CHE 344: Special Topics (Computational Chemistry)
Fall 2010
Lecture: Thursday 10:30-11:20, NHS 106B (the fishbowl)
Course website: homepages.gac.edu/~smiller3/courses/344-s10.htm

Instructors

Dr. Steve Miller

    Office: NHS 107B

    Office Hours: Thursday 11:30-12:30

              Thursday 1:30-2:30

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Dr. Amanda Nienow

    Office: NHS 106C

    Office Hours: Tuesday 10:30-11:30

              Thursday 9:00-10:00

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Catalogue Description

This course will examine modern computational chemistry methods and software. Topics will include an introduction to quantum mechanics, semiempirical methods, the Hartree-Fock self-consistent field (HF/SCF) formalism, basis sets, density functional theory, post-HF methods, and common calculation types. The course will also involve more advanced use of computational software (especially Gaussian 03). Students will be expected to carry out calculations, compare their results to values reported in the literature, and report their findings to the class as a whole.

Course Goals

1) Understanding the basic theory and utility of several calculation types, methods, and basis sets
2) Properly calculating and interpreting various molecular properties

Required Materials

None—Information will be made available in class, on the course website, and/or in the library as needed; students will be expected to conduct literature searches for additional materials.

Attendance

This course only meets for one hour per week, so it is important that you attend each meeting; attendance will be required and will be factored into your course grade via the participation component.

Grading

Course grades will be assigned based on four components:

Assignments	40%
Participation	10%
Final presentation	20%
Final paper	30%

Final grades will be assigned roughly according to the following scheme:

     A   85%
     B   75%
     C   60%
     D   55%
     F   <55%

These cutoffs may be adjusted at the end of the semester, but will not be raised (i.e. an 86% will always be an A or A-).

Assignments

Assignments will vary somewhat from week to week, but in general will be some combination of
    -performing one or more calculations
    -finding results previously reported in the literature
    -more traditional, paper-based homework

Participation

The participation component of your grade will be based on a combination of participating in classroom discussions and presenting results obtained for assignments to the rest of the class. The final presentation will not count towards your participation grade.

Final presentation and paper

You will be asked to investigate an interesting system of your choosing using appropriate computational methods. You will then present your findings to the class and compare them to any existing previously reported results (presentations will take place during finals week). You will also be expected to submit a written report of your project.

Additional Resources

Disability Services: Any student who has a physical, psychiatric/emotional, medical, learning, or attentional disability that may have an effect on the his/her ability to complete assigned course work should contact the Disability Services Coordinator (Laurie Bickett, lbickett@gustavus.edu or x6286) in the Advising Center, who will review the concerns and decide with the student what accommodations are necessary.

Help for students whose first language is not English: The Writing Center has a part-time tutor with professional training in ESL/ELL instruction on staff. Students can schedule work with this tutor by contacting the Writing Center. Students may bring their instructors documentation concerning their ELL status.