The purpose of the class project is to give you a chance to creatively apply the knowledge you have gained in the course of the semester about first-principles modeling of chemical systems to a short research problem of your own choosing. I hope it is something you can have fun in selecting and carrying out. The research problem could be of several types:

- A particular chemical problem that you would like to investigate, perhaps related to your own research interests or research project.
- A particular computational issue you would like to explore, such as the relative performance of some methods (basis sets, core potentials, ...) or algorithms for a particular type of calculation.
- A particular theoretical issue you would like to address, perhaps elaborating on a topic that we didnt have time to develop in class (e.g., solvation effects, excited states, relativity, ...).

The project has three requirements:

1. **Due March 16, 2015 (10%).** Provide in pdf, via email to Prof. Schneider, a brief (< 1 page) description of your proposed class project. Include (1) background about the problem area, including any relevant references, (2) the specific research question you propose to address, and (3) the computational plan for answering the research question. You may discuss this with Prof. Schneider or the TA before the due-date. You will receive feedback and suggestions shortly after you turn in the proposal.
2. **Due April 7, 2015 (10%).** Provide in pdf, via email to Prof. Schneider, a brief (≤ 2 page) summary of preliminary computational results, in particular highlighting any difficulties you have encountered.
3. **Due April 28, 2015 (80%).** Your pdf report will include an approximately six-page write-up of your project and results. The scientific and intellectual completeness is more important than any particular length. Include:

   (a) (5 pts) Cover page with title and name
   (b) (15 pts) Introduction to the problem area and specific question you are addressing,
   (c) (10 pts) Computational methods applied (software, methods, basis sets, etc.),
   (d) (20 pts) Results of your project, including narrative, Tables and Figures, as appropriate,
   (e) (15 pts) Discussion of the outcomes and their implications for the question you posed,
   (f) (5 pts) Conclusions summarizing outcomes and suggested future work.
   (g) (5 pts) References cited
   (h) (5 pts) Appendix including input files from your calculations as well as any other details that might be helpful in understanding the work.

   You will be graded on the appropriateness of your question, the thoughtfulness and execution of the approach, and the quality and thoroughness of the report of the results.

Sample projects from years past:

1. United Atom Force Field for Polyacetylene using Ab Initio Calculations and Thermal Conductivity of Single Chain Polyacetylene
2. Computational Measurement of Isothermal Compressibility for Simple Salts
3. Examination of the Conformations of Acetylcholine and its Agonists
4. Hydrogen Bond in Ionic Liquid, Carbon Dioxide and Water System
5. Ab Initio Catalyst Comparison for Ethylbenzene Synthesis from Alkylation
6. GGA Calculation of Strain Effects on $SrTiO_3$ BandStructure
7. Ethane Radical Reaction: A Comparison of Methyl Radical Termination and Hydrogen Abstraction
8. Computational Modeling of Uranyl and Neptunyl Structures
9. Computational Studies on some Ansa-Zirconocene Compounds
10. Binding of CO upon a Pt(111) Surface
11. Computational Method Comparison for Quadruple Bonded Metal Complexes
12. Amino Acid Zwitterions: An Investigation into the Modern Computational Methods of Solvation

