Chem 801: Selected Topics in Inorganic Chemistry

Electronic Structure and Bonding in Inorganic Materials, Spring 2020

Instructor: Daniel C. Fredrickson; 6329 Chemistry; 890-1567; danny@chem.wisc.edu
Office Hours: by appointment

Lectures: MWF 2:25-3:15pm; 2307 Chemistry; 1-3 credits

Overview: This course will cover the concepts and techniques necessary for the analysis of bonding, stability, and some physical properties on inorganic materials from electronic structure calculations.

Learning Outcomes: Students will be able to (1) interpret, discuss, and critically analyze the results of electronic structure calculations as presented in journal articles or encountered in their own research, (2) perform, interpret, and validate their own electronic structure calculations on periodic materials, and (3) use computer programming to streamline the workflow of electronic structure calculations and augment the ways in which the output of these calculations are analyzed.

Topics Covered (Tentative):

1. *Symmetry and electronic structure in periodic systems.* Translational symmetry and space group symmetry of crystals; the application of group theory to periodic structures; band structures; reciprocal space; Brillouin zones and average properties; bonding schemes for solids, such as the nearly-free electron model and the Zintl concept.

2. *Density functional theory (DFT) and electronic structure packages.* Formulation of DFT; self-consistent-field calculations with DFT; atomic potentials; DFT calculations with the ABINIT program.

3. *Theoretical tools for analyzing electronic structure.* Density of states (DOS) distributions and fat-bands; projected DOS distributions; crystal orbital overlap/Hamilton populations; indicators of electron localization; DFT-calibrated Hückel calculations; Fermi surfaces; Quantum Theory of Atoms in Molecules; other tools.

4. *Physical properties derived from electronic structure calculations, and other topics.* Conductivity; carrier mobilities; magnetic ordering; selected topics according to interests of students.

5. *Computer programming applied to electronic structure calculations.* Developing tools to aide the processing files and data; understanding the inner-workings of planewave DFT; translation of theoretical models into executable code.

Course website: TBD

Instructional mode: face-to-face.

Course designations and attributes: Counts toward 50% graduate coursework requirement

Prerequisites: Graduate or professional standing.

Expected background: Prior completion of Chem 608 and Chem 675 is recommended but not required.

Grading: Grades in this course will be determined by the completion of small pre-class problem sets, weekly group-based problem-sets focused on programming and calculations, and a final exam. For the 3 credit option, these components will be weighted as 25%, 50%, and 25% of the total possible points for the course, with the weights being adjusted as appropriate for other credit options. The final grades 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 difficulty of the assignments, but never upwards. Note that for the 3 credit option successful completion of all the problem sets guarantees a grade of at least B.

How the Credit Hours are Met: This course is offered for variable credit. One of these credits corresponds to the pre-class problem sets plus the final exam. The remaining two credits are associated with the group-based problem sets. Students are expected to engage in at least 45 hours of learning activities per credit.

Readings: Course notes, readings, and journal articles will be handed out in class. In addition, the following recommended books will be available in the instructor's outer office for reference:

R. M. Martin, *Electronic Structure: Basic Theory and Practical Methods.* Cambridge University Press: Cambridge, 2004.

C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids.* Oxford University Press: Oxford, 1972.

J. K. Burdett, *Chemical Bonding in Solids.* Oxford University Press: Oxford, 1995.

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 801: Tentative Course Calendar

Week, Day	Subject	Assignments
1, Jan. 22 (W)	Introduction; review of quantum mechanics	
Jan. 24 (F)	**Part 1: Basic crystallography.** Diffraction.	PPS#1
2, Jan. 27 (M)	Reciprocal space and the structure factor	PPS#2
Jan. 29 (W)	Space groups and symmetry operations	PPS#3
Jan. 31 (F)	*Group assignment 1:* CIF files to ABINIT input	
3, Feb. 3 (M)	Interpreting electron density: QTAIM	PPS#4
Feb. 5 (W)	*Group assignment 2a:* Computing Bader charges	
Feb. 7 (F)	*Group assignment 2b:* Electron density difference maps	GA#1 due
4, Feb. 10 (M)	**Part 2: Density functional theory.** Theorems.	PPS#5
Feb. 12 (W)	The Kohn-Sham Equation	PPS#6
Feb. 14 (F)	*Group assignment 3:* Density to diffraction	GA#2 due
5, Feb. 17 (M)	Self-consistent field calculations	PPS#7
Feb. 19 (W)	Exchange-correlation functionals	PPS#8
Feb. 21 (F)	*Group assignment 4:* Functionals of density	GA#3 due
6, Feb. 24 (M)	Pseudopotentials Pt. 1	PPS#9
Feb. 26 (W)	Pseudopotentials Pt. 2	PPS#10
Feb. 28 (F)	*Group assignment 5:* Operators on wavefunctions	GA#4 due
7, Mar. 2 (M)	The Kohn-Sham Equation in reciprocal space	PPS#11
Mar. 4 (W)	Derivation of semi-empirical models	PPS#12
Mar. 6 (F)	*Group work*	
8, Mar. 9 (M)	**Part 3: Wavefunctions in crystals.** Group theory review.	PPS#13
Mar. 11 (W)	Bloch's theorem; Bloch wavefunctions	PPS#14
Mar. 13 (F)	*Group assignment 6:* Band structure generation	GA#5 due
9	**Spring Break. No classes.**	
10, Mar. 23 (M)	Band structures of simple systems I	PPS#15
Mar. 25 (W)	Band structures of simple systems II	PPS#16
Mar. 27 (F)	*Group assignment 7:* Band structure survey	GA#6 due
11, Mar. 30 (M)	Brillouin zones and k-point meshes	PPS#17
Apr. 1 (W)	Symmetry in k-space	PPS#18
Apr. 3 (F)	*Group assignment 8:* Brillouin zones, Fermi surfaces	GA#7 due
12, Apr. 6 (M)	Density of states analysis	PPS#19
Apr. 8 (W)	Overlap populations	PPS#20
Apr. 10 (F)	*Group assignment 9:* Density of states	GA#8 due
13, Apr. 13 (M)	The electron localization function (ELF)	PPS#21
Apr. 15 (W)	Wannier functions, raMO analysis	PPS#22
Apr. 17 (F)	*Group assignment 10:* ELF and band electron densities	GA#9 due
14, Apr. 20 (M)	**Part 4: Models.** Fermi Surface nesting	PPS#23
Apr. 22 (W)	The nearly-free electron/Mott-Jones Model	PPS#24
Apr. 24 (F)	*Group assignment 11:* Fermi spheres and Jones Zones	GA#10 due
15, Apr. 27 (M)	The Zintl concept, polar intermetallics; Final exam distributed	PPS#25
Apr. 29 (W)	Magnetism: Stoner criterion, spin-polarization	PPS#26
May 1 (F)	Last day of class: donuts and group work.	GA#11 due

Final Exam due May 8, 2020, to be turned in via e-mail.