CHE 525/PHY 567 Final Project

For this project, you will choose a paper related to computational quantum chemistry from the literature, read it carefully, write a short review of it, perform some calculations related to the results of the paper, and write a report of your findings. You could choose a paper discussing the application of theory to a particular problem, one that includes both theoretical and experimental data, one presenting a new theoretical method, or even a completely experimental paper for which you think that theory could have helped solve the problem. You may not choose a paper on which you are an author, however, the paper may be related to your research. Some good journals to search for relevant papers would be:

- Journal of Physical Chemistry (A, B, C, or Letters)
- Journal of Chemical Physics
- Physical Chemistry Chemical Physics
- Journal of Chemical Theory and Computation
- Journal of Computational Chemistry

There will be several phases of the project, due on different days:

Phase 1. Select a paper and submit it to the instructors for approval.

Phase 2. Write a short (1-2 page) review of the paper. This review should include:

- a very brief summary of what the main results of the paper are,
- a very brief description of why the results are (or are not) interesting and important,
- an assessment of how well the data supports the results,
- and several specific suggestions of additional calculations that could be done to improve the paper, with an explanation of why these additional calculations would be valuable.

Phase 3. Perform the calculations that you proposed in Phase 2 and present the results in a brief report. Your report should include an introduction which motivates the work, a method section describing what you did so that someone could reproduce your results, a results section including text, figures, and tables demonstrating your findings, discussion of the significance of the results, and a conclusion which briefly states the most important outcomes of the work.