

Computational Chemistry

University of Missouri at Columbia - Chemistry 8330 - Fall Semester 2016

SYLLABUS

Professor: Dr. Rainer Glaser

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First Lecture: Monday, Aug 22, 2016, 11 am, A&S 303

Office Hours: W 1-2 pm, and by appointment

Course Web Site: http://faculty.missouri.edu/~glaserr/RG_T_FS16.html

Course Objectives: Applications of electronic structure theory have become a standard and powerful tool in chemistry research. It is the goal of this course to teach students the abilities to

- develop clear conceptual ideas and quantitative knowledge about methods of electronic structure theory,
- access research computing facilities and execute electronic structure computations with knowledge about input and output,
- read the contemporary research literature with an understanding of applications of electronic structure theory,
- identify a problem in their current research that is amenable to study with electronic structure theory,
- write a proposal on the application of electronic structure theory on a problem specific to the student's doctoral research,
- understand the culture of the field of computational chemistry and judge your own work and the work by others in that context.

Course Materials: Some of the content of this course is taken directly from the primary and secondary literature. You will be given reading lists for the various chapters containing the references to the literature discussed in this course. You will also be given a list of pertinent books on the various areas of computational chemistry. Consult them for details, references, and later on in your own research.

- (1) **REQUIRED.** Foresman, J. B.; Frisch, A. *Exploring Chemistry with Electronic Structure Methods*, 3rd edition, **2015**. Regular Price: \$45. Student price: \$35 (with shipping included in the USA and continental North America). <http://www.gaussian.com/g_prod/books.htm>
- (2) **RECOMMENDED.** Foresman, J. B.; Frisch, A. *Gaussian 09 User's Reference and I/Os Reference*, **2015**. Regular Price: \$65. <http://www.gaussian.com/g_prod/books.htm>
- (3) **REFERENCE.** Hehre, W. J.; Radom, L.; Schleyer, P. v. R.; Pople, J. *AB INITIO Molecular Orbital Theory*. Wiley-Interscience, **1986**.
- (4) **REFERENCE.** Cramer, C. J. *Essentials of Computational Chemistry: Theories and Models*. 2/e. Wiley, **2004**.

Assignments & Grading

There are no tests and no final. Assignments will be made weekly (beginning in the second week), usually on Wednesday, and the assignments need to be submitted in electronic form (for record keeping) and in printed form (for peer review) at the beginning of lecture usually on the following Wednesday. Writing assignments must be completed with MS Office Software and require other software available on Department of Chemistry computers and/or access to online materials available through Ellis Library. One of the Computer Rooms in the Department of Chemistry (South-East side, Schlundt Hall 101) has been reserved for CHEM 8330 for Fridays, 11 am - 1 pm throughout FS16. Most of the Friday meetings will take place in the Chemistry Computer Room (as posted in the online schedule and announced in class).

Assignments 1 - 8 may be the result of collaboration by pairs of students while Assignments 9 and 10 need to be performed individually. The collaboration applies to the assignments as well as the peer review of assignments (except for the peer review of the oral presentations). If you collaborate, then there will be one joint submission by each student pair and both students receive the same score for the assignment. All assignments will be evaluated by anonymous peer review in various forms. The peer review process will be implemented by the instructor and by undergraduate peer learning assistants. PLAs will be recruited from the enrolled undergraduate students and they can earn honors credit (learning-by-contract).

The peer review of the original submission results in a peer review score (PRSO) of up to 20 per assignment. Revision may be required depending on the PRSO.

If PRSO \geq 19: Your submission of assignment A% is accepted as is; no revision needed. :}

If $19 > \text{PRSO} \geq 15$: This will happen most usually. Read the peer review comments carefully, revise considering the reviewer comments, and submit the revision in electronic form by midnight of the day you received the peer review. Make your changes with TRACKING ON. I will look over the revision and you will have completed the assignment once I have a satisfactory revision on file (and no more peer review will be performed).

If PRSO < 15: This should happen rarely. Read the comments carefully, revise considering the reviewer comments, and submit the revision in electronic form before midnight at the end of the day of the next class meeting (i.e., usually Monday of the following week). Make your changes with TRACKING ON and, in addition, write in your email to me what changes were made and explain how these changes address the comments by the peer reviewers. I will look over the revision carefully. Your revision will be accepted once it scores above 15 points.

