Name: Dr. Brian Barngrover  
Department: Chemistry & Biochemistry  
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Phone: (936) 468-1568  
Office: M-124  
Student Hours: MWF 10:00 – 11:00 AM, M 2:00 – 4:00 PM; 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 1 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><strong>TOTAL POINTS</strong></td>
<td><strong>200</strong></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):**
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/academic_integrity.asp](http://www.sfasu.edu/policies/academic_integrity.asp)

**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/](http://www.sfasu.edu/disabilityservices/).

**MENTAL HEALTH:**
SFASU values students’ mental health and the role it plays in academic and overall student success. SFA provides a variety of resources to support student’s mental health and wellness. Many of these resources are free, and all of them are confidential.

**On-campus Resources:**
SFASU Counseling Services • [www.sfasu.edu/counselingservices](http://www.sfasu.edu/counselingservices)
Health and Wellness Hub (corner of E. College and Raguet) • 936-468-2401
SFASU Human Services Counseling Clinic • [www.sfasu.edu/humanservices/139.asp](http://www.sfasu.edu/humanservices/139.asp)
Human Services Room 202 • 936-468-1041

**Crisis Resources:**
Burke 24-hour crisis line 1(800) 392-8343
Suicide Prevention Lifeline 1(800) 273-TALK (8255)
Crisis Text Line: Text HELLO to 741-741