Computational Chemistry CHEM 5352
Physical & Environmental Sciences
Spring 2019

A. COURSE INFORMATION
Course number/section: CHEM 5352.001
Class meeting time: Lecture MWF 9:00 – 9:50 a.m
Class location: Lecture CS 108
Course Website: https://bb9.tamucc.edu/

B. INSTRUCTOR INFORMATION
Instructor: Tim Causgrove
Office location: CS 202
Office hours: W & F 11: 00 – 12:00 noon, M 3:00 – 4:00 p.m., W 1:00 – 3:00 p.m.
Telephone: 361-825-2399
e-mail: tim.causgrove@tamucc.edu
Appointments: arrange by e-mail to address above

C. COURSE DESCRIPTION
Catalog Course Description
The course will include the investigation of the uses and outcomes of computational chemistry, including both classical (non-quantum) simulations of molecular systems and quantum mechanical modeling of molecules. Emphasis will be on constructing an appropriate molecular model, performing the appropriate calculation, and interpreting the results of the calculation. Offered on sufficient demand.

Extended Course Description
Computational chemistry, both in the form of molecular dynamics simulations and quantum chemistry, is increasing in importance for predicting chemical behavior. This course will introduce students to both computational methods, the choices necessary for modeling a system, and methods of analyzing the results of simulations. Students will use a computational chemistry program to apply concepts learned to a system of their choice.

D. PREREQUISITES AND COREQUISITES
Prerequisites
CHEM 1412; MATH 2413; PHYS 1402 or PHYS 2426
Corequisites
None

E. REQUIRED TEXTBOOK(S), READINGS AND SUPPLIES
Required Textbook(s)
None

Optional Textbook(s) or Other References
None

Supplies
Scientific calculator

F. STUDENT LEARNING OUTCOMES AND ASSESSMENT

Assessment is a process used by instructors to help improve learning. Assessment is essential for effective learning because it provides feedback to both students and instructors. A critical step in this process is making clear the course’s student learning outcomes that describe what students are expected to learn to be successful in the course. The student learning outcomes for this course are listed below. By collecting data and sharing it with students on how well they are accomplishing these learning outcomes students can more efficiently and effectively focus their learning efforts. This information can also help instructors identify challenging areas for students and adjust their teaching approach to facilitate learning.

By the end of this course, students should be able to:

1. Identify the type of computational chemistry used in research articles
2. Determine appropriate approach to computational chemistry problems
3. Use either molecular dynamics or quantum chemistry software
4. Apply symmetry considerations to wavefunctions

G. INSTRUCTIONAL METHODS AND ACTIVITIES

This course is delivered through face-to-face lectures supplemented by PowerPoint outlines and assigned readings available on the internet. Coursework will involve reading and analyzing research articles. Class participation will be evaluated each class period based on preparedness for class. There will be two midterm exams and a final exam. Student work on a computational project will be presented in the format of a scientific paper.

H. MAJOR COURSE REQUIREMENTS AND GRADING

There will be two mid-term, in-class exams, one on (classical) molecular dynamics simulations and one on quantum mechanical calculations. The final exam will be in-class. There will be deadlines throughout the semester that will count as 10% of your grade. A computational project (to be developed in consultation with the instructor) is required that will be presented as a scientific paper.

<table>
<thead>
<tr>
<th>ACTIVITY</th>
<th>% of FINAL GRADE</th>
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<tbody>
<tr>
<td>Exams (2)</td>
<td>30</td>
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<tr>
<td>Class Participation</td>
<td>10</td>
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Overall grades for the course (three hours credit) will be assigned according to a ten-point scale: A for >90%, B for 80-89%, C for 70-79%, D for 60-69%, and F for <60%. Rounding is at the discretion of the instructor. Graduate students will have additional questions on exams and assignments that require a deeper knowledge of the subject matter compared to undergraduates. Graduate students will submit a “Supplemental Information” document along with their scientific paper.

