Chem 801, Spring 2018: Selected Topics in Inorganic Chemistry
Electronic Structure and Bonding in Inorganic Materials

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Office Hours: Tuesdays 2:25pm, and by appointment

Lectures: MWF 2:25-3:15pm; 8335 Chemistry; 1-3 credits

Description: 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.

Course Learning Objectives: 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. *Basic computer programming in c and Matlab.* Developing tools to aide the processing files and data; translation of theoretical models into executable code.

How the Credit Hours are Met: This course is offered for variable credit, with the completion of each of the three learning outcomes corresponding to one credit. Students are expected to engage in at least 45 hours of learning activities per credit.

Prerequisites: Graduate or professional standing, or permission from the instructor. 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 weekly problem sets. Each problem set will have three components: (1) Written problems to be solved without the use of a computer, (2) electronic structure analyses carried out using software freely available online, and (3) problems involving the creation of new programs. Students registering for less than three credits are only required to completed the components corresponding to the learning outcomes they have chosen.

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. 24 (W)	Introduction; review of quantum mechanics	
Jan. 26 (F)	**Part 1: Basic crystallography.** Diffraction.	
2, Jan. 29 (M)	Reciprocal space and the structure factor	**HW#1 Due**
Jan. 31 (W)	Space groups and symmetry operations	
Feb. 2 (F)	Using ABINIT: electron density	
3, Feb. 5 (M)	Interpreting electron density: QTAIM	**HW#2 Due**
Feb. 7 (W)	Electron density difference maps	
Feb. 9 (F)	**Part 2: Density functional theory.** Theorems.	
4, Feb. 12 (M)	The Kohn-Sham Equation	**HW#3 Due**
Feb. 14 (W)	Self-consistent field calculations	
Feb. 16 (F)	Exchange-correlation functionals	
5, Feb. 19 (M)	Pseudopotentials	**HW#4 Due**
Feb. 21 (W)	The Kohn-Sham Equation in reciprocal space	
Feb. 23 (F)	Implementation of DFT in ABINIT	
6, Feb. 26 (M)	Derivation of semi-empirical models	**HW#5 Due**
Feb. 28 (W)	**Part 3: Wavefunctions in crystals.** Group theory review.	
Mar. 2 (F)	Bloch's theorem; Bloch wavefunctions	
7, Mar. 5 (M)	Band structures of simple systems I	**HW#6 Due**
Mar. 7 (W)	Band structures of simple systems II	
Mar. 9 (F)	Brillouin zones and k-point meshes	
8, Mar. 12 (M)	Symmetry in k-space	**HW#7 Due**
Mar. 14 (W)	Band structures with ABINIT	
Mar. 16 (F)	Density of states analysis	
9, Mar. 19 (M)	Overlap populations, the electron localization function	**HW#8 Due**
Mar. 21 (W)	Wannier functions, raMO analysis	
Mar. 23 (F)	Fermi surfaces	
10	**Spring Break. No classes.**	
11, Apr. 2 (M)	**Part 4: Models.** Molecular crystals and Peierls distortions	**HW#9 Due**
Apr. 4 (W)	Fermi Surface nesting and charge-density waves	
Apr. 6 (F)	The nearly-free electron/Mott-Jones Model	
12, Apr. 9 (M)	The Zintl concept	**HW#10 Due**
Apr. 11 (W)	Polar intermetallics	
Apr. 13 (F)	**Part 5: Special topics.** Conductivity	
13, Apr. 16 (M)	Magnetism: Stoner criterion, spin-polarization	**HW#11 Due**
Apr. 18 (W)	Spin-orbit coupling	
Apr. 20 (F)	Angle-resolved photoelectron spectroscopy	
14, Apr. 23 (M)	Structural optimization, bulk-modulus	**HW#12 Due**
Apr. 25 (W)	Phonon band structures I	
Apr. 27 (F)	Phonon band structures II	
15, Apr. 30 (M)	Thermoelectrics	**HW#13 Due**
May 2 (W)	Superconductivity I	
May 4 (F)	Last day of class: Superconductivity II	