Chem 608: Symmetry, Bonding and Molecular Shapes

Fall 2018

Instructor: Daniel C. Fredrickson; 6329 Chemistry; 890-1567; danny@chem.wisc.edu
Office hours: 1381 Chemistry, M 8:00am-10:00am & F 12:30pm-1:30pm

Lectures: MWF 11:00-11:50am; 2307 Chemistry; 1-3 credits

Description: This course provides a solid background in elementary bonding theory and its application to understanding molecular geometry and reactivity. The course emphasizes qualitative methods applied to the bonding of elements from throughout the periodic table.

Overview: This course will cover bonding schemes that chemists use to rationalize and predict the structures and properties of molecules and solids, the roots of these schemes in quantum mechanics, and the role that symmetry plays in their application. Topics covered include group theory, the electronic structure of atoms, molecular orbital theory, bonding in main group and transition metal compounds, and band theory. About two-thirds of the class periods will follow the usual lecture format, while the remainder will be computer lab sessions in which the course's concepts will be implemented in Matlab programs and applied.

Learning outcomes: Students in this course will learn the fundamentals of symmetry and bonding, and how apply them to a wide range of chemical systems, ranging from transition metal complexes to polymers and solid state compounds. Students will also learn how to apply Hückel and extended Hückel molecular orbital calculations toward understanding bonding in a variety of compounds. In addition, students will gain experience in the translation of chemical concepts into computer code using Matlab.

Course website: None.

Topics Covered:

1. *Group Theory.* Symmetry operations and elements; mathematical groups; molecular symmetry groups (point groups); matrix representations; character tables; chemical applications.

2. *Atoms and Molecular Orbital Theory.* One-electron atomic theory; atomic orbitals; multi-electron atomic theory; homonuclear diatomics; heteronuclear diatomics; linear vs. bent triatomics; polyatomic molecules; approximate methods.

3. *Symmetry and Bonding in Molecular Systems.* Molecular shapes in main-group complexes; transition metal complexes and organometallic compounds.

4. *Symmetry and Bonding in Extended Systems.* Zintl phases; group theory applied to periodic structures (band theory); band structures for periodic systems.

Instructional mode: face-to-face.

Course designations and attributes: Advanced level; counts as L&S credit

How the credit hours are met: This course is offered for variable credit, with the lectures and readings providing the foundations for the completion of problem sets and a final exam. One credit is awarded for the successful solution of each half of the problem sets, while the third credit is earned in the preparation for and taking of the final exam. Students are expected to engage in at least 45 hours of learning activities per credit.

Prerequisites: Graduate/professional standing

Expected background: Chem 511 (Inorganic Chemistry) or equivalent
Chem 562 (Physical Chemistry/Quantum Mechanics) or equivalent

Grading: *3 credit option (recommended):* Grades will be based on 14 problem sets and the completion of the final exam. *2 credit option:* Grade will be based upon the completion of 14 problem sets. *1 credit option:* Grade will be determined based on 7 problem sets to be chosen in coordination with the instructor. Graduates will be determined based on the percentage of possible points achieved on these assignments using the following tentative ranges: 100-90% for **A**, 90-85 % for **AB**, 85-75% for **B**, 75-70% for **BC**, 70-60% for **C**, 60-50% for **D**, and 50%-0% for **F**. These ranges may be shifted downwards at the end of the semester to adjust for the difficult of the assignments, but never upwards.

Suggested textbooks: Course notes and journal articles will be handed out in class.
Additional recommended texts include:

A. Vincent, *Molecular Symmetry and Group Theory* (Wiley)
F. A. Cotton, *Chemical Applications of Group Theory* (Wiley-Interscience)
T. A. Albright, J. K. Burdett, M.-H. Whangbo, *Orbital Interactions in Chemistry* (Wiley-Interscience)

Academic Policies

ACADEMIC INTEGRITY: By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison's community of scholars in which everyone's academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to https://conduct.students.wisc.edu/academic-integrity/

ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES: McBurney Disability Resource Center syllabus statement: "The University of WisconsinMadison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform me of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. I will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA." http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

INSTITUTIONAL STATEMENT ON DIVERSITY: "Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals. The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world." https://diversity.wisc.edu/