I. COURSE CONTENT/SCHEDULE

Lecture Schedule:

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<tr>
<th>WEEK</th>
<th>TOPIC</th>
<th>DUE</th>
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<tr>
<td>1/14-18</td>
<td>Introduction to molecular dynamics simulations</td>
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<tr>
<td>1/23-25</td>
<td>Force fields and energy terms</td>
<td>Literature examples</td>
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<tr>
<td>1/28-2/1</td>
<td>Energy minimization vs. dynamics simulation vs. Monte Carlo</td>
<td>Decision on MD or quantum for your project</td>
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<tr>
<td>2/4-8</td>
<td>Ensembles, thermostats and barostats</td>
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<tr>
<td>2/11-15</td>
<td>Ergodicity, phase space and convergence</td>
<td>Installation/access to computational program</td>
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<td>2/18-22</td>
<td>Computational considerations</td>
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<tr>
<td>2/25-3/1</td>
<td>Exam #1</td>
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<tr>
<td>3/4-8</td>
<td>Basic concepts in quantum mechanics</td>
<td>Literature example for your chosen project</td>
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<tr>
<td>3/18-22</td>
<td>Ab initio: MO theory and SCF orbitals</td>
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<tr>
<td>3/25-29</td>
<td>Hartree-Fock method</td>
<td>Initial configuration of your project system</td>
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<td>4/1-5</td>
<td>Density functional theory calculations</td>
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<td>4/8-12</td>
<td>Exam #2</td>
<td>Outline of project</td>
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<td>4/15-19</td>
<td>Project development</td>
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<tr>
<td>4/22-26</td>
<td>Project development</td>
<td></td>
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<tr>
<td>4/29-5/1</td>
<td>Projects due</td>
<td>Project paper</td>
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<tr>
<td>5/8</td>
<td>Final Exam, 8:00 – 10:30 a.m.</td>
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Note: Changes in this course schedule may be necessary and will be announced to the class by the Instructor. The assignments and exams shown are directly related to the Student Learning Outcomes described in Section F.
J. COURSE POLICIES

- **Attendance/Tardiness**
  The student is expected to be on time and attend every class. If absent, it is the responsibility of the student to obtain any information that was missed from a classmate. Missed information includes not only lecture notes, but also any possible information regarding syllabus changes.

- **Late Work and Make-up Exams**
  There will be no make-up exams except as detailed below. In-class activities cannot be made up. No assignments are accepted after the start of the final exam.

- **Extra Credit**
  There will be no extra credit assignments.

- **Cell Phone Use**
  Don’t let that thing distract you.

- **Laptop Use**
  Any use of an electronic device (cell phone, tablet, laptop, etc.) during an exam is strictly prohibited. Any use of such a device will be considered an attempt to cheat on the exam and will result in a score of zero on the exam although more severe actions may be considered.

- **Missed Exam**
  Missing an exam does not entitle you to a make-up exam. Students with a university approved absence (athletics, university field trips, etc.) MUST contact the instructor well in advance of the scheduled absence to arrange for an early exam. A written excuse from the university department involved is required. Students who miss an exam without meeting the above requirements may be given a written exam that may be more difficult than the regular exam.

K. COLLEGE AND UNIVERSITY POLICIES

- **Academic Integrity (University)**
  University students are expected to conduct themselves in accordance with the highest standards of academic honesty. Academic misconduct for which a student is subject to penalty includes all forms of cheating, such as illicit possession of examinations or examination materials, falsification, forgery, complicity or plagiarism. (Plagiarism is the presentation of the work of another as one’s own work.) In this class, academic misconduct or complicity in an act of academic misconduct on an assignment or test will result in a failing grade.

- **Classroom/Professional Behavior**
  Texas A&M University-Corpus Christi, as an academic community, requires that each
individual respect the needs of others to study and learn in a peaceful atmosphere. Under Article III of the Student Code of Conduct, classroom behavior that interferes with either (a) the instructor’s ability to conduct the class or (b) the ability of other students to profit from the instructional program may be considered a breach of the peace and is subject to disciplinary sanction outlined in article VII of the Student Code of Conduct. Students engaging in unacceptable behavior may be instructed to leave the classroom. This prohibition applies to all instructional forums, including classrooms, electronic classrooms, labs, discussion groups, field trips, etc.

