARM 488

The high impact practice of undergraduate research at community colleges using the CCURI model

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The Community College Undergraduate Research Initiative (CCURI) functions as a national consortium of community colleges, four-year schools, government agencies, and private organizations dedicated to the development, implementation, and assessment of sustainable models for integrating an undergraduate research (UR) experience into community college STEM programs. The network has grown to over 50 institutions as of 2016. This sample size has provided opportunities for meta-analyses and novel research study designs aimed at uncovering the barriers associated with developing UR programs at a community college, and identifying the opportunities that arise as the result of the unique culture of the two-year institution. CCURI has collected data on best practices for integrating the research experience, and has developed a suite of recommendations that a community college could adopt as part of their program development efforts. In following these recommendations, it is believed that a community college would maximize the chance for success and optimize the probability of remaining sustainable over time. The future growth and sustainability of the undergraduate research experience at the two-year institution will require a better understanding of institutional-level change and a significant paradigm shift with respect to how we view the role of the community college in STEM education. Volunteer State Community College has used the model developing several undergraduate research projects in general and organic chemistry.

MARM 489

Mentoring undergraduate research in different college/university settings

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One innovative strategy that can improve higher education is the engagement of undergraduate students in doing research. Mentoring is one of the few opportunities that afford extended face-to-face and one-on-one instruction. However, mentoring undergraduate students in doing research is not the same in different types of colleges and universities. This paper gives insights on how undergraduate students are being mentored in different school settings namely: a third world country premier university, a big research public university, a small historically black college and a private university. The advantages and disadvantages of each setting will be discussed and emphasis will be given on how the presentor engages his students to do research at Pace University.

MARM 490

Undergraduate research through laboratory experience as special projects to enrich student college experience

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Undergraduate research projects were organized to give students independent lab based research experience based off of their immediate past knowledge and an opportunity to learn a new analytical technique with its application to soil environmental chemistry.

The first study involved determination of nitrates in a indigenously generated waste using Nitrate Ion selective electrode followed by comparison with solvent extraction-spectrophotometry. The students studied the relation of nitrates ions and soil pH.

The current study involves determination of Cadmium ion in soil with its minor speciations using ion selective electrode and compared with other methods of analysis. The local cultivated campus soil was dug out and treated for drying and homogenizing then cone-quartered and reduced to appropriate size. THE soil was added with Cd solution and allowed to dried and then analyses for the presence of Cd ions. The garden soil containing Cd gave no reading for acetic acid extractable mobile Cd ions and very low values for Nitric acid extractable occluded ions. The solid was then digested with aqua regia which then gave a high value of millivoltage for Cd ISE. Such behavior suggests that in fertile garden soil containing possible humic acid, the presence of Cd could be in complexed form mostly.

In both these studies, Undergraduate research has tremendously opened up the student thinking process with respect to academic learning. Students got to learn managing of the research methods and gave a good experience to their creativity.

MARM 491

The photo-enhanced Lewis acidity of aqueous methyl viologen

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Recent experiments (Henrich, J. D.; Suchyta, S.; Kohler, B. *J. Phys. Chem. B* 2015, **119**, 2737–2748) have suggested that the Lewis acidity of methyl viologen becomes greatly enhanced upon photoexcitation in aqueous solution. While Bronsted photoacids have been known for more than sixty years, methyl viologen is the first compound known to exhibit photoenhanced Lewis acidity. Although this behavior was identified by experiment, the mechanism for the enhanced Lewis acidity could not be determined. We have performed *ab initio* excited-state molecular dynamics simulations of aqueous methyl viologen in order to elucidate a mechanism for this behavior. On the basis of these simulations, we propose that a water molecule complexes with methyl viologen. A proton is released into solution from the water molecule, and the hydroxide ion adds covalently to the methyl viologen. The addition of the hydroxide ion provides access to a conical intersection that facilitates nonradiative decay. These simulations provide insight into a previously unknown photochemical pathway and will aid in the identification of other Lewis photoaicds.

MARM 492

Near-infrared spectroscopy of ethynyl radical, C_2H

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The ethynyl radical, C_2H, is a reactive intermediate important in various combustion processes, and widely observed in the interstellar medium. C_2H radical also has a special interest due to its complex vibronic coupling involving three electronic species: a $X\,^2\Sigma^+$ground state and degenerate components of the first excited electronic $A\,^2\Pi$ state. The $A\,^2\Pi$ state has term energy value of 3700 cm^{-1}, is comparable to the C-H stretch frequency of approximately 3300 cm^{-1} in the $X^2\Sigma^+$ state. In the laboratory, C_2H radicals can be made via 193 nm photolysis of CF_3C_2H. Diode laser transient absorption was used to record Doppler-limited spectra between 7000 and 7130 cm^{-1}. Two interleaved, rotationally resolved bands were observed and assigned to a $^2\Sigma$ - $^2\Sigma$ transition at 7088 cm^{-1} and a $^2\Pi$ - $^2\Sigma$ transition at 7108 cm^{-1} in this work. The $^2\Sigma$ and $^2\Pi$ symmetry are results of a mixture of vibrationally excited X states and different zero-order A-state bending levels: a $^2\Sigma^+$ symmetry combination of $X(0,2^0,3)$ and $A(0,3,0)^0\kappa$ and a $^2\Pi$ symmetry combination of$X(0,3^1,3)$ and $A(0,0,2)^1$. The mixing of vibrational excited $X\,^2\Sigma^+$ states with the electronic $A\,^2\Pi$ state leads to characteristic features in the high resolution spectroscopy, distinctive photophysics as well as unusual reaction kinetics.

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MARM 493

Monitoring dimerization of radical anions by vibrational spectroscopy

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The delocalization of charges is among the factors controlling charge and exciton transport in conjugated molecules. Thus, it is considered to play an important role in the performance of a wide range of molecular technologies. Dimerization reactions are well-suited to investigate the spatial

delocalization of charges. While dimerization reactions of radical cations are well investigated, studies on radical anions are still scarce. Radical anions of aromatic hydrocarbons are known to dimerize with neutral counterparts, through which an electron is considered to delocalize over the two molecules. Yet, due to the lack of a method to quantify delocalization of electrons, it has been difficult to study and clarify the exact nature of dimer radical anions. Here, by using time-resolved infrared (TRIR) detection coupled with pulse radiolysis, we show that radical anions of 4-*n*-alkyl-4‘-cyanobiphenyls (nCB) undergo dimerization reactions. We have recently demonstrated that nitrile *ν*(C≡N) vibrations respond to the degree of electron localization of nitrile-substituted anions: we can quantify the changes in the electronic charges from the neutral to the anion states in the nitriles by monitoring the *ν*(C≡N) IR shifts. Probing the shifts of the nitrile IR vibrational band allows us to unambiguously show that an electron is delocalized over the two nCB molecules, confirming the formation of dimer radical anions. Experimental findings are corroborated by electronic structure calculations. The present study provides clear evidence of spatial delocalization of electrons over intermolecular complexes.

MARM 494

EPR and NMR studies of radiation damaged polymers

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Kapton ((Polyimide) is used in space missions due to its high durability even in harsh environments. Though there have been some EPR and NMR studies on proton and heavy nucleus- irradiated Kapton, very few works have been performed on effects due to the electron irradiation.[1, 2, 3] The main objective of this research is to examine the relationship between free radical concentrations, chemical structure of electron irradiated Kapton and its optical and electric properties, using EPR and NMR spectroscopy. For the purpose, 90 KeV electron-irradiated (in vacuum) 1 Mil Kapton (Polyimide) film is used provided by our collaborators at AFRL.From our preliminary observations, for samples exposed to two different environments, the formation and subsequent decay of the free radical concentrations attributed to radiation damage was recorded. This signal decay agrees well with the ageing recovery mechanism being probed by our collaborators through electrical conductivity measurements. Similar experiments are being performed for the irradiated PVDF films from US ARL. It is observed that the recovery time for PVDF is much longer than Kapton.
Both ^{13}C and ^{1}H NMR measurements are planned to search for structural evidence of bond scission. The effects of annealing the irradiated film in vacuum, inert atmosphere (Ar) and air is also being used to study the ageing recovery mechanism.

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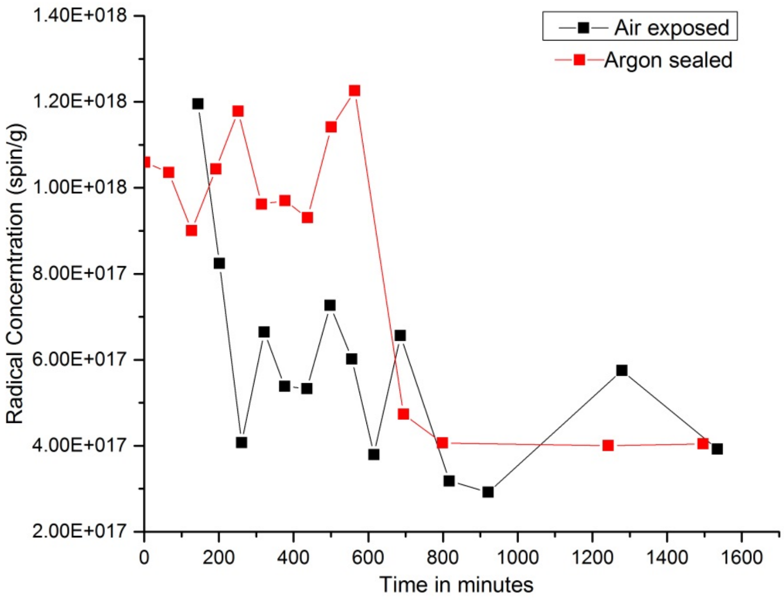

Figure 1: Plot for time decay of radical concentration of New Kapton samples

MARM 495

Radiation and radical chemistry of ionic liquids for energy applications

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Ionic liquids are becoming an important component of many advanced devices and technologies. A fair number of these applications, such as photoelectrochemical solar cells, high-performance batteries and recycling of spent nuclear fuel, expose ionic liquids to extreme conditions where they are subject to ionization or to the injection of excess charges. It is thus important to understand what happens to ionic liquids under those conditions, and the unique combination of properties they possess leads to significant differences in behaviour compared to familiar liquids. From the standpoint of ionization phenomena, the most important of these properties are: 1) the molecular-scale structural heterogeneity of ionic liquids, in which distinct polar, non-polar and interfacial environments may exist; and 2) dynamical heterogeneity characteristic of glassy fluids combined with significant viscosities, which extend the dynamical response of ionic liquids over several orders of magnitude in time. This presentation will explore ionization processes in ionic liquids as revealed by diverse radiation chemistry techniques, and the influence of ionic liquid properties on the ensuing chemical reactivity. This work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences and Biosciences under contracts DE- SC0012704 (BNL) and DE-AC02-06CH11357 (ANL).