Chem 608: Tentative Course Calendar

Week, Day	Subject	Assignments
1, Sept. 5 (W)	**Quantum Mechanics**— Review	
Sept. 7 (F)	**Quantum Mechanics**— *Postulates lab* (PS#1)	
2, Sept. 10 (M)	**Atoms**— H atom	
Sept. 12 (W)	**Atoms**— Atomic Orbitals, *Atoms lab* (PS#2)	
Sept. 14 (F)	**Atoms**— Many electron atoms	**PS#1 Due**
3, Sept. 17 (M)	**Atoms**— Electronic states	
Sept. 19 (W)	**Atoms**— *Quantum mechanical integrals lab* (PS#3)	
Sept. 21 (F)	**MO Theory 1**— H_2	**PS#2 Due**
4, Sept. 24 (M)	**MO Theory 1**— *MO Lab 1* (PS#4)	
Sept. 26 (W)	**MO Theory 1**— N_2,	
Sept. 28 (F)	**MO Theory 1**— *MO Lab 2* (PS#5)	**PS#3 Due**
5, Oct. 1 (M)	**Group Theory**— HHe, CO	
Oct. 3 (W)	**Group Theory**— *MO Lab 3* (PS#6)	
Oct. 5 (F)	**Group Theory**— Symmetry operations, elements	**PS#4 Due**
6, Oct. 8 (M)	**Group Theory**— *Symmetry Operations Lab* (PS#7)	
Oct. 10 (W)	**Group Theory**— Mathematical groups, point groups	
Oct. 12 (F)	**Group Theory**— Point groups	**PS#5 Due**
7, Oct. 15 (M)	**Group Theory**— Point groups; *Point Groups Lab* (PS#8)	
Oct. 17 (W)	**Group Theory**— Matrix representations	
Oct. 19 (F)	**Group Theory**— Character tables	**PS#6 Due**
8, Oct. 22 (M)	**Group Theory**— Using character tables	
Oct. 24 (W)	**Group Theory**— Chemical applications	
Oct. 26 (F)	**MO Theory 2**— *Group Theory Lab* (PS#9)	**PS#7 Due**
9, Oct. 29 (M)	**MO Theory 2**— H_2O: linear or bent?	
Oct. 31 (W)	**MO Theory 2**— *MOs of H_2O lab* (PS#10)	
Nov. 2 (F)	**Main Group Molecules**—Molecular shapes	**PS#8 Due**
10, Nov. 5 (M)	**Main Group Molecules**—Molecular shapes	
Nov. 7 (W)	**Main Group Molecules**— *AL_3 lab* (PS#11)	
Nov. 9 (F)	**Main Group Molecules** — *Walsh diagrams lab* (PS#12)	**PS#9 Due**
11, Nov. 12 (M)	**Transition metal complexes**— Octahedral	
Nov. 14 (W)	**Transition metal complexes**— Electron configurations	
Nov. 16 (F)	**Organometallics**— *d orbitals lab* (PS#13)	**PS#10 Due**
12, Nov. 19 (M)	**Organometallics**—Zeise's salt	
Nov. 21 (W)	**Organometallics**—$(C_6H_6)Cr(CO)_3$, The isolobal analogy	**PS#11 Due**
Nov. 23 (F)	*Thanksgiving recess; no class*	
13, Nov. 26 (M)	**Band Theory**— Complex representations	
Nov. 28 (W)	**Band Theory**— Bloch's Theorem, Crystal orbitals, H lattices	
Nov. 30 (F)	**Band Theory**— C chain, Graphene	**PS#12 Due**
14, Dec. 3 (M)	**Band Theory**— Analyzing bonding;	
Dec. 5 (W)	**Band Theory**— *Band structure lab* (PS#14)	
Dec. 7 (F)	**Band Theory**—Crystal symmetry, k-space, *Final Distributed*	**PS#13 Due**
15, Dec. 10 (M)	**Band Theory**— *Band structures lab 2*	
Dec. 12 (W)	**Last day of class.** Coffee, donuts, discussion of final	

PS#14 and take-home final exam due Tuesday, Dec. 18, 2018 at 2:25 pm in Chemistry room 6329.