Computational Research  
CHEM 2175.021 Math 124 TBA  
Spring 2024

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Student Hours: M 10:00 am – noon, M 1:30 pm – 3:30 pm, T 11:00 am – noon; other times by appointment

Course Description: Computational and theoretical study of the chemical problems utilizing density functional theory.

Course Objective: To provide students with a guided self-exploration of computational and theoretical chemistry research by problem solving involving critical thinking and how to apply these methods to systems of interest.

Student Learning Outcomes:  
The student is expected to be able do the following, upon completion of this course:

▪ Set up and run a geometry optimization.  
▪ Basic structure of molecular and atomic systems used in chemistry such as Lewis structures, molecular geometry, bonding theories, and periodic trends.  
▪ Analyze quality of results and draw conclusions based on results.  
▪ Calculate enthalpy reaction energies

Honor Justification: This course is for 2 credit and spans 15 weeks. The course requires students to prepare by completing literature search and review of related materials outside of the regularly scheduled upon research time. The students will also use that time to prepare and write their research paper over the research that was performed. During research time, students will be actively engaged in research by setting up, submitting, and analyzing calculations. From these calculations students will draw conclusions and increase their critical thinking and quantitative reasoning. These activities average at a minimum 3 hours of work each week to prepare outside of time spent engaging with the content.

Text and Materials: Professional Laboratory Notebook

Course Calendar: TBA

Grading Policy:  
Notebook – The student will develop and maintain a professional research notebook. The notebook will be a hard copy of jobs ran and energies calculated, as well as a place for the student to write down ideas and conclusions. The notebook will be checked periodically during the semester and is due Wednesday during Finals’ week. The notebook is worth 100 points

Research Summary – A one page summary of the semester’s research is due at the same time as the student’s notebook. The summary is worth 100 points.
Method of Evaluation:

<table>
<thead>
<tr>
<th>ITEM</th>
<th>POINT VALUE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Notebook</td>
<td>100</td>
</tr>
<tr>
<td>Research Paper</td>
<td>100</td>
</tr>
<tr>
<td>TOTAL POINTS</td>
<td>200</td>
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**Grading Scale (Based on 200 Total Points Possible)**

**This Course is Pass/Fail 139 pts or more to pass**

200-179 = A; 178-159 = B; 158-139 = C; 138-119 = D; 119-0 = F

**Attendance Policy:**

Students must attend research as agreed upon with the professor.

**Academic Integrity (A-9.1):**

The Code of Student Conduct and Academic Integrity outlines the prohibited conduct by any student enrolled in a course at SFA. It is the responsibility of all members of all faculty, staff, and students to adhere to and uphold this policy.

Articles IV, VI, and VII of the new Code of Student Conduct and Academic Integrity outline the violations and procedures concerning academic conduct, including cheating, plagiarism, collusion, and misrepresentation. Cheating includes, but is not limited to: (1) Copying from the test paper (or other assignment) of another student, (2) Possession and/or use during a test of materials that are not authorized by the person giving the test, (3) Using, obtaining, or attempting to obtain by any means the whole or any part of a non-administered test, test key, homework solution, or computer program, or using a test that has been administered in prior classes or semesters without permission of the Faculty member, (4) Substituting for another person, or permitting another person to substitute for one’s self, to take a test, (5) Falsifying research data, laboratory reports, and/or other records or academic work offered for credit, (6) Using any sort of unauthorized resources or technology in completion of educational activities. Plagiarism is the appropriation of material that is attributable in whole or in part to another source or the use of one’s own previous work in another context without citing that it was used previously, without any indication of the original source, including words, ideas, illustrations, structure, computer code, and other expression or media, and presenting that material as one’s own academic work being offered for credit or in conjunction with a program course or degree requirements.

Collusion is the unauthorized collaboration with another person in preparing academic assignments offered for credit or collaboration with another person to commit a violation of any provision of the rules on academic dishonesty, including disclosing and/or distributing the contents of an exam. Misrepresentation is providing false grades or résumés; providing false or misleading information in an effort to receive a postponement or an extension on a test, quiz, or other assignment for the purpose of obtaining an academic or financial benefit for oneself or another individual or to injure another student academically or financially.

**Withheld Grades Semester Grades Policy (5.5):**

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 coursework 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 to compute the grade point average. For additional information, go to https://www.sfasu.edu/policies/course-grades-5.5.pdf.

**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/.

**STUDENT WELLNESS AND WELL-BEING:**
SFA values students’ overall well-being, mental health, and the role it plays in academic and overall student success. Students may experience stressors that can impact both their academic experience and their personal well-being. These may include academic pressure and challenges associated with relationships, emotional well-being, alcohol and other drugs, identities, finances, etc.

If you are experiencing concerns, seeking help, SFA provides a variety of resources to support students’ mental health and wellness. Many of these resources are free, and all of them are confidential.

**On-campus Resources:**
**The Dean of Students Office** (Rusk Building, 3rd floor lobby)
www.sfasu.edu/deanofstudents
936.468.7249
dos@sfasu.edu

**SFA Human Services Counseling Clinic** Human Services, Room 202
www.sfasu.edu/humanservices/139.asp
936.468.1041

**The Health and Wellness Hub  “The Hub”**
Location: corner of E. College and Raguet St.
To support the health and well-being of every Lumberjack, the Health and Wellness Hub offers comprehensive services that treat the whole person – mind, body and spirit. Services include:

- Health Services
- Counseling Services
- Student Outreach and Support
- Food Pantry
- Wellness Coaching
• Alcohol and Other Drug Education
www.sfasu.edu/thehub
936.468.4008
thehub@sfasu.edu

Crisis Resources:
• Burke 24-hour crisis line: 1.800.392.8343
• National Suicide Crisis Prevention Text: 9-8-8
• Suicide Prevention Lifeline: 1.800.273.TALK (8255)

Crisis Text Line: Text HELLO to 741-741
Instructor reserves the right to change the syllabus at any time.