MARM 496

Effect of various anions of pyrrolidinium-based ionic liquids on yield of solvated electrons and reactivity observed by picosecond radiolysis technique

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Ionic liquids (ILs) are been proposed and looked upon as an alternative solvent to meet the complex challenges of future nuclear fuel cycles. The unique properties of ILs can be used to design a novel and efficient IL-based nuclear separations schemes capable of processing spent nuclear fuel. However under such extreme conditions, radiation stability of IL-based system will affect the efficiency and selective separation of spent nuclear fuel. Several research groups have investigated the radiation stability of different hydrophobic ILs by understanding there degradation mechanism via final product analysis using various methodologies.[1-2] Radiolytically-generated excess electrons on a time scale of nanoseconds can determine the consequent radiation chemistry and the accumulation of radiolytic damage in ILs.[3-4] Picosecond pulse radiolysis technique provide an opportunity to study such intermediate species in ILs which are of interest in recycling of spent nuclear fuel. In the present work yield and solvation process of electron and there reactivity in various anions such as bis(trifluoromethylsulfonyl)amide (NTf_2), bis(fluorosulfonyl)imide (FSI), dicyanamide (DCA) of pyrrolidinium based ILs (Fig. 1) are been studied using picosecond radiolysis technique.

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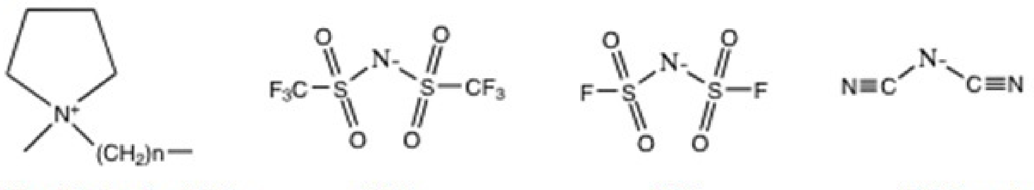
Figure 1



Pyrrolidinium Cation (n = 3, 9) NTf_2 FSI DCA anions

MARM 497

The speciation of technetium (VII) in the presence of bistriflamidic acid in ionic liquids

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Technetium-99 (^{99}Tc $t_{1/2}$: 2.1x 10^5 years; β_{max}: 293.7 keV) is a high-yield (6%) fission product in light-water reactors, which presents major challenges in separations and containment technologies. The use of ionic liquids as a possible alternative media for separations is being explored. In order to access the potential use of ILs for separations, a fundamental understanding of the interactions of the extracted species ,TcO_4^-, and ILs must be understood. The speciation of technetium (VII), TcO_4^- over varying concentrations of Bis((trifluoromethyl)sulfony)imide ($HNTf_2$) in ionic liquids (IL) has been studied. $HNTf_2$ is a known super acid and recently been shown to be an even stronger acid when dissolved in (IL) bearing the NTf_2 anion. This superacid-IL system was used to study the speciation of the pertechnetate ion in the presence of non-aqueous acidic media. N-alkylammonium pertechnetate salts were combined with varying concentrations of $HNTf_2$ in an IL with the corresponding cation as the Tc salt and anion as the acid and were studied using UV-VIS, ^{1}H and ^{99}Tc NMR. Preliminary results suggest that the TcO_4^- anion is protonated in the IL and forms $HTcO_4$ (pertechnic acid). Pertechnic acid is typically generated using large amounts of a non-coordinating acid Sulphuric acid (>9M) in aqueous media. The species formed in acid-IL solution is observed using far less acid (<100mM). We report here on our findings

MARM 498

Evidence of the Hofmeister effect in the extraction of copper from aqueous to ionic liquid phase

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We present the results of experiments on extractions of copper (II) salts from water to protic ionic liquids (ILs). The ILs are chosen to coordinate strongly with copper, eliminating the need for chelating agents such as crown ethers. Intriguingly, the extent of extraction depends strongly on the identity of the anion in the copper salt, and the pattern follows the Hofmeister series. The results are interpreted with reference to current thinking about IL nanostructure, and suggest that the hydrophobic/hydrophilic interface intrinsic to ILs may play an important role in solvation in the IL phase.

MARM 499

Surface studies of an ionic liquid on copper and gold

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Ionic liquids are now widely recognized as useful electrochemical materials. ILs typically present quite low vapor pressures, rendering them fully compatible with ultrahigh vacuum surface and thin film methods. For many applications, it is the surfaces and interfaces of ILs where many of the functional properties are defined and realized. This work examines structural and chemical properties of the interaction of ILs with copper and gold substrates, focusing on the interface. Ultrathin films of 1-methyl-3-octylimidazolium bis(trifluoromethylsulfonyl)amide ($Im_{1,8}^+$ / NTf_2^-) were prepared by physical vapor deposition, with film thicknesses from sub-monolayer to multilayers. The films were characterized using x-ray photoelectron spectroscopy, ultraviolet photoelectron spectroscopy and scanning tunneling microscopy. Results suggest a stronger interaction with Cu(100) than with Au(111).

MARM 500

Self-organized organic nanoparticles of hydrophilic metalloporphyrin as a catalyst for the selective oxidation of olefins under ambient conditions

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Metalloporphyrins have been studied extensively for their catalytic activity such as for oxidative degradation of volatile organic compounds, hydroxylation of alkanes and epoxidation of alkenes. However, their supramolecular systems are comparatively new and the study of their self-organised nanoaggregate systems is currently under investigation. A study has been conducted on the preparation of self-organised organic nanoparticles of water soluble porphyrins such as 5,10,15,20- tetrakis(4-sulfonatophenyl) porphyrinato iron (III) chloride [FeTPPS], and have been tested for their catalytic activity using different organic substrates, mostly water soluble aromatics. The oxidized products of these substrates have been analyzed by UV-Vis and GC-MS. The catalytic oxidation products from metalloporphyrin NP reactions are different from those already reported for solution phase reactions. The TON for these NP catalyzed reactions depends upon the size of NP and also upon the nature of oxygen source used for these reactions. Our hypothesis is that the differences in their catalytic activity is because of differences in the mechanism between the NP and solution phase reactions.

MARM 501

Photo-physical characterization of porphyrin conjugates

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Porphyrins are aromatic heterocyclic organic compounds with interesting photo-physical properties. Due to the aromaticity of the macrocycle, these compounds tend to absorb intensely in the visible light region. This makes them practical for applications in diagnostic tracking and alternative therapies such as photo-dynamic therapy (PDT). The latter application works by taking advantage of production of reactive oxygen species (ROS) to trigger an apoptotic pathway in cells. However, organic dyes are limited in their effectiveness because of their low solubility and low up-take in cells. Most dyes are conjugated with groups that impart water solubility or with groups that increase cell-uptake or selectivity for a particular cell line. The goal of this project was to characterize and test the efficiency of an array of porphyrin-conjugates, utilizing either tannic acid or hyaluronic acid, as targeting vectors. Tannic acid and hyaluronic acid contain many carboxylic acid and alcohol groups which are available for linking more than one photosensitizer. This makes it possible to direct multiple photo-active molecules into cells of interest, via endocytosis. Photo-physical characterization of conjugates include UV-vis spectroscopy, steady-state fluorescence, and lifetime based on fluorescence. Generation of ROS was measured with an indirect method using fluorescence that determines the reaction between singlet oxygen (an important ROS) and a commercially available chemical sensor known as Singlet Oxygen Sensor Green (SOSG). Moreover, we also studied the cell uptake of these conjugates by fluorescence microscopy imaging.

MARM 502

Study of multi-target directed ligands: Copper binding selectivity and inhibition of reactive oxygen species formation

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Alzheimer's disease (AD) is the most prevalent form of dementia, affecting over 5 million Americans and 28 million people worldwide. It is predicted that by 2050, the number of people age 65 and older with AD will increase to 13.8 million Americans. Currently, AD is the only disease among the top 10 causes of deaths in America that does not have a cure or treatments to slow the progression. Under the amyloid cascade hypothesis, a 39-42 residue amyloid-b (Ab) peptide is linked to plaque Ab depositions or partially aggregated soluble Ab that trigger a neurotoxic cascade resulting in AD pathology. Intracellular tangles in the brain, and production of reactive oxygen species (ROS) are hallmarks of AD that result in neuronal death. Due to the mounting evidence supporting the implication of some metal ions like Cu^{2+} and Zn^{2+} in the progression of AD, our study focused on the role of Cu^{2+}. Using a multi-target directed ligand design (MTDL) approach, two compounds (AM29 and AM49) were studied for metal ion selectivity and ROS inhibition. Focus was placed on finding the selective binding to Cu^{2+} over other biologically relevant metal ions, and the correlation between Cu^{2+} binding and the ability of the compounds to inhibit the Cu^{2+}-catalyzed ROS formation. UV-Visible spectroscopy and fluorescence spectroscopy were used to acquire data in our experiments. Results demonstrate a high degree of selectivity for Cu^{2+} versus Ca^{2+}, Mg^{2+}, Zn^{2+}, Mn^{2+} and Fe^{2+}, which could have important implication in preventing side effects. Additionally, both multi-target compounds were able to inhibit to a 98% extent the Cu^{2+}-catalyzed ROS formation. In conclusion, the compounds herein studied represent a novel and promising alternative for the treatment of AD.

