Class Syllabus  
Spring 2020  
CHE 541/471  
Computational Chemistry

Name: Dr. Brian Barngrover  
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Office: M-124  
Student Hours: W 11:00 am – noon, W 3:00 – 4:00 pm, MT 1:30 – 3:00 pm; other times by appointment

Text and Materials:
Non-programmable calculator with scientific notation.

COURSE CALENDAR:
Material will be covered in the following section order with approximate class time.  
Introduction to Theory, Computation, and Modeling (1 week)  
Molecular Mechanics (2 weeks)  
Molecular Orbital Theory (2 weeks)  
Semiempirical Implementations (1 week)  
Ab Initio Implementations (2 weeks)  
Electron Correlation (2 weeks)  
DFT (2 weeks)  
Spectroscopic Properties (1 week)  
Condensed Phase (1 week)  
Simulations of Molecular Ensembles and Thermodynamic Properties (1.5 weeks)

GRADING POLICY:
Calculations (25%): I will assign computational sets throughout the semester. You must submit work on the cluster to receive credit.  
Exams (75%): We will have two exams throughout the semester. The exams will occur the weeks of: March 2nd and May 4th. The first two will be given in the evening. The last exam will occur during the scheduled finals exam time.

Grading scale - A= 90 - 100%; B= 80 - 89%; C= 70 - 79%; D= 60 - 69%; F= below 60%

ATTENDANCE POLICY:  
Attendance of class is mandatory. A total of four unexcused absences will result in the student being dropped from the class with a grade of "F". There will be no make-up exams.

ACADEMIC INTEGRITY (A-9.1):  
Academic integrity is a responsibility of all university faculty and students. Faculty members promote academic integrity in multiple ways including instruction on the components of academic honesty, as well as abiding by university policy on penalties for cheating and plagiarism.  
Definition of Academic Dishonesty  
Academic dishonesty includes both cheating and plagiarism. Cheating includes but is not limited to (1) using or attempting to use unauthorized materials to aid in achieving a better grade on a
component of a class; (2) the falsification or invention of any information, including citations, on an assigned exercise; and/or (3) helping or attempting to help another in an act of cheating or plagiarism. Plagiarism is presenting the words or ideas of another person as if they were your own. Examples of plagiarism are (1) submitting an assignment as if it were one's own work when, in fact, it is at least partly the work of another; (2) submitting a work that has been purchased or otherwise obtained from an Internet source or another source; and (3) incorporating the words or ideas of an author into one's paper without giving the author due credit.

Please read the complete policy at http://www.sfasu.edu/policies/4.1-student-academic-dishonesty.pdf.

Any student found cheating will be subject to the penalties as stated in the Student Code of Conduct handbook; including but not limited to a score of zero on exam, expulsion from the class or expulsion from the University.

**WITHHELD GRADES SEMESTER GRADES POLICY (A-54):**
Ordinarily, at the discretion of the instructor of record and with the approval of the academic chair/director, a grade of WH will be assigned only if the student cannot complete the course work because of unavoidable circumstances. Students must complete the work within one calendar year from the end of the semester in which they receive a WH, or the grade automatically becomes an F. If students register for the same course in future terms the WH will automatically become an F and will be counted as a repeated course for the purpose of computing the grade point average.

The circumstances precipitating the request must have occurred after the last day in which a student could withdraw from a course. Students requesting a WH must be passing the course with a minimum projected grade of C.

**STUDENTS WITH DISABILITIES:**
To obtain disability related accommodations, alternate formats and/or auxiliary aids, students with disabilities must contact the Office of Disability Services (ODS), Human Services Building, and Room 325, 468-3004 / 468-1004 (TDD) as early as possible in the semester. Once verified, ODS will notify the course instructor and outline the accommodation and/or auxiliary aids to be provided. Failure to request services in a timely manner may delay your accommodations. For additional information, go to http://www.sfasu.edu/disabilityservices/.

**CLASSROOM BEHAVIOR POLICY:**
To ensure a classroom environment conducive to learning, any forms of classroom disruptions will not be tolerated (examples but not limited to – talking, use of cell phones/beepers, sleeping, reading other material, eating/drinking). Students who violate these rules will be asked to leave. Repeat offenders will be subject to disciplinary action in accordance with University policies as described in the Code of Student Conduct. http://www.sfasu.edu/policies/student-code-of-conduct-10.4.pdf

**SEMESTER WITHDRAWALS:**
Last day to withdraw from the course without obtaining WP or WF grade is March 18th.