Day/Time: T 9:25 am - 10:40 am  
Location: SSMB 327  
CRN: 23017

Instructor Information

Kristin D. Krantzman  
E-mail: krantzmank@cofc.edu  
Office: SSMB Rm 116

Office Hours:
M  2:00-2:50 pm  
T  11:00-11:50 am  
W  1:00-1:50 pm  
F  11:00-11:00 am  
and by appointment

Course Description: An introduction to computer modeling of various properties and structures of molecules, thermodynamic properties and structures of simple crystals, and the kinetics of chemical reactions. 
Prerequisite: CHEM 231.

Course Schedule (Tentative)

<table>
<thead>
<tr>
<th>Dates</th>
<th>Class Topics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jan. 11</td>
<td>Introduction to Computational Chemistry and WebMO</td>
</tr>
<tr>
<td>Jan. 18, Jan. 14</td>
<td>Geometry Optimization and Frequency Calculations</td>
</tr>
<tr>
<td>Feb. 1, Feb. 8, Feb. 15</td>
<td>Model Chemistries</td>
</tr>
<tr>
<td>Feb. 22</td>
<td>Electron Density, Electron Potential and Reactivity</td>
</tr>
<tr>
<td>Mar. 1</td>
<td>Infared/Raman Spectroscopy and Thermodynamics</td>
</tr>
<tr>
<td>Mar. 15</td>
<td>UV/Vis and NMR Spectroscopy</td>
</tr>
<tr>
<td>Mar. 22</td>
<td>Transition States</td>
</tr>
<tr>
<td>Mar. 29, Apr. 5</td>
<td>Molecular Dynamics Simulations</td>
</tr>
<tr>
<td>Apr.12, Apr. 19</td>
<td>Project Presentations</td>
</tr>
</tbody>
</table>

Information in this syllabus can change with appropriate notice.
**Student Learning Outcomes**

This course is not designed to prepare the student as a “quantum” chemist. It is designed to introduce modeling and, in particular, molecular modeling as another tool that chemists can use along with tools such as IR, Raman, UV-Vis, and NM R spectroscopy in their everyday work.

*Upon satisfactory completion of this course, the student would be expected to*

- recognize and understand various types of modeling that are used commonly by chemists.
- gain experience with a typical molecular modeling user interface for constructing molecular models and for interpreting molecular modeling calculation results.
- understand and choose the appropriate theoretical method(s) and basis set(s) for a given calculation based on desired accuracy and computational “expense”.
- calculate and interpret single point, optimized, and transition structure energies for a molecule.
- calculate and interpret simple molecular properties such as geometry and dipole moment.
- calculate and interpret electron density, electron potential, and reactivity diagrams for molecules.
- calculate and interpret theoretical values of IR, Raman, UV-Vis and NM R spectra and associated thermochemical properties.
- set up, perform and analyze molecular dynamics simulations of a protein in an aqueous solution.
- formulate, design, perform the calculations, and interpret the results of a molecular modeling “experiment/exercise” suitable for use in an undergraduate chemistry class.

**Evaluation of Student Performance**

**Grading Scale**

<table>
<thead>
<tr>
<th>Letter Grade</th>
<th>Percentage</th>
<th>Letter Grade</th>
<th>Percentage</th>
<th>Letter Grade</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>93-100</td>
<td>B-</td>
<td>80-82</td>
<td>D+</td>
<td>72</td>
</tr>
<tr>
<td>A-</td>
<td>90-92</td>
<td>C+</td>
<td>78-79</td>
<td>D</td>
<td>71</td>
</tr>
<tr>
<td>B+</td>
<td>87-89</td>
<td>C</td>
<td>75-77</td>
<td>D-</td>
<td>70</td>
</tr>
<tr>
<td>B</td>
<td>83-86</td>
<td>C-</td>
<td>73-74</td>
<td>F</td>
<td>&lt;70</td>
</tr>
</tbody>
</table>

**Homework Assignments** 75 %

Homework assignments will be made each class period. The assignments are due at the beginning of the next class period.

**Independent Project** 25 %

The final project will be to develop and write a complete first-draft handout for a molecular modeling “experiment/exercise” suitable for use in one of our classes. Students will give an oral presentation about their final project during the last to weeks of class. More guidance and information will be given later in the semester.

**Late Assignments**

A penalty of 10 % will be deducted for each day that a homework assignment is submitted past the deadline.
College and Class Policies

**Attendance Policy**
Attendance is expected at all classes. However, do not attend class if you are sick or under quarantine. Students are responsible for all information presented in class whether they are present or not.

