CHEM [redacted]/6171
Applications of Inorganic Chemistry in Current Energy Research

Spring [redacted]

Syllabus and Logistics

[redacted]

Course Schedule:

1. Lecture/Discussion

10:05-10:55 AM Mon, Wed, Fri in MoSE 1222

2. Take-Home Exams

Midterm Exam: **Due In Class, Fri February 28**

Final Exam: **Due to My Office, 11:30 AM Fri May 2**

Course Materials:

Required Books

There is no required textbook for this course.

Reading assignments will come from supplied references and/or literature packets on T-Square. An introductory inorganic chemistry text, such as *Shriver & Atkins Inorganic Chemistry*, will likely be useful for background reading and reference. Many are available in the library, along with other helpful resources, including the reserve texts listed below.

Reserve Books

1. *Advanced Inorganic Chemistry*, 6th ed. by F. A. Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann

2. *Chemical Applications of Group Theory*, 3rd ed. by F. A. Cotton

3. *Symmetry and Spectroscopy: An Introduction to Vibrational and Electronic Spectroscopy*, by D. C. Harris and M. D. Bertolucci

4. *Physical Methods for Chemists*, 2nd ed. by R. S. Drago

5. *Chemistry of the Elements*, 2nd ed. by N. N. Greenwood and A. Earnshaw (available electronically via the GT Library)

Course Policies and Expectations:

Class Communication and T-Square

All supplied course materials will be available via the web at T-Square. These will include homework assignments, references and literature packets, and lecture slides.

You will occasionally receive class information via email from me to your Georgia Tech account. Some announcements may not be communicated in class. Therefore, it is important for you to check your email regularly. Email from me will **contain CHEM 4803/6171 in the subject line.** If you use an alternative email address it is your responsibility to have messages from your Georgia Tech account forwarded to the alternative address.

The best way to contact me is via email. My email address is jake.soper@chemistry.gatech.edu. For any communication concerning the class, please **add CHEM 4803 or CHEM 6171 to the subject line**, and be sure to identify yourself by name in the message. I will try to answer all email in a timely fashion (<24h).

Please make me aware of any issues that may arise. I've found that more communication makes for a better course and a more enjoyable semester. I aim to be very available. Feel free to contact me in person, by email, or by a note left my mailbox.

Lecture

Computers and cell phones are not permitted during lecture.

Slides used in class will be posted to the **Resources** section of the CHEM 4803/6171 T-Square site. I will not post copies of my lecture notes. If you miss a lecture, it is your responsbility to copy lecture notes from a classmate.

Class attendence and participation are mandatory. Everyone benefits if you come to class prepared to be an active participant in the learning process. To encourage class participation, problem sets based on reading assignments from current literature will be due appoximately once a week. Homework policies are provided below.

Reading/Problem Sets

Problem sets will be due approximately once per week. The problem sets are based on reading assignments from current literature, and are designed to test comprehension and stimulate critical review.

Problem sets will be due in class, at the beginning of class. Unless you make me aware of exceptional circumstance before the assignment is due, I will not accept late homework or homework turned in outside of the classroom. Problem sets will comprise 20% of your overall class grade. Problem sets will be graded on a scale of 0-5 points. Points will be deducted for failing to make a good attempt at all of the assigned questions. I also reserve the right to deduct points for unwillingness to participate in classroom discussions of the homework questions.

At the end of the semester, your total homework points earned will be normalized to 20. For example: If a total of 13 problem sets are assigned over the course of the semester, then there are 65 possible points. If you earn 55 of these points, you have 55/65 = 0.85 of the possible homework points (i.e. 17/20).

You are encouraged to work together with your classmates on the problem sets, but each student is required to write up and turn in solutions in their own words. You are allowed to ask me questions. You are free to use any online or library resources in researching your answers (including SciFinder and the primary literature), but all submissions must be written in your own words. If your answer derives from another source, cite this in your homework. Any plagarism, including copying from classmates, will be considered a violation of the Georgia Tech Academic Honor Code.

Exams

One take-home midterm exam will be given during the semester. It will be distributed on later than Friday February 21, and be due in class (at 10:05 AM) on Friday February 25.

A take-home final exam will distributed no later than Wednesday April 23, and be due on Friday May 2 at 11:30 AM, the final exam period set by the Georgia Tech Registrar's office.

Take home exams will detail the allowed resources and rules for colloboration. All students, except those with a conflict as defined by the Registrar, must turn in the exams by the deadlines above. Late or missing exams, without a documented excuse, will receive a failing (F) grade.

