MoleCVUE Workshop on Computational Chemistry in the Undergraduate Curriculum

Coordinator: Carl Salter (salterc@moravian.edu)

Talk Title: "Introducing Molecular Models"

Presenters: Carl Salter, Jim Foresman, Will Polik, and Kevin Range

Schedule:

9:00 am:	"Introducing Molecular Models", Carl Salter
9:30 am:	"Exploring Chemistry with Electronic Structure Calculations", Jim Foresman
10:15 am:	"Using WebMO throughout the Chemistry Curriculum to Explore Molecular Shapes, Conformations, Energy Surfaces, Spectroscopy, Orbitals, and Symmetry", Will Polik
11:15 am:	"Computational Exercises in General Chemistry", Kevin Range
12:00 pm:	Lunch
1:00 pm:	Workshop: Develop activities using Gaussian and WebMO
4:00 pm:	Report out

Workshop description: WebMO is a web-based interface to modern computational chemistry programs (Gamess, Gaussian, Molpro, Mopac, NWChem, PQS, PSI, Quantum Espresso, VASP, Q-Chem, Tinker). Using just a web-browser, users can draw 3-D structures, run calculations, and view results. WebMO is simple enough for novice users (reasonable defaults are provided, and result are presented graphically) but flexible enough for experts (full access to input and output files is provided, and job types can be customized).

Workshop topics will include:

* Overview of WebMO features and capabilities
* Drawing molecules using the WebMO Editor
* Running various job types
* Visualization of results using the WebMO Viewer
* Importing and exporting structures and jobs
* Customization WebMO job types
* Using WebMO on Apple and Android portable devices
* Installation and administration of a WebMO server

This is a hands-on workshop suitable for high-school and college faculty. Participants are encouraged to bring their own Windows, Mac, or Linux laptop or Apple iPad. In addition to workshop activities, a WebMO developer will be available for questions and individual consultation.

Time: Monday, June 5 from 9 am-5 pm

Room: Tower 1

Notes: This room fits 40 banquet style. There are other MoleCVUE talks and activities that are part of the technical session on Sunday afternoon and Tuesday morning.