MARM 503

Pulsed field gradient NMR study of ion transport in lithium-ion battery electrolytes for aerospace applications

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The main advantages of lithium-ion batteries are its high specific energy, high energy density, low self-discharge rate, long cycle life, low weight, and wide temperature ranges of operation. However, for certain applications, such as aerospace and remote planetary exploration, there is a need for improving the low temperature performance. The aim of the present work is to evaluate different formulations of electrolytes for lithium ion batteries. The base electrolytes used are LiPF6 in a mixture of liquid carbonates; these electrolytes were prepared by collaborators at the NASA's Jet Propulsion Lab (JPL). We are interested in the effect of certain liquid and solid additives on low temperature ion transport. Nuclear Magnetic Resonance (NMR) spectroscopy is a technique of choice for measuring structural and dynamic properties of complex mixtures. Specifically, PFG (Pulsed Field Gradient) NMR allows for the determination of self-diffusion coefficients of each component of the liquid mixture: cations, anions, and solvents. In order to attain a better fundamental understanding of the chemistry of commonly used electrolytes, we performed PFG NMR variable temperature experiments, ranging from -20°C to 30°C on modified carbonate LiPF6 electrolytes in a 400 SB Bruker Avance III Spectrometer. From the measured self-diffusion coefficients of the anions, cations, and the solvents, one can calculate the Li+ transference number and the degree of cation-anion association. Our results will be discussed in the context of electrochemical performance data provided by our colleagues at JPL. Particular attention was given to the influence of the polarity of the solvent and the effect of additives.

MARM 504

Measuring the nanomechanical properties of tomato cuticles using atomic force microscopy

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The tomato cuticle is attached to the plant cell wall and possesses two components: cutin and waxes. Tomato fruit is subjected to stresses from environmental, biotic, and mechanical factors, leading to decreased crop yield and economic losses. It is important to understand the fundamental links between chemical composition and biomechanical properties of tomatoes. This project assesses the influence of cutin deposition on the nanomechanical properties of the tomato cuticle using Atomic Force Microscopy (AFM). The Young's modulus of the glossy surface of dewaxed and waxy tomato outer cuticles from wild type (M82) and two RNAi-silenced cultivars (deficient in cutin synthase enzymes CUS1 and CUS2) were compared under controlled humidity (60%). The results were used to investigate if inhibition of the expression of the CUS1 and the CUS2 genes would result in significant differences in the elasticity of tomato cuticles. A downward trend in Young's modulus (M82, CUS2 and CUS1) was observed for the glossy surface of the dewaxed samples. This indicated that the elasticity of tomato cuticle is positively correlated to cutin deposition within the sample. Higher cutin deposition in the sample leads to higher values for the Young's modulus. However for the waxy samples, CUS1 and CUS2 displayed a higher Young's modulus than M82. It was concluded that in the absence of epicuticular waxes, as compared with the wild-type M82 cultivar, cutin deficiency in CUS1 and CUS2 contributes to a lower resistance to deformation and decreased stiffness of the cuticles in the absence of waxes. However, for the waxy samples the scenario is quite the opposite, with CUS2 and CUS1 having higher Young's modulus values than M82. This trend can be attributed to the higher proportion of waxes to cutin in the CUS-silenced cuticles. In the future, these results will be correlated with findings from NMR and mass spectroscopy to better understand the underlying changes in chemical composition that produce cultivar-specific differences in nanomechanical performance.

MARM 505

Understanding the formation and size distribution of porous poly(*o*-toluidine) microspheres

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Poly(*o*-toluidine) (POT), a derivative of polyaniline, belongs to a class of intrinsically conducting polymers having unique electronic and optical properties. We have developed a simple method to prepare highly porous POT microspheres, which may be useful as electroactive microreactors, scaffolds for catalysis, and encapsulants for drug delivery. Briefly, *o*-toluidine and ammonium persulfate are rapidly mixed in aqueous acidic solution to obtain granular POT, which is converted into porous spheres upon addition of excess 4M ammonium hydroxide. FTIR spectra indicate that spherical and granular POT are chemically identical, but that the spheres contain unpolymerized *o*-toluidine (OT). SEM images show that the morphology depends strongly on the concentration of OT and that spheres are not formed in its absence. We propose that the rapid change to an alkaline environment produces a water-in-oil-in-water double emulsion. The spheres are formed when unreacted OT forms droplets that dissolve granular POT, and the pores are formed by water droplets trapped in the polymer matrix. The spheres are polydisperse in size. Approximately 65% are 1-5µm in diameter, 20% are 6-10µm, 5% are >10µm, and 10% are <1µm. Preliminary SEM data suggest that reducing the amount of granular POT available to dissolve in the OT droplets may inhibit the formation of larger spheres and other non-spherical objects.

MARM 506

Green and microscale flavone synthesis

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This project continues the synthesis of several flavones as a part of an undergraduate research project in the Organic II lab at Volunteer State Community College. Several flavones were synthesized using green methods, taking advantage of green solvents and catalysts. The use of green solvents minimizes exposure and reduces the generation of hazardous waste products. Microscale synthesis allows for a cost effective/high impact laboratory experiments for students of organic chemistry. UV- Vis fluorescence spectroscopy techniques with analytes were conducted at various pH levels to measure samples from this study, as well as, previous samples from prior syntheses. Melting points were determined for all products including intermediates throughout the series of reactions. Thin Layer Chromatography with ImageJ also provided characterization.

MARM 507

Partial sulfonation of polyaniline nanofibers

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Polyaniline (PANI) is a well-known conductive polymer that is easily prepared as high surface area nanofibers. Composites of PANI nanofibers with gold nanoparticles (Au-NPs) may result in new materials with novel optical and electronic properties for sensors and other devices. We have observed that sulfonated PANI, with its negatively charged substituents, can attract positively charged Au-NPs, thereby increasing the extent of NP deposition. However, sulfonation increases the water solubility of PANI, ultimately degrading the desirable nanostructure. We hypothesize that degradation may be limited if PANI is only partially sulfonated, leaving the fiber core insoluble while providing sufficient charge at the surface to attract positive NPs. PANI nanofibers are prepared from 0.8M aniline and 0.1M ammonium persulfate in acidic solution. The product is deprotonated in ammonium hydroxide, and then sulfonated by exposure to dilute sodium metabisulfite. The addition of sulfonate groups has been confirmed by FTIR spectra. Longer exposures to the salt increase the extent of sulfonation, which leads to increasingly soluble and degraded nanofibers as seen in SEM images. The deprotonated form of PANI is known to be more readily sulfonated than its protonated form. We are therefore exploring partial deprotonation via timed exposure to NH_4OH as another route to limit and eventually control the extent of sulfonation.

MARM 508

Toxicity of e-juices

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E-cigarettes have taken a recent rise in popularity due to the idea that they pose a lesser health risk than traditional cigarettes. This idea, however, is contrary to the current scientific literature that was reviewed. E-cigarettes have been found to have a host of various toxins with a broad range of harmful effects. Many of the toxins identified were carcinogenic. In order to determine the risk factors associated with smoking e-cigarettes data from various experiments were accumulated in order to extrapolate mathematical values that could propose realistic risk factors. The collected and extrapolated values were arranged as graphs representing a risk value per wattage of vaping for 11 different e-cigarette juices.

MARM 509

Determination of elemental arsenic and leachable arsenic in aquifer sediment samples of Bangladesh

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Groundwater aquifer is a principle source of drinking water and irrigation water for billions of people worldwide. Consequently, there is growing public concern about chronic exposure to geogenic contaminants in groundwater that pose a serious health risk to over hundred millions of people in several countries including Bangladesh, India, China, Myanmar, Pakistan, Vietnam, Nepal and Cambodia. In Bangladesh, arsenic (As) contamination of groundwater is threatening both drinking water supply and food production. Rice production in Bangladesh has more than doubled over the last decades to meet the rising food demand of the growing population. Aquifer sediments were collected from two sites of coastal city Chittagong, Bangladesh. Total 30 core samples at 1.5 meter intervals were collected from each site. The samples were packed in Chemplex XRF (X-ray Fluorescence Spectrophotometry) sampling cups on site and carried to US laboratory to run by the optimized handheld XRF for elemental abundance particularly heavy metals including Pb, Cd, Cu, Zn, As, Fe, Mn. Dry samples were digested with 1.2M HCl at 100^{o}C for 1 hour to detect the leachable arsenic. A digestion procedure was modified and optimized to detect the leachable arsenic in the sediment samples by using Econo-Quick testing arsenic field kits, a product of Industrial Testing Systems. The preliminary results obtained from the depth profile for sedimentary arsenic showed consistency with the groundwater arsenic profile, measured on site by ETS test kits in existing private wells at different depths. Interestingly, this modified method could be used to monitor the arsenic accumulation in paddy field caused by the irrigation with contaminated groundwater. It has great implication to evaluate fate and transport of arsenic in aquifers of Bangladesh and elsewhere which is one of the most important factor in assessment strategy.

MARM 510

Enantioselective synthesis of actinopolymorphol B and its analogs

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An enantioselective synthesis of actinopolymorphol B is currently in development along with the synthesis of its analogs. The reaction schemes to synthesize these molecules will be presented. Noyori's

asymmetric hydrogenation of ketones will be utilized to install the stereochemistry of the molecule. The conditions to form the key aldehyde intermediate of this synthesis has been optimized. Also, using a recently developed methodology for the functionalization of alkynes, the analogs of actinopolymorphol B can be formed. The compounds to be synthesized are structurally related to medicinal agents and their biological activities will be screened. The molecules will be tested for growth inhibitory effect of many human cancer cell lines and antibacterial activities with collaboration with the other research groups.

MARM 511

Visible light-driven energy transfer: Hybrid-engineered nanostructures versus plasmonic resonance in solar cell applications

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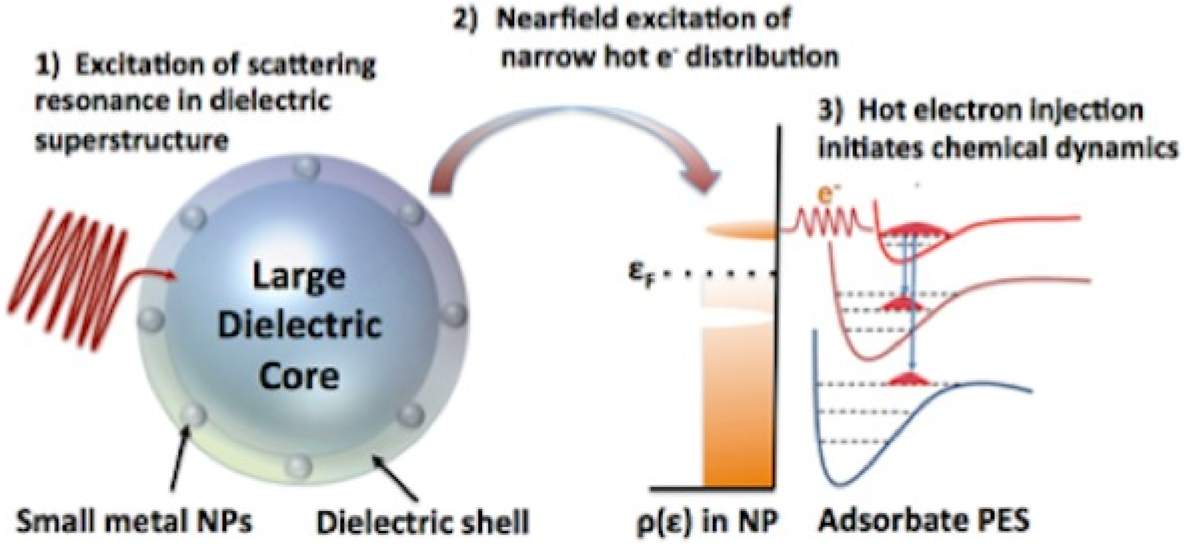
We will report on our efforts to elucidate the properties of engineered nanostructures that we hypothesize can enable a new paradigm of visible light-driven energy transfer we call "Scattering Mediated Hot-Electron Transfer". (SMHET). In addition, we hypothesize the excitation state distribution of these electrons have a longer lifetime than electrons excited via plasmonic resonance, which is an optical resonance on metal nanoparticles with potential applications for light-driven energetic electron transfer that have been widely explored.