Grade Changes

Request for re-grades must be made in writing within one week of the date that the graded exam or problem set is returned.

Proposal/Review Project

Each student will submit and present a written proposal and critical review project to the class in April. The project will be worth 25% of your overall class grade. Detailed instructions will be provided at a future date.

Course Grades

Midterm Exam	25 points (25%)
Final Exam	30 points (35%)
Problem Sets	20 points (20%)
Proposal/Review Project	25 points (25%)
TOTAL	**100 points**

Grading Scale

A	Excellent	90.1-100%	90.1-100 points
B	Good	80.1-90.0%	80.1-90.0 points
C	Average	70.1-80.0%	70.1-80.0 points
D	Fair	60.1-70.0%	60.1-70.0 points
F	Failing	<60.1%	<60.1 points

I reserve the right to adjust this grading scale, but the cut-offs can only be lowered so that any adjustments will only benefit students. Adjustments are not guaranteed, and any that are made will be done at the end of the semester after all grades are calculated.

Studens enrolled in CHEM 4803 and 6171 will be given the same exams and problem sets, and graded indentically, however final grades will be independently calculated for the two classes. **This means a different grading scale may be applied to CHEM 4803 vs. CHEM 6171.** I expect the mean grade in both classes to be a B, unless a class is exceptionally good or exceptionally bad.

Learning Disabilities

Student learning disabilities documented through ADAPTS will be honored as detailed to the instructor. Please inform both me within the first week of the course or as soon as possible.

Academic Honesty

It is expected that all students are aware of their individual responsibilities under the Georgia Tech Academic Honor Code, which will be strictly adhered to in this class. All violations of the Honor Code will be reported to the Office of Student Affairs. For questions involving any Academic Honor Code issues, please consult me, the teaching assistants, or honor.gatech.edu.

Course Schedule and Aims:

Aims

The class covers applications of inorganic chemistry in current energy research as well as fundamental principles of coordination chemistry and reaction mechanisms relevant to these topics. Ideally one informs the other and builds an understanding of the theories and mechanisms governing energy conversion and storage in chemistry and biology. Core concepts will be taught by examinations of recent primary research literature in the areas listed below.

2014 Lecture Schedule

Below is a tentative outline/ordering of topics I'm planning to cover in this course. This list may be revised—and topics may be added or dropped—as we progress through the semester. As the course develops, I will regularly update this online schedule in an attempt to stay current.

1.0 Powering the Planet

1.1 Chemical challenges and opportunities in energy research

2.0 Metal–Ligand Multiple Bonds

2.1 Electronic structures of tetragonal oxo–metal complexes
2.1.1 the oxo wall
2.2 Oxo–metal complexes in non-tetragonal ligand fields
2.2.1 "violations" of the oxo wall
2.2.2 reactive oxo intermediates
2.2.3 electronic designs for O–O bond formation

3.0 Water Splitting, Part I

3.1 Water oxidation
3.1.1 thermodynamics
3.1.2 water oxidation catalyts and mechanisms for O–O bond formation
3.1.2.1 enzymatic
3.1.2.2 homogeneous
3.1.2.3 heterogeneous

4.0 Proton Coupled Electron Transfer (PCET)

4.0.1 definitions and elementary steps
4.1 Theory and mechanisms
4.1.1 thermochemistry
4.1.2 theoretical treatments
4.1.3 linear free energy relationships and PCET kinetics

5.0 Water Splitting (Part II), Hydrogen Production

5.0.1 Thermodynamics of H2 activation
5.1 Hydrogenases
5.2 Homogeneous catalysts
5.2.1 hydrogenase models
5.2.2 small molecule catalysts and photocatalysts
5.3 Heterogeneous catalysts and electrode materials

6.0 PCET in Energy Conversion and Storage

6.1 O_2 reduction
6.1.1 enzymatic
6.1.2 synthetic catalysts and fuel cells
6.2 CO_2 reduction
6.2.1 thermodynamics of CO_2 reduction
6.2.2 mechanisms: enzymatic CO_2 reduction, homogeneous catalysis and electrocatalysis
6.3 N_2 fixation
6.4 PCET at metal–oxide nanoparticle surfaces

7.0 Metal–Organic Framework (MOF) Materials

7.1 Synthesis and geometric principles
7.2 Structure–property relationships
7.3 Selective catalysis
7.4 CH_4/H_2 storage
7.5 CO_2 capture and selective gas adsorption