Chemistry 8021 **Computational Chemistry** 4 Credits
Spring Semester 2014

Guidelines for Final Critical Analysis of a Paper (8021 Requirement Only)

1. The paper should be chosen from the literature. Work dated 2008 or beyond is preferable, but earlier papers will be considered on a case by case basis. You are not merely allowed, but you are *encouraged* to pick a paper germane to your own research interests. Simultaneous presentation of experimental results is fine, however more than 50% of the paper should be devoted to computation/theory.

2. The chosen paper must be approved by me; provide a copy either in person or by email (pdf).

3. **The deadline for choosing a paper is Friday, April 18.**

4. The form of your analysis should be 4-8 pages in length including references, figures, etc. (18-point-spacing, 12 point Times font, one inch margins). I've got to read *lots* of these (in addition to all the final exams), and I will appreciate conciseness *enormously* by about halfway through.

You should address the following areas at a minimum:

a. What are the objectives of the study?

b. What are the most significant conclusions drawn from the study?

c. How does the employed level of theory impact on the research? Were there issues which could not be adequately addressed? Are the conclusions dependent on assumptions implicit to the theory?

d. What comparisons are made to experiment, if any? What is the overall trustworthiness of the paper in your opinion?

e. How could you improve on the current results? [*Don't* assume you have infinite computational resources! Put yourself in the authors' place and try to design either improvements or extensions of their work that could reasonably be carried out.]

5. If you have time and inclination, you are free to use your class accounts to do calculations of your own relevant to the subject of your paper. However, you might wish to discuss these calculations with me if you are in any doubt as to how much time they might take.

6. Your analysis will be due by no later than the final exam, i.e., May 15th at 1:30 PM. **Please email an electronic version as a pdf file to me at cramer@umn.edu.**

7. Grading will be based on clarity and style of the writing (30 points), depth and accuracy of the scientific analysis (40 points), and the degree to which the chosen paper was particularly challenging and/or analyzed with a high degree of creativity and initiative (30 points).