Because light harvested from the sun represents a sustainable and renewable energy source, light initiated energetic electron transfer has attracted considerable attention as an emerging paradigm for solar energy conversion. This method of electron transfer involves structures that can harvest solar photons and invest their energy into electronic motion, creating so-called “hot electrons”. Subsequently, hot electrons excited on the harvesting structure deposit energy into energy accepting materials such as photovoltaic cells. Ideally, structures that can mediate transfer of energy between solar photons and acceptors can be constructed from cheap and earth abundant materials, as opposed to the traditionally expensive materials used in plasmonic resonance, such as gold and silver.

Theoretical and computational methods are being used to elucidate the first step in the SMHET mechanism, which is a process we call Scattering Mediate Absorption. Based on results from rigorous Mie theory and Finite-Difference Time-Domain calculations, we find that light with specific energy content can be efficiently channeled into the metal nanoparticles decorating the surface of silica core structures, and that the specific energy content can be tuned by changing only the radius of the silica core. We observe this effect in a wide variety of metals with different optical properties.



MARM 512

Hierarchical nanoparticles in photodynamic therapy

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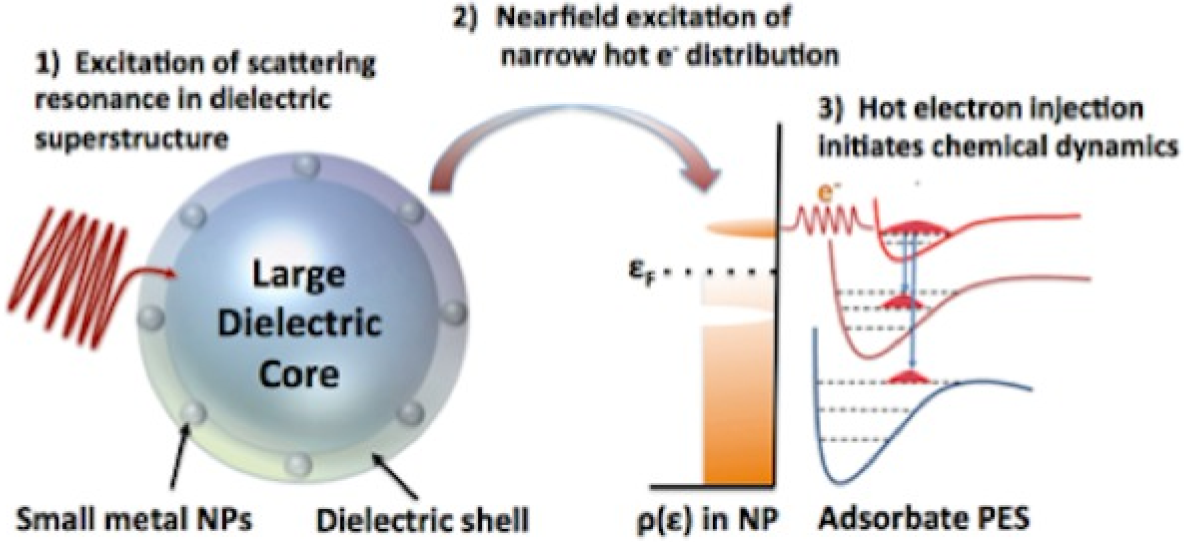
We will be presenting theoretical results analyzing the photophysics in novel hierarchical nanoparticles that will allow us to assess the potential for these hierarchical nanoparticles to be used as photosensitizers in photodynamic therapy (PDT).

Photodynamic therapy uses light to excite or activate a photosensitizer that has been targeted to a specific tissue, which elicits a cellular response that ultimately leads to cell death via generation of reactive oxygen species and radicals that cause irreversible damage to the cell. It is both a curative and palliative therapy for cancers of the skin, esophagus, lungs, bladder, head and neck cancer, as well as non-cancer ailments such as psoriasis, actinic keratosis, periodontitis and acne.

Quantum dots have been investigated as potential photosensitizers in PDT due to their highly controllable photophysics and potential to mediate optically-initiated energy transfer. We have observed highly tunable photophysics and optically-driven energy transfer mediated by hierarchical nanoparticles, which we propose arises from a new phenomena we call Scattering Mediated Hot-Electron Transfer (SMHET). We will present results from theory and simulation aimed at elucidating the mechanism of SMHET, and we will evaluate the potential of these hierarchical nanoparticles to serve as safe and efficient photosensitizers for PDT.



Schematic of a hierarchical nanoparticle and the mechanism of scattering mediated hot electron transfer.

MARM 513

Fusing a green fluorescent protein to SCO2139, a *S. coelicolor* rhomboid protease

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Cell membranes are controlled borders with the outside world and serve as organizers of cell signaling, metabolic pathways and ultra-structure assembly. Proteases that reside within the cell membrane play an important role in regulating these events, although it is still not clear how they function. Rhomboids are intramembrane proteases found in all forms of life that have been implicated in several human diseases. Streptomycetes are gram positive soil bacteria that produce secondary metabolites with antibiotic and anti-tumor biological activities. The production of these natural products relies on a cell signaling system, not fully understood, that integrates environmental, physiological and stress signals. We propose that rhomboid proteases play a role in their cell communication. Using bioinformatics we identified four putative rhomboid genes in Streptomyces coelicolor, the model organism for the Streptomyces genera and demonstrated that SCO2139 is a functional rhomboid protease. To elucidate the function of SCO2139 we have built a green fluorescent protein-rhomboid protease fusion. The purification and characterization of the fusion protein and its oligomeric state will shed light into the native structure of this intramembrane protease.

MARM 514

Oxidation of meso-substituted tri and tetra porphyrins

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Porphyrins are pertinent to the metabolism of living organisms as they are found to be the active components in numerous biological systems. The synthesis by use of a modified Adler method, purification and characterization of tri and tetra meso substituted porphyrins comprised of p-anisaldehyde, p-tolualdehyde, and p-pyridine carboxaldehyde groups is the primary focus of our research. Upon running NMR and UV-Vis spectrums possible chlorin impurities were found. Chlorin has essentially the same chemical formula as a porphyrin aside from a single double bond in the porphyrin ring. This suggests that our porphyrins have not reached complete aromaticity. To counter this occurrence, we will be subjecting our synthesized porphyrins to 2,3-dichloro-5,6-dicyanobenzoquinone, DDQ, which will oxidize the bonds in our porphyrins that have not successfully formed double bonds. Once completed UV-Vis and NMR analysis of porphyrins oxidized with DDQ compared to their starting material. We speculate that the use of DDQ will further purify our porphyrins to permit delivery of our porphyrins to cancer cells by the use of liposome carriers.

MARM 515

Vibrational analysis of cysteine: Copper^{2+} interaction

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Alpha-synuclein, a cytosolic protein mainly found in neural tissue, is of great interest to Parkinson's research as it is a major component of Lewy bodies – the pathological characteristic of Parkinson's disease. Studies have proposed a cysteine residue coordinating with a copper moelcule, initiating its aggregation, leading to the Lewy bodies. To confirm a cysteine can complex with a copper, both computational and experimental analysis of cysteine and copper solutions were executed, via of Raman spectroscopy and Gaussian 09 W/Gauss View 05 software, respectively. With the addition of metal to the cysteine solution, the S-H mode at 2690 cm^{-1} disappears and S-C mode at 1063 cm^{-1} shifts to 1044 cm^{-1} – confirming thiol-metal complexing. Should this trend be observed with vibrational analysis of the *Alpha-synuclein*, its aggregation may be confirmed as caused by same cysteine-metal coordination as observed.

MARM 516

The effects of roasting on the reduction of hexavalent chromium by coffee

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Batch experiments were performed to investigate the application of commercial roasted coffee and raw coffee for detoxification of hexavalent chromium [Cr(VI)] contaminated solution. When 2g of ground raw coffee was mixed with 40 mL of 50 mg/L of Cr(VI) solution, all Cr(VI) disappeared immediately while approximately 75% of initial Cr(VI) was removed within 30 minutes in the presence of commercial roasted coffee. In addition to the mass of applied coffee, the reaction temperature for the roasted coffee affected hexavalent chromium reduction rate. The reaction rate increased as the temperature increased. For the raw coffee, the reduction rate was too fast to identify the significant change of the reduction rate as a function of reaction temperature. The experimental results confirmed that both roasted and raw coffees are great candidates for non-toxic, environmental friendly reducing agents for the remediation of hexavalent chromium contaminated solution with low maintenance and significantly less secondary contamination. The roasting activity may reduce the availability of potential electron donors in the coffee or discharge the reducing agents slowly to the solution resulting in the slower Cr(VI) reduction rate than that with the raw coffee.

