Chemistry 791: Bonding: from Molecules to Solids
https://sakai.unc.edu/portal/site/bonding

Mon. / Wed. / Fri., 8-8:50 AM in Venable G307  Fall 2013

Description: Bonding: from Molecules to Solids will use the viewpoint of chemistry to understand the electronic properties of molecules, solids, and surfaces. Beginning with a molecular orbital (MO) description of molecules, we then build up complexity as we move towards 3-D extended solids. Along the way we cover 1-D systems (e.g., conjugated polymers) and 2-D materials (from benzene to graphene). The overarching goal is to learn how to apply a chemists’ intuition for bonding in molecules to larger structures while also identifying those cases where not to apply that intuition – i.e., to appreciate why a chemists’ understanding sometimes fails when moving beyond molecular dimensions.

Professor: Scott Warren, Ph.D.
E-mail: sw@unc.edu
Phone: 919-966-0994
Pre-requisite: Physical chemistry
Office Hours: Tuesdays, 4:30 to 5:30 pm in Kenan A808 or by appointment.

Texts: No texts are required. When there is a reading assignment, copies of the relevant text will be placed on Sakai. With the exception of “Orbital Interactions in Chemistry”, the following texts have been placed on reserve in the science library.

Honor Code:
The University of North Carolina at Chapel Hill has had a student-led honor system for over 100 years. Academic integrity is at the heart of Carolina and we all are responsible for upholding the ideals of honor and integrity. The student-led Honor System is responsible for adjudicating any suspected violations of the Honor Code and all suspected instances of academic dishonesty will be reported to the honor system. Information, including your responsibilities as a student is outlined in the Instrument of Student Judicial Governance. Your full participation and observance of the Honor Code is expected.

Class policies:
1. Please be familiar with the UNC honor code: http://studentconduct.unc.edu
2. You are welcome to work together on homework assignments or in preparing for exams. It is your responsibility to identify the working situation that best helps you learn the course material. You are not allowed to work together on exams.
3. If you cannot attend an exam, please let me know as soon as possible. A make-up exam will be scheduled.
4. Assignments not turned in on time (i.e., in class on their due date) will lose 10% of their value for each day they are late.
5. Cell phone use is not permitted in class or during exams.
6. Please maintain an atmosphere that is respectful to others and conducive to learning.

Class content:

I. Atoms and molecules
   Atomic orbitals
   Molecular orbitals
   Perturbation theory

II. 1-D
   Orbitals and bands in 1-D
   Metals, semiconductors and insulators
   Conjugated polymers
   Conductivity and mobility
   Polaron theory

III. 2-D
   Orbitals and bands in 2-D
   Graphene and other examples of 2-D materials

IV. 3-D
   3-D band structures: theory
   3-D band structure: examples
   Polarons in 3-D
   Pauling and Hume-Rothery rules

V. Advanced topics
   Surfaces and chemisorption
   Molecular electronics
   Solar devices
Grading:
Class grades will be calculated as follows:
- Exam 1: 100 points
- Exam 2: 100 points
- Final exam: 200 points
- Homework: 500 points
- Research proposal: 100 points
- Total: 1000 points

Exam information:
Three exams will be given on the following dates:
- Sept. 27
- Nov. 1
- Finals week (after Dec. 5)
Questions on the final exam will be divided equally between content covered before Nov. 1 and the content covered after Nov. 1.

Research Proposal:
Students will write an original research proposal (due Nov. 25) that applies the course content to a topic of their own interest. The proposal will have a length of five double-spaced pages, not including references, and have three sections: (1) Introduction, which identifies an important research problem, (2) Research Plan, which develops the approach and methods used to address that problem, (3) Impact, which describes how the proposal has advanced basic understanding or improved the prospects for applications.

Each proposal will be submitted without personal identifying information and will be peer-reviewed by two anonymous classmates as well as by me. The grade will be based on a weighted average of the three reviews.