Computational Chemistry Workshops

Hosted by
Dr. Desiree M. Bates
Computational Chemistry Leader

September 13, 2011:

- *Accessing Phoenix*
- *Basic shell commands*
- *Text editor (VI)*
- *Gaussview and Maestro*
- *Computational software packages and Visualization Software @ UW*

September 20, 2011:

- *What is a potential energy surface?*
- *Geometry optimizations*
- *Calculating Harmonic Vibrational Frequencies*
- *Energy Points*

October 4, 2011:

- *Reaction Pathways*

October 18, 2011:

- *Calculating Thermodynamic Quantities*

November 1, 2011:

- *Convergent Quantum Mechanical Methods*
- *What is Density Functional Theory?*
- *Basis Sets*

November 15, 2011:

- *What is Molecular Modeling?*
- *Glide: docking calculation with Schrodinger Software Suite*

Room 1381 at 2:00 pm
Prior to meeting please have an active phoenix account
To get one, email clusteradmin@chem.wisc.edu