- **Statement of Civility**
  Texas A&M University-Corpus Christi has a diverse student population that represents the population of the state. Our goal is to provide you with a high quality educational experience that is free from repression. You are responsible for following the rules of the University, city, state and federal government. We expect that you will behave in a manner that is dignified, respectful and courteous to all people, regardless of sex, ethnic/racial origin, religious background, sexual orientation or disability. Behaviors that infringe on the rights of another individual will not be tolerated.

- **Deadline for Dropping a Course with a Grade of W (University)**
  I hope that you never find it necessary to drop this or any other class. However, events can sometimes occur that make dropping a course necessary or wise. **Please consult with your academic advisor, the Financial Aid Office, and me, before you decide to drop this course.** Should dropping the course be the best course of action, you must initiate the process to drop the course by going to the Student Services Center and filling out a course drop form. Just stopping attendance and participation WILL NOT automatically result in your being dropped from the class. Please consult the Academic Calendar ([http://www.tamucc.edu/academics/calendar/](http://www.tamucc.edu/academics/calendar/)) for the last day to drop a course.

- **Grade Appeals (College of Science and Engineering)**
  As stated in University Procedure 13.02.99.C2.01, Student Grade Appeal Procedures, a student who believes that he or she has not been held to appropriate academic standards as outlined in the class syllabus, equitable evaluation procedures, or appropriate grading, may appeal the final grade given in the course. The burden of proof is upon the student to demonstrate the appropriateness of the appeal. A student with a complaint about a grade is encouraged to first discuss the matter with the instructor. For complete details, including the responsibilities of the parties involved in the process and the number of days allowed for completing the steps in the process, see University Procedure 13.02.99.C2.01, Student Grade Appeal Procedures. These documents are accessible through the University Rules website at [http://www.tamucc.edu/provost/university_rules/index.html](http://www.tamucc.edu/provost/university_rules/index.html), and the College of Science and Engineering Grade Appeals webpage at [http://sci.tamucc.edu/students/GradeAppeal.html](http://sci.tamucc.edu/students/GradeAppeal.html). For assistance and/or guidance in the grade appeal process, students may contact the chair or director of the appropriate department or school, the Office of the College of Science and Engineering Dean, or the
Office of the Provost.

- **Disability Services**
  The Americans with Disabilities Act (ADA) is a federal anti-discrimination statute that provides comprehensive civil rights protection for persons with disabilities. Among other things, this legislation requires that all students with disabilities be guaranteed a learning environment that provides for reasonable accommodation of their disabilities. If you believe you have a disability requiring an accommodation, please call (361) 825-5816 or visit Disability Services in Corpus Christi Hall 116.

  If you are a returning veteran and are experiencing cognitive and/or physical access issues in the classroom or on campus, please contact the Disability Services office for assistance at (361) 825-5816.

  [http://disabilityservices.tamucc.edu/](http://disabilityservices.tamucc.edu/)

- **Statement of Academic Continuity**
  In the event of an unforeseen adverse event, such as a major hurricane and classes could not be held on the campus of Texas A&M University–Corpus Christi; this course would continue through the use of Blackboard and/or email. In addition, the syllabus and class activities may be modified to allow continuation of the course. Ideally, University facilities (i.e., emails, web sites, and Blackboard) will be operational within two days of the closing of the physical campus. However, students need to make certain that the course instructor has a primary and a secondary means of contacting each student.

L. **OTHER INFORMATION**

- **Academic Advising**
  The College of Science & Engineering requires that students meet with an Academic Advisor as soon as they are ready to declare a major. The Academic Advisor will set up a degree plan, which must be signed by the student, a faculty mentor, and the department chair. Meetings are by appointment only; advisors do not take walk-ins. Please call or stop by the Advising Center to check availability and schedule an appointment. The College’s Academic Advising Center is located in Center for Instruction 350 or can be reached at (361) 825-3928.

**GENERAL DISCLAIMER**

I reserve the right to modify the information, schedule, assignments, deadlines, and course policies in this syllabus if and when necessary. I will announce such changes in a timely manner during regularly scheduled lecture periods.