**Academic Integrity Statement**
Each student is responsible for their own individual work—although group discussion and/or helping each other is encouraged.

One of the core values of the College is academic integrity. This course is conducted under the Honor Code (http://deanofstudents.cofc.edu/policies-and-procedures/honor-code-and-code-of-conduct.php) of the College of Charleston. Students at the College are bound by honor and by their acceptance of admission to the College to abide by the Code and to report violations. Faculty members are required to report violations of the Honor Code or Code of Conduct to the Office of Student Affairs. Conviction of an Honor Code violation in this class will result in the grade of "F" for the course. Please consult the department's Policy on Scientific Integrity (http://chemistry.cofc.edu).

**Accommodations for Students with Disabilities**
This College abides by section 504 of the Rehabilitation Act of 1973 and the Americans with Disabilities Act. If you have a documented disability that may have some impact on your work in this class and for which you may require accommodations, please see an administrator at the Center of Disability Services/SNAP, 843.953.1431 or me so that such accommodation may be arranged.

**Attendance Verification**
Only students officially registered (graded or auditing) for this course may attend class. During the week following the drop/add deadline, the professor will verify student enrollments in this course. Any student appearing on the class roll but determined not to have attended the class even once will be removed.

**OAKS**
OAKS, including Gradebook, will be used for this course throughout the semester to provide the syllabus and class materials and grades for each assignment, which will be regularly posted.

**Inclement Weather, Pandemic or Substantial Interruption of Instruction**
If in-person classes are suspended, faculty will announce to their students a detailed plan for a change in modality to ensure the continuity of learning. All students must have access to a computer equipped with a web camera, microphone, and Internet access. Resources are available to provide students with these essential tools.
College and Class Policies (cont.)

**Mental & Physical Wellbeing**
At the college, we take every student's mental and physical wellbeing seriously. If you find yourself experiencing physical illnesses, please reach out to student health services (843.953.5520). And if you find yourself experiencing any mental health challenges (for example, anxiety, depression, stressful life events, sleep deprivation, and/or loneliness/homesickness) please consider contacting either the Counseling Center (professional counselors at [http://counseling.cofc.edu](http://counseling.cofc.edu) or 843.953.5640 3rd Robert Scott Small Building) or the Students 4 Support (certified volunteers through texting "4support" to 839863, visit [http://counseling.cofc.edu/cct/index.php](http://counseling.cofc.edu/cct/index.php), or meet with them in person 3rd Floor Stern Center). These services are there for you to help you cope with difficulties you may be experiencing and to maintain optimal physical and mental health.

**Inclusion**
The College of Charleston offers many resources for LGBTQ+ students, faculty and staff along with their allies.

- Preferred Name and Pronoun Information
- On Campus Gender Inclusive facilities
- Campus Resources
- College of Charleston Reporting Portals
- National Resources for Faculty & Staff
- GSEC Reports
- Documenting LGBTQ Life in the Lowcountry (CofC Addlestone Library Special Collections Project)

**COVID-19 Reminders**
For the health and safety of yourself and those around you, you are required to wear a face-covering over both your nose and mouth while inside all campus buildings (you should do the same inside other public buildings). This mask should fit well; there should not be gaps anywhere between your face and the mask. Also remember that students, faculty, and staff should not come to campus when they feel unwell.


The CDC’s guidance has changed over the course of the pandemic as new data and new variants have emerged; check the latest info for yourself: [https://www.cdc.gov/coronavirus/2019-ncov/if-you-are-sick/quarantine.html](https://www.cdc.gov/coronavirus/2019-ncov/if-you-are-sick/quarantine.html)
and find CofC’s info here: [https://cofc.edu/back-on-the-bricks/](https://cofc.edu/back-on-the-bricks/).

The easiest thing to do is to contact Student Health about your particular situation to get their guidance: [https://studenthealth.cofc.edu/](https://studenthealth.cofc.edu/) If you cannot attend class due to a COVID-related situation, contact your instructors as soon as possible for help in making up assignments.

CofC Student Health requests that you inform them of positive COVID testing results and any close contact with someone who is COVID-positive, so they can monitor the campus health situation and give you personalized healthcare. CofC holds regular free testing events on campus for anyone in the campus community to get tested for COVID infection. CofC also holds free vaccination events on campus for all students. Vaccination remains the best way to protect yourself, your family, and those around you.