MARM 517

Interaction of catalase with nanoceramics as monitored by different spectroscopic methods

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Nanomaterials are materials with morphological features on the nanoscale with special properties that stem from their small dimensions. The fascinating and useful properties of nanomaterials make them versatile materials in various fields of science, ranging from material science to medicine. Due to the potential application of nanomaterials, it is imperative to understand the interactions of nanomaterials with various biomolecules. In this study, the interactions of four nanomaterials—aluminum oxide, silicon oxide, tin oxide, and zinc oxide—with the enzyme, catalase, were investigated by various spectroscopic methods (absorbance, fluorescence and circular dichroism). Results showed aluminum oxide significantly reduced absorbance and emission of the catalase in comparison to the other nanoceramics. Silicon oxide and zinc oxide, however, had a significant initial change in emission and absorption, but did not have a substantial overall change like silicon oxide. The tin oxide decreased the absorbance and emission of the catalase slightly. The changes in the conformation of catalase upon mixing with the nanoceramics were also observed.

MARM 518

Use of molecularly imprinted polymer to improve the analysis of naproxen in environmental water samples

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Pharmaceuticals are continually released into the environment. Because of their physical and chemical properties, they can accumulate in sediments, sludge, and soils, inducing adverse effects in terrestrial organisms. However, due to the very limited methods permitting the detection of these low-level concentration compounds in such complex matrices, their concentrations in environmental samples remain largely unknown. Among these pharmaceuticals are NSAIDs or nonsteroidal anti-inflammatory drugs, a class of drugs that provides antipyretic (fever reducing), analgesic (pain-killing) and anti-inflammatory effects. In this study, naproxen, an over the counter NSAIDs, has been used as the target analyte in the development of sampling pretreatment method using commercially available molecularly imprinted polymer (MIP). The naproxen in environmental water samples was extracted using MIP and then analyzed using high performance liquid chromatography (HPLC). Using the same source of samples, the use of MIP improved the analysis as higher amount of naproxen was found in comparison to the analysis made use of Oasis HLB, which is presently used in the analysis of naproxen. A shorter extraction time was also observed.

MARM 519

Comparative analyses of phenol content and antioxidant properties of Philippine tea samples

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The phenol content and antioxidant properties of the water extracts of seven commercial fruit and medicinal plant based teas from the Philippines were evaluated and compared to one another. The total phenolic content, determined by the Folin-Ciocalteu method varied from 23.2 mg/g (bitter melon) to 91.49 mg/g (Pito-pito dried herbal tea) mg of gallic acid equivalent/g dry tea. The antioxidant properties were evaluated using the 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay system, which showed 80% to 100% inhibition or reduction of the DPPH. The 2,2-azinobis (3-ethyl-benzothiazoline-6-sulfonic acid (ABTS) assay was also performed and showed the same results as that of DPPH assay. A general trend in terms of antioxidant activities and total phenol content can be observed as pito-pito dried herbal tea showed 100% inhibition of both DPPH and ABTS.

MARM 520

Binding interaction of nanoceramics (metal oxides) with human serum albumin

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Nanomaterials are defined as materials with at least one external dimension in the size range from approximately 1-100 nanometers. The properties of nanomaterials make them versatile materials in various fields of science, ranging from material science, energy, to medicine. This study was conducted because the knowledge on the interactions of nanomaterials with different biomolecules is limited. The interaction of nanoceramics (aluminum oxide, silicon oxide, titanium oxide and zinc oxide) with human serum albumin (HSA)—the most abundant protein constituent of blood plasma— was investigated by various spectroscopic methods (absorbance, fluorescence and circular dichroism). Results showed aluminum oxide significantly changes in terms of reduced absorbance, emission, and CD profile in comparison to the other nanoceramics. Absorbance reduction in samples with silicon oxide was also observed. The nanoceramics also reduced the emission intensity in the samples of HSA. Interestingly, a peak was observed at around 420 nm for zinc oxide and 410 nm for aluminum oxide and silicon oxide as the amount of nanomaterials being added increased.

MARM 521

Antioxidant activities of different bee propolis extracts

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Propolis, a natural resinous substance collected by honeybees from buds and exudates of plants, is believed to be used in the beehive as a protective barrier against enemies. Like other bee products known to be natural medicine, propolis contains beneficial activities such as antibacterial, antioxidative, antiviral, antimicrobial and many more. Depending on the season, bee species, vegetation, and the area of collection, the chemical composition of propolis are qualitatively and quantitatively variable. In this study, the antioxidant activity of the extracts from propolis samples obtained from various parts of the world (Europe, Australia, USA and the Philippines) were determined. Based on the results, the methanol

extracts have higher antioxidant activity than dichloromethane extracts. We also relate the chemicals/phenolics found in extracts with the antioxidant activity.

MARM 522

Effect of pH on the spectroscopic properties of several hydroxycinnamic acid derivatives

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Hydroxycinnamic acids are a class of aromatic acids and hydroxy derivatives of cinnamic acid. These compounds account for about one third of the phenolic compounds in our diet. Hydroxycinnamic acids are of great interest because they are potent antioxidants. This study observed the effect of pH on the spectroscopic properties (absorbance and fluorescence) of caffeic acid, coumaric acid, ferulic acid and sinapic acid. Computational calculations on absorbance were also carried out and compared with the experimental results. The absorbance and fluorescence spectra blue shifted from pH 3 to pH 7 and then red shifted from pH 7 onwards. Emission intensity was also observed to increase with increasing pH in ferulic acid and sinapic acid. However, caffeic acid, only increased in emission intensity up to pH 10. The emission intensity of coumaric acid decreased from pH 3 to pH 7 and increased and remained the same at higher pH. Theoretical calculations agree with experimental results in absorbance where in there is a blue shift from pH 3 to pH 7 and then a red shift from pH 7 onwards.

MARM 523

Phytochemical study and evaluation of larvicidal activity (*Aedes aegypti*) and termiticide (*Nasutitermes sp.*) of extracts *Morinda citrifolia* L. (Noni)

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The use of plants with insecticidal properties and larvicides for pest control has shown great success in comparison with the use of synthetics. This study points to the *Morinda citrifolia* L. (Noni) as a viable and ecological alternative to the problems caused by the action of pathogens carried by mosquito larvae *Aedes aegypti*, causing the death of thousands of people each year, dengue victims. It also discusses the feasibility of its use as an insecticide for termites arboreal *Nasutitermes sp*. The ethanol extract of Noni fruit was produced and obtained by cold maceration technique in the Laboratory of Environmental Biotechnology Empress State University Maranhão. And the phytochemical analysis showed the presence of triterpenoids and antroquinonas, these substances, responsible for power Noni larvicide and insecticide. Tests with the ethanol extract in different proportions: 100:1 mg / ml; 250:1 mg / ml; 500:1 mg / ml, determined the death of 100 % in larvae of the mosquito *Aedes aegypti* and termite genus *Nasutitermess spp* with analysis of 1 hour and 24 hours after validation. So the use of *Morinda citrifolia* L. (Noni) shows that it is a good option in control of larvae and insects, because of their insecticidal and larvicidal activity, low cost, availability in the Brazilian Northeast and ease of cultivation in different regions of the country and the world.

Keywords: *Morinda citrifolia* L., larvicidal, insecticide.

Table 1 . Mortality of larvae (*Aedes aegypti*) 24 hours

Treatment x Proportion	**100:1 mg/ mL**	**250:1 mg/ mL**	**500:1 mg/ mL**
Ethanol Extract	100%	100%	100%
Extract Hydroalcoholic 70%	100%	100%	100%
Extract Hydroalcoholic 50%	100%	100%	100%
Aqueous Extract	10%	10%	50%
Treatment x Proportion	**1: 20 mg/ mL**	**2,5: 20 mg/ mL**	**5: 20 mg/ mL**
Aqueous solution dry Extract	40%	6.60%	33,3%
Treatment x Proportion	**Alcohol 92,8%**	**Alcohol 70%**	**Alcohol 50%**
Test Negative	100%	100%	100%
Treatment x Proportion	**100mg/ L**	**0.1 grams**	-
Test Positive (temephos)	100%	100%	-

Table 2. Mortality of termites (*Nasutitermes sp.*) 24 hours

Treatment x Proportion	**100:1 mg/ mL**	**250:1 mg/ mL**	**500:1 mg/ mL**
Aqueous Extract	36.6%	40%	100%
Treatment x Proportion	**1: 20 mg/ mL**	**2,5: 20 mg/ mL**	**5: 20 mg/ mL**
Aqueous solution Dry Extract	70%	27%	80%
Treatment x Proportion	**1: 8 mL/ mL**	**3: 8 mL/ mL**	**6: 8 mL/ mL**
Dilution extract hydroalcoholic 50%, ratio 100: 1 mg / ml	47%	53%	63,4%
Tratamento x Proporção	Álcool 92,8%		
Teste Negativo	100%		
Tratamento x Proporção	**100mg/ L**		
Teste Positivo (Temephos)	100%		

MARM 524

Synthesis and characterization of silver nanoparticles and nanoprisms

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Preliminary results on the changes in particle size distribution and particle shape as a function of reagent concentration and pressure in the growth of silver nanoparticles are presented. UV/Visible, dynamic light scattering and TEM are used to characterize the silver nanoparticle distributions and to correlate particle shape/size with reaction parameters in order to probe the reaction mechanism. We discuss the possible mechanisms that lead to the growth of nanoparticles in particular shapes depending on reaction conditions.

MARM 525

Exploring fulgides with optoelectronic properties: Synthesis

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It has been previously shown that fulgides, after the Latin word *fulgere* which means to glitter or shine, may be exploited as molecular switches and molecular memory devices. In order to understand better their photochromic properties, we report on our efforts to synthesize 2,3-bis(diphenylmethylene)succinic acid *via* Stobbe condensation, with spectroscopic data (NMR, IR, MS) to confirm the product.

MARM 526

Esterification of succinic acid derivatives using dimethyl carbonate

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Dimethyl carbonate is touted as a “green” methylating agent as it is a safer alternative to methyl halides, exhibits low toxicity, and is biodegradable. It has been previously shown that precise reaction control may be achieved using this reagent with mono-carboxylic acids. We explore the use of dimethyl carbonate for the esterification of bis-carboxylic acids, such as derivatives of succinic acids.

MARM 527

Microwave-promoted Strecker synthesis

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The Strecker synthesis is a three-component reaction that gives alpha-amino nitriles, which are precursors of alpha amino acids. It has been reported that the use of microwaves enhances the rate of synthesis for these molecules, which is beneficial for short-lived radionuclides like carbon-11, used in positron emission tomography (PET). We explore the microwave synthesis of alpha-amino acetonitrile under cryogenic conditions, and characterize the product mixture by mass spectrometry.

