University at Buffalo
The State University of New York

CHE 512, Spring 2019: Computational Chemistry and Electronic Structure

Syllabus Revision 2. Last updated: January 23, 2019

Time and Location: Tue/Thu 09:30 – 10:50, Talbert 106, North Campus

Instructor: Prof. Jochen Autschbach
Instructor email: jochena@buffalo.edu, Phone: 645-4122
Instructor's Office Hours: Wed 3:00 – 4:00 pm, NSC 313, or by appointment
Faculty mailboxes are located inside the Chemistry Department's main office, NSC 359

Important dates (please confirm with the official UB academic calendar):
Beginning of classes: Monday, Jan 28
Spring Break: Mon, Mar 18 to Sat, Mar 23
End of classes: Friday, May 10
There is no final exam

Course web site: UBLearns, `https://ublearns.buffalo.edu`. The course web site contains down-loadable (PDF) versions of the syllabus, homework, additional course information, and announcements regarding the course. The instructor uses UBLearns to contact students by email. Make sure that your email address in UB's computer systems is up to date, and check your email periodically.

Learning Outcomes

The students will acquire knowledge about various electronic structure methods, molecular orbital theory, molecule-field interactions and time-dependent phenomena, and basic practical skills in computational chemistry. The latter will be assessed via homework scores. For the homework, some computations will be carried out at UB's CCR. Knowledge in all topics will be assessed by the exam scores.

Textbook:

There is no required textbook. Reading material will be provided to the registered students as handouts.

Optional textbooks and other resources: See the *Library resources guide* posted at UBLearns. There are, in particular, several sources listed with problems and worked-out solutions for self-study.

Course Content:

Molecular orbital theory, the nature of the chemical bond, Hartree Fock method, electron correlation, molecule-field interactions, dynamic response & linear and nonlinear optical and spectroscopic properties.

Exams, Assignments, Grades, Policies

The course's grade will be based on two graded homework assignments, and two mid term exams. Grade details: Two homework sets counting 20% each toward the final grade Two mid-term exams counting 30% each toward the total grade. The final weighted percent scores (100% max.) will be rounded to the nearest integer and then converted into letter grades as follows (the ranges are inclusive): 0 – 45 = F, 46 – 50 = D, 51 – 55 = D+, 56 – 60 = C-, 61 – 65 = C, 66 – 70 = C+, 71 – 75 = B-, 76 – 80 = B, 81 – 85 = B+, 86 – 90 = A-, 91 – 100 = A.

There is no 'extra credit' available; no exceptions. Regarding incomplete grades, see `http://undergrad-catalog.buffalo.edu/policies/grading/explanation.shtml#incomplete`

You are welcome to use a Computer Algebra System (CAS) such as Wolfram Alpha, Mathematica, or Maple for your homework, as long as you include printouts of the CAS sessions to show your work. Also, variable names need to be explained, the steps need to be annotated if necessary, figures need to be labeled properly, etc. The instructor will not try to decipher incomprehensible CAS code or guess what a plot is showing. The instructor often uses Mathematica for calculating some of the answers to homework problems for a course. UB has a campus license for several CASs. You can access those, and other software, via UB's Virtual Computing Lab. Instructions: `http://www.buffalo.edu/ubit/service-guides/software/my-virtual-computing-lab.html`

Completed homework is due by the end of the lecture on the due-date listed on the assignment (usually one week after the homework was handed out). Late homework: 25% deduction off the total score per periods of 48 hrs late, starting at the end of class on the due-day. Homework will be handed out in class. It usually gets posted at UBLearns on the same day. However, if you miss the class and the instructor does not post the homework on-line for technical or other reasons, this is not an excuse for failing to hand in your homework. Attend all lectures.

Homework extensions without penalty, and requests for make-up tests, require *documentation* of a family or medical emergency or a similarly acceptable excuse.

Academic integrity as defined in UB's official guidelines is strictly enforced. Make sure you know what is meant by 'academic integrity' according to the guidelines posted at `http://undergrad-catalog.buffalo.edu/policies/course/integrity.shtml`

Students with special needs: Please inform me of any special needs and register with UB's Accessibility Resources as soon as possible. Go to
`http://www.student-affairs.buffalo.edu/ods/` for further details.