You will be provided periodically with class performance measures (i.e., average, standard deviation, minimum and maximum scores) to assess your relative performance. Letter grades will be assigned at the end of the course based on your average performance; Assignments 1 – 8 and 10 (20 each) and with Assignment 9 counting double (40). If you complete all assignments (that is, all assignments have been accepted), depending on the average original peer review score $\langle \text{PRSO} \rangle = \text{sum of all your scores} / 11$, you will earn a grade of “A” if $\langle \text{PRSO} \rangle \geq 19$, “A-” if $\langle \text{PRSO} \rangle \geq 18$, “B+” if $\langle \text{PRSO} \rangle \geq 17$, “B” if $\langle \text{PRSO} \rangle \geq 16$, “B-” if $\langle \text{PRSO} \rangle \geq 15$, and so on. You can improve your assignments in the revision process, but the preparation of high quality original submissions matters for your scores.

In addition, students can improve their grades by provision of exemplary work (which will be posted as sample with your approval, eight opportunities) and by delivery of an outstanding oral presentation (top three presentations) and/or submission of an outstanding final paper (top three papers). Each special recognition improves the grade by one notch. For example, a student with an average original peer review score of 17.5 and one assignment posted as sample will receive an “A-”.

Attendance

Attendance is a requirement in this course, and only one unexcused absence is tolerated. If you miss a class for a legitimate reason (sickness, conference, interview, *etc.*), please provide some form of acceptable written proof (in electronic form if possible). Every unexcused absence will reduce your grade by one notch. Since most assignments are produced by pairs of students, it hardly ever happens that an assignment is missed. However, if you know in advance that you or your group will not be able to complete an assignment for a valid reason, talk to the instructor at the time the assignment is made.

Academic Integrity: Academic integrity is fundamental to the activities and principles of a university. All members of the academic community must be confident that each person's work has been responsibly and honorably acquired, developed, and presented. Any effort to gain an advantage not given to all students is dishonest whether or not the effort is successful. The academic community regards breaches of the academic integrity rules as extremely serious matters. Sanctions for such a breach may include academic sanctions from the instructor, including failing the course for any violation, to disciplinary sanctions ranging from probation to expulsion. When in doubt about plagiarism, paraphrasing, quoting, collaboration, or any other form of cheating, consult the course instructor.

Students with Disabilities: If you anticipate barriers related to the format or requirements of this course, if you have emergency medical information to share with me, or if you need to make arrangements in case the building must be evacuated, please let me know as soon as possible.

If disability related accommodations are necessary (for example, a note taker, extended time on exams, captioning), please register with the Disability Center, S5 Memorial Union (573-882-4696, <http://disabilitycenter.missouri.edu>), and then notify me of your eligibility for reasonable accommodations. For other MU resources for persons with disabilities, click on “Disability Resources” on the MU homepage.

Intellectual Pluralism: The University community welcomes intellectual diversity and respects student rights. Students who have questions or concerns regarding the atmosphere in this class (including respect for diverse opinions) may contact the Departmental Chair or Divisional Director, the Director of the Office of Students Rights and Responsibilities (<http://osrr.missouri.edu/>) or the MU Equity Office (equity@missouri.edu; <http://equity.missouri.edu/>). All students will have the opportunity to submit an anonymous evaluation of the instructor(s) at the end of the course.

Academic Inquiry, Course Discussion and Privacy - Faculty not allowing recording: University of Missouri System Executive Order No. 38 lays out principles regarding the sanctity of classroom discussions at the university. The policy is described fully in Section 200.015 of the Collected Rules and Regulations. In this class, students may not make audio or video recordings of course activity, except students permitted to record as an accommodation under Section 240.040 of the Collected Rules. All other students who record and/or distribute audio or video recordings of class activity are subject to discipline in accordance with provisions of Section 200.020 of the Collected Rules and Regulations of the University of Missouri pertaining to student conduct matters.

Those students who are permitted to record are not permitted to redistribute audio or video recordings of statements or comments from the course to individuals who are not students in the course without the express permission of the faculty member and of any students who are recorded. Students found to have violated this policy are subject to discipline in accordance with provisions of Section 200.020 of the Collected Rules and Regulations of the University of Missouri pertaining to student conduct matters.