Computational Ligand Redox
CHE 275.007 Math 132 Friday 12:00-1:00/Chemistry 307 TBA
Fall 2018

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Office Hours: MF 9:00-10:00 AM; Thurs. 2:00 PM- 4:00 PM; other times by appointment

Course Description: Introduction to computation bioinorganic research

Course Objective: To provide students with a guided self-exploration of computational 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:
▪ Perform experimental procedures relevant to their project
▪ Explain and articulate the goals and outline of work for their project
▪ Analyze quality of results and draw conclusions based on results
▪ Develop plan for project completion and presentation for CHE 470

Text and Materials: Professional Laboratory Notebook

Course Calendar: see end of document

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. The student will also attend the group CHE 275 course meeting.

Fulfil All Requirements of CHE 275 seminar class. (see course schedule below)

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>
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</thead>
<tbody>
<tr>
<td>Notebook</td>
<td>100</td>
</tr>
<tr>
<td>Research Summary</td>
<td>100</td>
</tr>
<tr>
<td>TOTAL POINTS</td>
<td>200</td>
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</tbody>
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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/).
<table>
<thead>
<tr>
<th>Topic</th>
<th>Date</th>
<th>Instructor or Presenter</th>
<th>Notes/Assignments</th>
</tr>
</thead>
</table>
| Research at SFA Chemistry and Biochemistry Department                | August 31 | Janusa                  | - Students assigned to Research Advisors  
Assignment #1: Meet with your research professor to discuss project(s). Submit a project topic and a 1-paragraph narrative why you want to work on that topic in the next class  
Assignment #2: Students meet with advisor for further discussion/action on the project and submit a 1-paragraph narrative of that meeting, signed by both, in the next class |
| Safety Training                                                      | September 7| Franks                  | - Students submit assignment #1  
Assignment #2: Students prepare a typed 1-page summary of review of at least 5 current (≤ 10 years) articles relevant to their proposed research. List cited references on a second page following the guidelines above. Assignment should be signed on both pages by advisor and student and brought to next class |
| SFA Library Resources – how to do a literature search               | September 14| Library Staff           | - Students submit assignment #2  
Assignment #3: Students prepare a typed 1-page summary of review of at least 5 additional current (≤ 10 years) articles relevant to their proposed research. List cited references on a second page following the guidelines above. Assignment should be signed on both pages by advisor and student and brought to next class |
| Library resources – doing the actual literature search               | September 21| Library Staff           | - Students submit assignment #3  
Assignment #4: Students participate in in-class literature search  
Assignment #5: Students prepare a typed 1-page summary of review of at least 5 additional current (≤ 10 years) articles relevant to their proposed research. List cited references on a second page following the guidelines above. Assignment should be signed on both pages by advisor and student and brought to next class |
| Writing a good proposal                                             | September 28| Odunuga                 | - Students submit assignment #4  
Assignment #5: Students write ‘Introduction/Literature Review’ portions of their proposal. Assignment should be typed, signed by both advisor and student, and brought to next class. Give a copy of the assignment to your advisor for correction.  
Assignment #6: Students make changes to ‘Introduction/Literature Review’ as corrected by advisor. Students bring copies containing advisor’s comments and corrected version (signed by both) to next class |
| Ethics in Research                                                  | October 5  | Odunuga                 | - Students submit assignment #5  
Assignment #7: Students write ‘Methodology and Objectives’ portions of their proposal. Assignment should be typed, signed by both advisor and student, and brought to next class. Give a copy of the assignment to your advisor for correction. |
| Maintaining a good laboratory notebook                              | October 12 | Odunuga                 | - Students submit assignment #6  
Assignment #8: Students make changes to ‘Methodology and Objectives’ as corrected by advisor. Students bring copies containing advisor’s comments and corrected version (signed by both) to next class |
| Use of Excel – General operation, Graphs, charts etc.              | October 19  | Fry                     | - Students submit assignment #7  
Assignment #9: Students prepare a typed 1-page summary of review of at least 5 additional current (≤ 10 years) articles relevant to their proposed research. List cited references on a second page following the guidelines above. Assignment should be signed on both pages by advisor and student and brought to next class |
| Simple Statistical Analysis using Excel                             | October 26  |                        | - Students submit assignment #8  
Assignment #10: Students write ‘Synopsis and References (minimum 6)’ portions of their proposal. Assignment should be typed, signed by both advisor and student, and brought to next class. Give a copy of the assignment to your advisor for correction. |
| Opportunities in the department and after graduation (Welch, patent course, SURE etc.) Discuss Welch application | November 2  | Harris                  | - Students submit assignment #9  
Assignment #11: Students submit the following in assigned Drop boxes on D2L by 11 a.m.  
1. Complete Proposal signed by advisor and student  
2. “Skills” narrative signed by advisor and student  
3. Survey  
If applicable, a completed and signed Welch Proposal to Carrie Stover |
| Fundamentals of Scientific Writing (http://acswebinars.org/sainani)  | November 9  | Odunuga                 | - Students submit assignment #10  
Assignment #12: Students write a 1-page narrative, minimum 500 words, of the research skills and experience they have learned in their advisor’s laboratory. Assignment should be typed, signed by both advisor and student, and brought to next class. Give a copy of the assignment to your advisor for correction. |
| Presentations by former student(s)                                 | November 16|                        | - Students submit assignment #11  
Assignment #13: Students submit assignment #12  
Assignment #14: Students make changes to complete proposal as corrected by advisor. Students bring copies containing advisor’s comments and corrected versions of (1) Synopsis and References and (2) complete proposal. Both should be signed by advisor and student. |
| Practical aspects of giving a PowerPoint presentation               | November 30| Odunuga                 | - Students submit assignment #12  
Assignment #15: Students make further changes to complete proposal and ‘Skills’ assignments as directed by advisor. |
| Final class                                                         | December 7 | Odunuga                 | - Students submit assignment #13  
Assignment #16: Students submit the following in assigned Drop boxes on D2L by 11 a.m.  
1. Complete Proposal signed by advisor and student  
2. “Skills” narrative signed by advisor and student  
3. Survey  
If applicable, a completed and signed Welch Proposal to Carrie Stover |