MARM 528

Synthesis of polymers based on epoxidized soybean oil

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Plant-derived polymers are explored as greener alternatives to petroleum-based plastics, because of their potential as renewable, biodegradable, and carbon-neutral products. Epoxidized soybean oil (ESO) is a commercially successful plant-derived product which is used as plasticizers, UV cure agents, pigment dispersants, and fuel additives. We report our efforts in the synthesis of polymers based on epoxidized soybean oil, with a goal towards the development of high-molecular weight polymers.

MARM 529

Ionic liquid solutions for cellulose and chitin dissolution

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Cellulose and chitin are found in the cell wall of plants and in the shells of insects and crustaceans, respectively. These polysaccharides are extremely abundant and contain a variety of characteristics that make them highly utilizable in fields like energy, and biomedicine. Due to the highly structured nature of cellulose and chitin, containing many hydrogen bonds, there are very few substances that can dissolve them into useable forms. However, ionic liquids have proven to be very efficient in dissolving cellulose and chitin and can be very eco-friendly. The method of dissolution through the use of ionic liquids must still be refined to ensure the most efficient process. We synthesized various quaternary ammonium salts which may be ionic liquids. These salts will be dissolved in various solvents, and the resulting solutions will then use to try to dissolve cellulose and chitin. Following the dissolution, we will regenerate the dissolved products and recover the ionic liquids used.

MARM 530

Synthesis and characterization of $[Rh^{III}(NNN)(NN)L]^{n+}$

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Several complexes of the general formula, $[Rh^{III}(NNN)(NN)Cl]^{2+}$, have been synthesized (where NNN = 2,2:6,2–terpyridine, 4–chloro–2,2:6,2–terpyridine, 4–(4–chlorophenyl)–2,2:6,2–terpyridine, 4–methyl–2,2:6,2–terpyridine and NN = 2,2–bipyridine, 1,10–phenanthroline, 4,4–dimethyl–2,2–bipyridine, 3,4,7,8–tetramethyl–1,10–phenanthroline and 4,4–dimethoxy–2,2–bipyridine). These complexes were synthesized using a modified literature procedure. All complexes were precipitated as the PF_6^- salt, without any purification, with yields ranging from 60% to 90%. Complexes were characterized using

NMR and UV–Vis. Crystallization, for X–ray diffraction, of these products are currently being investigated. Continuing trials to convert the chloride complex to the triflate have shown interesting results, however with low yields. Optimization of these products are currently being performed. The complex of $[Rh^{III}(NNN)(NN)(OTf)]^{2+}$ will be synthesized with $pyPorH_2$ (pyridylporphyrin) and its analogs to study their photochemical and photophysical properties.

MARM 531

Determination of the ionization constant of weak carboxylic acids using microscale freezing point depression measurements

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Freezing point depression is a colligative property that is related only to the number of particles in solution but not to the nature of the solute. For the first time the ionization constant of a carboxylic acid is determined in a non-traditional titrimetric method. The values obtained are also the first ones ever recorded at 0°C. The project uses microscale freezing point depression measurements to calculate this physical property using the Van't Hoff factor. The investigation involves the study of several carboxylic acids($Ka=10^{-2} – 10^{-3}$) . The ionized fraction of the solute is measured through a derived equation that correlates the freezing point depression temperature. The measured Ka values of various carboxylic acids were determined at various aqueous concentrations (1.00M, 0.50M, 0.25M, 0.10M). The experiment is fast, uses extremely low concentrations of the solute and the results are easily reproducible.

MARM 532

Isolation and identification of antibiotic-resistant bacteria from New York City soil samples

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Antibiotic resistance in pathogenic bacteria is a growing medical problem. As an urban environment, New York City puts an enormous amount of pressure on its natural areas. As part of the Soil Joint Seed Project we are focused on the isolation and identification of antibiotic resistant bacteria found in soil. The project as a whole is concerned with the effects and implications that resistant bacteria could have towards human health and the environment. Soil samples were collected from three sites that range from “pristine” to “polluted” according to varying degrees of human influence: Thain Forest (pristine), Central Park (intermediate), and Newtown Creek (polluted). Serial dilutions of 10^{-3}, 10^{-4}, and 10^{-5} were prepared with 0.2 ml of dilution added into R2A plates. To ensure bacterial growth only, antifungals nystatin and cycloheximide were added. After pure cultures were obtained, bacterial isolates were plated onto R2A + penicillin, R2A + kanamycin, and R2A + penicillin and kanamycin to test for antibiotic resistance. Colonies were further studied via gram staining and microscopy. Preliminary results shows that there are gram-positives and gram-negatives among the cultured isolates. In addition many isolates are showing antibiotic resistance. Further studies will involve identification of species via Biolog and DNA sequencing along with determination of resistance mechanism by PCR primers specific to resistant genes. Prevalence of the isolates in the microbial community will also be determined by comparison to metagenomic sequencing results.

MARM 533

Synthesis of pyrrolidinium ionic liquids bearing symmetrical and asymmetrical fluorous anions

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The non-volatile nature of ionic liquids (ILs) together with their inherent conductivity and other attractive physical properties make them suitable as alternative solvents for many applications. Pyrrolidinium ionic liquids are among the most common ILs studied in recent years particularly when paired with the fluorine containing NTf_2^- anion. The physical properties of these ILs can be tuned by variation in the length of the alkyl side chains and symmetry of the ions. We report here on a series of *N*-ethyl-*N*-methyl pyrrolidinium and *N*-methyl-*N*-octyl pyrrolidinium ILs bearing several symmetrical and asymmetrical fluorine containing anions. The cations were synthesized by reaction of *N*-methylpyrrolidine with 1-bromoethane or 1-bromooctane. The pyrrolidinium bromide salts were then converted to the ionic liquids via metathesis in water with the symmetrical or asymmetrical lithium or potassium salts of the fluorous anions. The structures of the ILs were confirmed using H-1 and C-13 Nuclear Magnetic Resonance (NMR) spectroscopy. The ILs will be characterized for their physical properties including conductivity, viscosity and thermal profile.

MARM 534

The effect of alkyl versus ether side chains on the physical properties of ionic liquids

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Ionic liquids (ILs) are low melting salts composed of cations and anions of dissimilar sizes that are selected to obtain desired properties. However, their high viscosities impede their adoption in many large scale processes. Ether side chains have been shown to lower the viscosity of ILs. In this project, we have synthesized a series of ten pyrrolidinium ionic liquids bearing ether and alkyl side chains of varying lengths (4 to 10 atoms in length), and 10 analogous imidazolium ionic liquids. Their physical properties, such as viscosity, conductivity and thermal profile were measured and compared. X-ray diffraction was also used to study the intermolecular interactions between the ions. Results reveal a dramatic decrease in viscosity with the substitution of alkoxy (ether) side chains for alkyl side chains on the pyrrolidinium cation. However, as the length of the ether chain increases there is negligible change in the viscosity (of about 50 cP). In contrast, a consistent increase in the viscosity was observed as the length of the alkyl side chain increases. These results provide significant insight on the choice of starting materials for researchers designing ILs for specific applications.

MARM 535

Microbiomes associated to plant roots in NYC soil

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The presence of microbes in the soil has important influences on both the environment and on human health. We are interested in characterizing the structure of the microbial community of the soil associated with roots of plants from three contrasting sites in New York City: 1- the Thain family forest at the New York Botanical Garden (NYBG) (pristine forest); 2- the marshes in Newton Creek (heavily contaminated soil) and 3- Central Park (a green space exposed to pollutants). To determine the diversity and composition of the soil community, we have extracted and amplified bacterial community DNA using primers specific to the 16S rRNA gene. The amplicons have been sequenced and analyzed. As a preliminary assessment of the possible implications for human health, we have characterized each microbiome by analyzing the distribution of antibiotic resistance genes. This is an exploratory hypothesis-generating project as it will generate data to address environmental and human health problems.

MARM 536

Ruthenium interactions with ethanol upon microwave irradiation

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Recently, microwave assisted preparation represents a major breakthrough in synthetic chemistry methodology. This method provides a rapid and homogenous heating of the entire sample and enhances reaction rates allowing the formation of uniform nucleation centers for nanoparticles. In addition, this method is energy efficient and environmentally friendly. In this study, we investigated the interactions of ruthenium chloride with anhydrous ethanol. Ethanol is often used as a solvent for nanoparticle synthesis. It was observed that either a green or blue complex forms depending on the concentration of the solution, and the temperature and duration of microwave irradiation. Mid-IR and UV-Vis Spectroscopy were used to analyze the ruthenium solutions.

MARM 537

Rapid analysis of organic micro-contaminants in complex environmental matrices using direct sample injection GC-MS

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Direct sample injection (DSI) represents a promising but under-utilized modification to traditional GC/MS that is specifically designed to facilitate the semi-quantitative analysis of messy samples with little to no cleanup. In DSI, milligram quantities of sample are placed in a disposable glass vial and heated in a programmed temperature vaporizing (PTV) injector. Solvent (if present) is vented through the split valve at moderate temperature. Next, volatile sample components are loaded onto the GC column – or directly into the MS – via rapid heating, while solids and nonvolatile components that may be present in the sample are retained in the sample vial. In doing so, DSI provides enhanced method detection limits commonly associated with large volume injection techniques, while also minimizing the need for sample pre-processing and cleanup. Thus, it is a powerful tool for screening studies and exploratory

investigations. This presentation summarizes efforts to develop and optimize a DSI GC/MS method for monitoring the photo-transformation of the pesticide trifluralin in aqueous suspension and and on solid surfaces. The influence of carrier/extraction solvent ID and temperature conditions are discussed, and overall method performance is compared to that obtained by traditional splitless injection. Accuracy and precision of the DSI method was found to be comparable to conventional GC-MS analysis, and the additional method sensitivity afforded by the method facilitated the identification of multiple photolysis products and a variety of co-incident organic micro-contaminants that were not targets of the study.

