

Computational Project and Paper Presentations

1. **Computational Project.** Choose from:

- **Gaussian electronic structure project.** Carry out several new calculations on a system of interest to your research, and submit a written summary of your findings. The study can take any of several forms, including
 - (a) comparing the geometries, isomerization energies, equilibrium constant, or other molecular properties predicted using different methods and basis sets to experimental values; *or*
 - (b) calculating the reaction diagram for a simple reaction of interest, and estimating the rate constant; *or*
 - (c) predicting a full spectroscopic work-up (NMR, IR, UV/vis) using various methods for comparison to experiment.

Other possibilities are available.

- **Variational or Perturbation Theory project.** Choose a 1-D or 2-D potential energy function – for example, a Lennard-Jones, or double-well system – and predict the energies and wavefunctions using the variational method or perturbation theory. use of a symbolic math program such as MAPLE is encouraged.

Biochemists: we may have to limit your molecule of interest to a small reactive site or enzyme cofactor so that the structure is still amenable to a quantum mechanical treatment.

Write a brief, draft proposal for your project, summarizing what you would like to study. You do not need to provide detail as to the methods – I will expect that it will be up to me to recommend an approach, and to help limit the scope of the project so that it is workable. E-mail your draft proposal to me by 5pm Friday, Mar 12. I will respond within a few days, so that by 5pm on Friday Mar 19 you can email me a project proposal that we both agree on. We may agree at any later time to expand or reduce the scope of the project, as your work progresses.

You should be working on your project no later than April 1.

2. **Paper presentation.** Chem 713 students will also present a roughly 20-minute lecture to the class, based primarily on one or two papers. Each presentation will be critiqued by students and the instructor, and comments will be consolidated by the instructor. Students are graded based on both their presentation and on their participation in the evaluations of their classmates. You should email me your topic, relevant reference(s), and preferred presentation date as soon as possible, and we should have the assignments finalized no later than Fri Mar 26.