

# CHEM 8840B: Computational Chemistry

## Class Project Guidelines

The class project is your chance to gain practical experience with the tools of computational chemistry. If possible, you are encouraged to select a project related to your research interests, since this will give you more direct experience with how computational chemistry methods can assist your own work. However, if you are studying something like the denaturation of DNA, this is probably not feasible...

*Please prepare a class project proposal to turn in one week from today. I will review the proposed projects (which can be fine-tuned later) to make sure they sound feasible.*

*Your project should use methods of computational chemistry to help answer a chemically interesting question.*

You may opt to use any of the computational chemistry methods discussed in class, including molecular mechanics (force field) methods, semiempirical methods, and *ab initio* electronic structure methods. As a rough guideline, *ab initio* methods should be reserved for systems with about 20 atoms or fewer, while semiempirical and molecular mechanics methods might be feasible for systems of up to a few dozen atoms. The molecular mechanics and semiempirical methods are available in HyperChem, while Q-Chem will be used for the *ab initio* computations (either via the HyperChem graphical interface on the PC's, or via the text interface on the IBM SP2, your choice).

Some suggestions for possible projects are given below:

1. Structures and relative energies of different conformations of a molecule.
2. Energetics of a reaction (reaction enthalpy and activation barriers: energies of reactants, products, and transition states).
3. Thermodynamic properties of a molecule (including heat of formation).
4. Absorption and/or emission spectra of a molecule.
5. Charge density of a molecule and its implications for reactions governed by electrostatic effects.
6. Substituent effects on structures and/or energetics.
7. Vibrational frequency predictions to explain spectra.
8. Rotational constant predictions to explain spectra.
9. Candidate molecules for unusual bonding, etc.