MARM 538

Evaluating the efficacy of source reduction strategies on fecal bacteria concentrations in Mill Neck Creek, NY

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Mill Neck Creek is a tidal estuary on the north shore of Long Island with a long-standing history of pathogen contamination. The creek is a major freshwater tributary to Oyster Bay andCold Spring Harbor, two culturally, ecologically, and economically important water bodies, which has prompted New York State to establish a total maximum daily load (TMDL) for pathogens in the system. The TMDL uses fecal indicator bacteria as surrogates for enteric pathogens believed to be entering the waterbody through improper or illegal sewage disposal, and subsequently diminishing its recreational and commercial value. It prompted multiple pollution reduction strategies, most notably a $13.2 million project to re-sewer houses near Mill Neck Creek's headwaters, which was completed in 2012. This study represents a first attempt to evaluate the impact of these source reduction efforts on pathogen levels in Mill Neck Creek. Combined geospatial and temporal analysis of fecal bacteria concentrations in the waterbody over the past fifteen years indicate that although major reduction strategies targeted the headwaters of Mill Neck Creek, bacterial concentrations in the waterbody continue to exhibit pronounced spatial dependence that is indicative of elevated and persistent pathogen loading from that region. However, parametric and nonparametric analysis indicate that creek-wide bacterial concentrations are decreasing with time, and are significantly lower ($p < 0.05$) after 2012, when major sewer infrastructure upgrades were completed. Current efforts are devoted towards apportioning levels of pathogen reduction between natural (e.g., reductions that may be attributable to flow, season, and tidal mixing) and anthropogenic forcing.

MARM 539

Developing a pollen supplement diet for honey bees

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Honey bees are essential pollinators in life. Together with other types of bees, they pollinate one third of the food we eat, contributing over $14 billion of pollination services to agriculture in the USA. But honey bees are dying in alarming numbers since 2006. Of the 2.6 million managed colonies in the USA, 30-45% die every year. The disappearance of honey bees is becoming unsustainable for commercial beekeepers and the impact on the USA economy could be disastrous. There are many different factors that point to the disappearance of honey bees, which include flowerless landscapes, monoculture farming, parasite-related diseases, and pesticides. It is believed that these factors lead to malnutrition, which weakens the

bee's immune system making them susceptible to diseases. Here we show preliminary biochemical results towards the development of a well-balanced pollen supplement diet for honey bees. This diet consists of proteins, carbohydrates, lipids, vitamins and minerals. The approach is based on the robustness of the process used to make corn syrup. We demonstrate the kinetics for the enzymatic digestion of starch in a mixture of ground grains using μ-amylase and glucoamylase. Our results indicate that glucoamylase alone can completely digest starch into glucose building blocks. This observation suggests that glucoamylase can be used to develop a pollen supplement for honey bees from a mixture of ground grains. This diet can be used to feed honey bees when pollen resources are scarce.

MARM 540

Horizontal transfer of rhomboid proteases of archea

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Rhomboid proteins are intramembrane serine proteases with either six or seven transmembrane domains that cut other proteins and release the products extracellularly. These proteases are present in all forms of life though their functions are quite diverse. They have very low sequence conservation and different functions across taxa, including: controling EGF receptor signaling in *Drosophila* and *Caenorhabditis elegans*, cleavage of adhesins in apicomplexan parasites, and regulation of mitochondrial morphology in yeast and multicellular eukaryotes. In terms of prokaryotes, *Streptomycetes* have a maximum of 5 rhomboid genes, while mycobacteria have only two, which may be involved in cellular signaling.

Using phylogenetic and genomic analysis, this study compares the structure and number of rhomboids in archea genomes. Furthermore, these genes are products of both vertical and horizontal transfer reiterating that idea that genes are commonly transferred, specifically amongst single celled organisms providing novel phenotypes.

MARM 541

Extract from *Plantago lanceolata* has an important mucolytic effect on the respiratory tract mucus

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Mucous is typically produced from cells found in mucous glands. The body's natural reaction to inflammation and infection is to increase mucus production and its viscosity, as in chronic bronchitis or in COPD (Chronic Obstructive Pulmonary Disease). From our viscosity experiments we determined that the use of a *Plantago Lanceolata* (PL) extract decreased mucus viscosity by 15% in our initial experiments w/o incubation. We consider this decrease in viscosity a reassuring validation of our hypothesis. We foresee that PL extract can be an effective treatment of acute and chronic bronchitis, COPD and alleviate symptoms of cystic fibrosis.

MARM 542

Exploration of DNA barcoding using 16S rRNA gene in invertebrates

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16S rRNA is a commonly used region in DNA barcoding to identify a particular bacterial species. Mitochondrial 16S rRNA gene is used often because it is a powerful tool for population genetics and phylogenetic studies. It is found in multiple copies and is a highly conserved region for identification of species. In our project, we decided to use several invertebrate samples that were collected from different locations in and around Queensborough Community College campus to test if the 16S rRNA gene model will work to cluster various invertebrate taxa. The DNA from these invertebrate samples was extracted using the Zymo-Spin^{TM} Genomic DNA kit. Barcoding region from these samples was amplified using specific primers for the 16S barcoding regions by using PCR. The PCR products were sequenced and the results were compared. Then the sequences from invertebrate samples were corroborated using BLAST. After identification of the species, phylogenetic tree was made from 16S rRNA gene sequences. Our results show that there is appropriate taxon clustering and phylogenetic resolution based on previously published data.

MARM 543

Identification of plankton species in the Hempstead harbor region

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The Coalition to Save Hempstead Harbor (CSHH) has been working in the development of a report card for Hempstead Harbor with the purpose of clearly communicating the health of the harbor to the general public. At the beginning of May 2015 there were reports of “sludge” and large pollen slicks mixed possibly with an algal bloom in the harbor. Water clarity suddenly came fore as a primary indicator of the health of the harbor, overshadowing the work that has been done with dissolved oxygen and bacteria. Samples were collected and tested for bacteria, but other tests needed to be done in order to definitively eliminate other forms of pollution.

The body of water has been monitored and measured for water temperature, salinity, dissolved oxygen (DO), pH, secchi depth, turbidity (in NTUs), nitrates, and ammonia. All parameters were consistent throughout the season except for turbidity. We hypothesized different phytoplankton might be responsible for the increase in turbidity.

This research project was done to better understand this phenomenon by looking at water samples collected from several stations and using DNA Barcoding to identify the plankton that may be causing a bloom. DNA was extracted from the water samples, and via PCR the *rbcL* gene was target for amplification and sequencing. Sequence analysis was done via DNA Subway and our results revealed *Bathycoccus prasinos* (Picoplankton), and to our surprise species like *Cucumis sativus* and *Cucumis melo* were most prevalent.

MARM 544

Long-term study of the factors impacting water quality at the Hempstead harbor

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The purpose of this research is to advance the public attention in keeping and repairing the local environment to its full environmental and economic potential. We worked together with The Coalition to Save Hempstead Harbor (CSHH) who had gathered data from 2005 – 2015. The scope of the water-monitoring program has expanded over the years. Chronic sewage spills from inadequate wastewater-treatment plants that were sited along Hempstead Harbor and the drastic cutbacks to Nassau County Department of Health's water-quality monitoring program were the stirring factors that led to this effort. For this project, six factors, Water Temperature, Air Temperature, Water pH, Dissolved Oxygen, Salinity were analyzed over an 11 year time period so that we can report some trends. Our analysis shows that Water temperature and air temperature stayed stable. Except for three stations the Water Salinity stayed the same. There seems to be a lot of change in the Dissolved Oxygen levels which correlates with changes in the Turbidity levels.

MARM 545

Exploration of DNA barcoding using the CO1 gene in invertebrates

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The mitochondrial CO1 gene has long been the standard locus for DNA barcoding of animals. Its mutation rate is fast enough to distinguish recently diverged species while its sequence remains highly conserved between closely-related species. Here, CO1 barcodes were amplified from a diverse array of 37 invertebrate species.

Samples were acquired and identified from several entomology research laboratories and the local environment around Queensborough Community College in Bayside, New York. DNA was extracted from these samples, and the barcoding region was amplified by PCR. The forward and reverse strands of the PCR products were then sequenced and aligned in order to build consensus sequences, and the correct identifications of the samples from the barcoding sequences were confirmed using BLAST. Using these CO1 barcoding sequences, a phylogenetic tree was constructed with software available from Cold Spring Harbor.

The efficacy of the CO1 gene as a universal invertebrate barcoding region was then examined by comparing the resulting phylogenetic tree to established phylogenetic relationships between the species involved in this study. CO1 data shows appropriate taxon clustering and phylogenetic resolution.

MARM 546

Isolation, identification, and characterization of microorganisms associated with sanitization stations

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In the fall of 2015, a study began at the Biological Sciences and Geology Department of Queensborough Community College to isolate, identify and characterize microorganisms associated with sanitization stations. The aim was to determine if some isolates are pathogenic. Samples were taken from the Administration, Library and Art buildings and streaked on Tryptic Soy Agar (TSA). Using TSA and the T-streak technique, bacterial colonies were isolated into pure cultures for physical and biochemical

testing. Preliminary results indicate that there was bacterial growth in all the sampled sanitization stations at the three locations. Gram staining results shows that all the isolates are Gram-positive bacteria, mainly Bacillus and Cocci forms. The Cocci isolates did grow on blood agar but did not show alpha- or beta-hemolysis. Further testing of the isolates is underway.

MARM 547

Antiphospholipid antibody and MiR106b mediated the expression of tissue factor in breast cancer cell lines

Irene Sun[1], *irenefsun@gmail.com, Elaine Lin*[2]*, Regina Sullivan*[1]*, Andrew V. Nguyen*[1]*. (1) Biological Sciences and Geology, Queensborough Community College, Bayside, New York, United States (2) Cell, Developmental & Cancer Biology , Oregon Health & Science University, Portland, Oregon, United States*

A link between coagulation and clinical outcome of patients with cancer has been well established. Tissue factor (TF), a transmembrane glycoprotein known originally as the initiator of blood coagulation cascade, has recently been demonstrated to modify cancer microenvironment and angiogenesis. We have recently shown that anti-phospholipid antibody (aPL) mediate breast cancer tumor progression in xenograft model by up regulation of TF. We have further demonstrated that aPL stimulates TF expression in less aggressive tumor cell line (MDA-MB-468) but not aggressive cell line (MDA-MD-231), which expressed endogenously high level of TF. In our examination of the mechanism by which aPL stimulation leading to TF up regulation, we have discovered that microRNAs (miRs) play a significant role. Using the two cells with different endogenous expression of TF, we showed that miR106b is highly expressed in MDA-MB-468 compared to MDA-MB-231. Treatment of MDA-MB-468 with miR106b inhibitor released the inhibition of TF expression suggesting that miR106b negatively regulate TF expression. Our preliminary data show that aPL modifies miR106b expression in MDA-MB-468.

MARM 548

Structural feature and modification of keratin fiber by carbonyl-containing compounds

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Styling methods such as perm-waving and or straightening are traditionally based on the use of chemicals to alter keratin fiber structure. Mechanistically, some of these methods are based on cleavage of the cystine disulfide covalent bonds that are present in keratin. Herein we describe a new approach using heat activation of a cyclic compound in a 5 or 6-membered ring, e.g., an alkylene carbonate. Thermal properties of keratin structure were also characterized by transient electro-thermal technique (TET). The results correlate well with measurements of spin diffusion by solid-state NMR and cryo-electron microscopy.

MARM 549

Peptidomimetic structure and function: Synthetic peptide macrocycles with potential as anti-thrombosis agents and short artificial peptide helices and turns

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Peptide structure and function are intrinsically linked and exquisitely exploited in studies of protein-protein interactions and pertinent in the development of novel first generation pharmaceuticals. We are currently creating inhibitors of the binding event between collagen and van Willebrand factor (vWF), which is implicated in the initiation of pathogenic thrombosis. Our cyclic peptidomimetics connect in a head-to-tail fashion, offering improved stability over disulfide-cyclized literature peptides known to compete with vWF for binding collagen. Using a competition ELISA, we have assessed the ability of our novel compounds for displacing vWF from collagen, to moderate success, and continue to improve our designs. Our cyclic peptides are tested in a stability assay, exposed to a panel of proteases in reducing conditions to determine their ability to withstand the cellular environment, as compared to the literature peptides and linear controls. These studies represent an example of first generation macrocyclic peptide-based pharmaceutical design. In independent work, we built off of our previously developed short alpha- and beta-peptide helical scaffolds and synthesized several peptides that use primary sequence to influence helical control. Using CD spectroscopy we analyzed which permutations improved helical character and melting characteristics and are using our beta-peptide scaffold to study a protein-protein interaction involved in cancer. Additionally, we have defined a new minimal epitope for beta-turn motifs, also examined using CD spectroscopy. Overall, our results from both major studies inform future peptidomimetic designs, especially in the development of short, structured peptides with biological function.

MARM 550

Exploring the proteolytic susceptibility of peptoid oligomers

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Peptoids are an important family of peptidomimetic oligomers with significant therapeutic potential. Peptoids are constituted from N-substituted glycine units joined through tertiary amide linkages that may deter binding within the active site of protease enzymes. Currently, peptoids are believed to be resistant to all major classes of proteases. In turn, the molecule can circumvent in vivo degradation, which may enhance their pharmacological potential. As investigators evaluate peptoids as drug molecules, further investigation of mechanisms for petoid metabolism will prove valuable. There are numerous endopeptidases, including collagenase, that specifically recognize proline residues in the active site and then catalyze hydrolysis of the adjacent amide bond. Proline shares a similar N-substituted side chain structure as peptoids. Therefore, it is possible that proteases capable of cleaving at proline positions could likewise degrade peptoid oligomers. To investigate this hypothesis, we have synthesized canonical peptide substrates to proline-specific proteases, along with their corresponding peptoid analogs. The susceptibility of these oligomers to enzyme-mediated hydrolytic cleavage can therefore be compared. These studies allow us to further assess the pharmacological attributes of peptoid molecules.

MARM 551

Phosphoproteomics of human immunodeficiency virus -1

***Manjeet Kaur**, manjeet.kaur1@yorkmail.cuny.edu. Chemistry, York College, Jamaica, New York, United States*

Novel strategies have been developed in the last few decades to counter the viral pathogenesis of HIV-1 in human T cells. My research focuses on post-translational modification of HIV proteins: TAT, REV and NEF and study their biological significance in HIV infection. The investigation requires identification and characterization of well conserved phosphorylated sites in these HIV proteins. This requires running CLUSTALW that provides amino acid sequences of HIV proteins from 12 different strains from which well conserved motifs in these proteins are extracted. Phosphorylation prediction tools such as NetPhosK, GPS and KinasePhos are used to predict potential phosphorylation sites in these proteins in order to predict the specific kinases responsible for bringing phosphorylation on specific sites. This is followed by running kinase assays on these HIV peptides which is analyzed by MALDI-MS. Several phosphorylation sites are found in these proteins and their biological significance in HIV mechanism is still need to study.

MARM 552

The role of calcium in the mechanism of N-methyl-4-phenylpyridirum (MPP+) toxicity toward dopaminergic cells

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Parkinson's disease (PD) is the second most common neurodegenerative disease behind Alzheimer's disease. PD is characterized by the irreversible degeneration of dopaminergic neurons in the substantia nigra, a region in the midbrain, causing symptoms of tremors, muscular rigidity, and bradykinesia. Increasing evidence suggests that environmental factors and toxins play roles in the etiology of PD. Although many specific examples of environmental factors associated with PD have been identified, the discovery of the specific dopaminergic toxicity of neurotoxin N-methyl-4-phenylpyridum (MPP^+) provided the greatest stimulus for PD research.

MPP^+ selectively destroys dopaminergic neurons and induces the symptoms of PD in humans and other primates. The proposal that specific uptake of MPP^+ through dopamine transporter (DAT) followed by mitochondrial complex I inhibition has been widely accepted as the cause of specific dopaminergic toxicity. Our preliminary studies using model dopaminergic MN9D and SH-SY5Y, non-dopaminergic PC12, and liver HepG2 cell lines show that DAT is not essential for the efficient cellular uptake or toxicity of MPP^+. While $MPP^+$is taken up into all four cell lines, it is highly toxic only to MN9D cells. MPP^+ uptake into MN9D is mediated by an unknown mechanism which is highly sensitive to extracellular calcium, but insensitive to extracellular sodium. These findings are inconsistent with the above proposal. Furthermore, we show that uptake of MPP^+ is effectively inhibited by unrelated pharmacological agents such as benzamil, verapamil, and mibefradil, although these inhibitors did not protect dopaminergic cells from MPP^+ toxicity. These and other findings suggest the toxicity mechanism of MPP^+ may be due to the perturbation of the calcium metabolism that results in dopaminergic cell death.

MARM 553

Toxicity of host-guest formulations of isozyme-selective carbonic anhydrase inhibitors

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Controlled drug delivery systems (DDSs) have progressed over the last six decades. The appropriate administration of drugs through various routes in the body is essential for achieving optimal spatial and temporal delivery of the drug in the organism and the efficient reach of diseased sites. The host-guest complexation of drug molecules with macrocycles, such as crown ethers, cyclodextrins, cucurbiturils and calixarenes, have gained increasing attention in the last two decades, with new generation drug delivery technologies being developed based on these complexes.

The purpose of the study was to generate and characterize novel host-guest complexes of pyridinium-sulfonamides as selective and efficient carbonic anhydrase inhibitors (CAIs). We will present recent results in the complexation of pyridinium sulfonamides with several classes of hosts mentioned above in a comparative manner, together with the toxicity induced by different hosts and by their complexes with the pyridinium sulfonamide guests in vitro, using 2D and 3D cellular models. We will correlate this toxicity of the host-guest complexes with the physicochemical properties of these nanocarriers for drawing structure-property relationships.

MARM 554

Optimization of 1,2,4-triazolopyridines as inhibitors of human 11β-hydroxysteroid dehydrogenase Type 1 (11β-HSD-1): Discovery of clinical candidate BMS-823778

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11β-hydroxysteroid dehydrogenase Type 1 (11β-HSD-1),also known as cortisone reductase is an NADPH-dependent enzyme which is highly expressed in key metabolic tissues that include adipose tissue, liver as well as the central nervous system. The biology, chemistry and toxicology of 1β-hydroxysteroid dehydrogenase Type 1will be discussed as well as the discovery by Bristol Myers Squibb of the clinical candidate BMS-823778.

Hotel-Subway- Metro Shuttle

Bus 1 - 7:00 AM - 9:00 AM

1. Executive Boulevard - **Shell Gas Station: 1 Enterprise Blvd, Yonkers, NY 10701**
2. Cross County/Hyatt - **South Entrance, Chipotle - 5510 Xavier Drive #5510, Yonkers, NY 10704**
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4. 242nd St Subway - **242nd St. Broadway, NY 10471**
5. CMSV - **6301 Riverdale, Bronx, NY 10471**

Bus 2 - 7:00 AM - 9:00 AM

1. 242nd St. Subway - **242nd St. Broadway, NY 10471**
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Only one shuttle is providing service on the loop 242nd St. Subway (242nd St. Broadway, NY 10471) and CMSV (6301 Riverdale, Bronx, NY 10471) on Friday and Saturday (June 10th and 11th).

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Bus 2 - 6:00 PM - 8:00 PM

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Bus - 9:00 PM - 10:00 PM

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8:45 AM – 11:00 AM – Villa, Sharp, HH, Founders – Every 30 Minutes

11:30 AM – 1:30 PM – Villa, Sharp, HH, Founders – Every 15 Minutes

1:30 PM – 4:30 PM – Villa, Sharp, HH, Founders – Every 30 Minutes

5:00 PM – 6:00 PM – Villa, Sharp, HH, Founders- Every 30 Minutes

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Planet Wings	5981 Broadway (718) 884-9464	Bronx, NY 10471
Beccofino Restaurants	5704 Mosholu Ave, (718) 432-2604	Bronx, NY 10471
Riverdale Pizza	5654 Riverdale Ave (718) 549-4750	Bronx, NY 10471
Riverdale Steak House	5700 Riverdale Ave (718) 549-9946	Bronx, NY 10471
Lee's Chinese Kitchen Inc	5979 Broadway (718) 543-3811	Bronx, NY 10471
Golden Phoenix Chinese Restaurant	5646 Riverdale Ave (914) 966-1801	Bronx, NY 10471
New China Restaurant	5690 Mosholu Ave (718) 543-7400	Bronx, NY 10471
Riverdale Pie Guys	5784 Mosholu Ave (718) 708-6130	Bronx, NY 10471
New Nagoya LTD	5786 Mosholu Ave (718) 432-8886	Bronx, NY 10471

New King's Wok Kitchen	6669 Broadway (914) 528-8222	Bronx, NY 10471
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Cornyn Coach'n Four Restaurant	602 S Broadway (914) 969-3070	Yonkers, NY 10705
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*** All Prices are a la carte unless otherwise noted

Hours of Operations

Breakfast to Lunch:
8:00 AM—2:00 PM
Dinner: 4:00 PM—6:00 PM

2mato

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