Class Syllabus

Ch120a: Nature of the Chemical Bond Units: 3-0-6 – Winter term 2012

Personnel

Instructor:
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Teaching Assistants:
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Locations and Hours:

Lecture:
MWF 2pm 134 Beckman Institute (Auditorium)
Office hours:
Friday 3-4 pm in BI 134 (Auditorium), immediately following class

Prerequisites:

Some knowledge of quantum mechanics and chemistry. (It is sufficient to have learned the material in Ma2, Ph2, Ch1, but nice to have some exposure to material covered in courses such as Ph12, Ch21, Ch41)

Overview:

Ch120a aims to provide a conceptual understanding of the chemical bond sufficient to semi-quantitatively predict the structures and properties of materials.

The philosophy is similar to that of Linus Pauling, who revolutionized the teaching of chemistry by including the concepts from quantum mechanics (QM), but not its equations. We also include the new understanding that has resulted from QM calculations over the last 40 years. We develop an atomistic QM-based understanding of the structures and properties of chemical, biological, and materials systems. This course is aimed at experimentalists and theorists in **chemistry**, **materials science**, **chemical engineering**, **applied physics**, **biochemistry**, **physics**, **geophysics**, and **mechanical engineering** with an interest in characterizing and designing molecules, drugs, and materials.

Courses in QM often focus more on applied mathematics rather than physical concepts. We start by understanding some of the essential differences between quantum and classical mechanics, one of which is the description of kinetic energy. These ideas are used to understand why atoms are stable and why chemical bonds exist. We then introduce the role of the Pauli principle and spin and proceed to use these basic concepts to predict the structures and properties of various classes of materials. These include molecules and solids spanning the periodic table.

Applications include:

- **Organics:** Resonance, strain, and group additivity. Woodward-Hoffman rules for pericyclic reactions, and reactions with dioxygen and ozone.
- **Semiconductors:** Focus on Si and GaAs, donor and acceptor impurities, surface reconstruction, and surface reactions.
- **Transition metal systems:** Role of *s* and *d* character in bonding in organometallic reaction mechanisms. (E.g. metathesis, oxidativeaddition, and reductive elimination). *Examples*: the Grubbs ROMP catalysts and the Periana $CH_4 \rightarrow CH_3OH$ catalysts.
- **Ceramics:** Oxides and ionic materials, relation between covalent and ionic character in bonding, concepts of ionic radii and packing in determining structures and properties. *Examples*: silicates, perovskites, and cuprates
- **Metals and metal alloys:** Bonding in bulk structures, chemisorption, and reaction on their surfaces
- **Hypervalent systems:** XeF_n, ClF_n, IBX chemistry
- **Bioinorganics:** Electronic states in oxy-hemoglobin and cytochrome P-450
- **Superconductors:** Fundamental mechanisms, applications to organic and cuprate systems

Grading, Homeworks, Resources, Collaboration Policy/Honor Code

• **Grading** There will be eight problem sets, a midterm exam, and a final exam. The final exam counts for 50% of the total grade in the course. The midterm exam and the sum of the homeworks each are 25% of the total grade.
• **Homeworks** Homeworks will be assigned on Fridays and will be due back on the following Wednesday **at 2pm**. TA's will aim to have all homeworks graded by the following Friday. The lowest-graded homework will be dropped from the total grade, however you are encouraged to make a serious attempt at every problem as the final exam will be consist of topics cumulative over all homeworks. Attending TA hours, especially on Monday, is strongly recommended.
• **Resources** Lecture summary guides, lecture material, and supplemental reading will be posted online at the class website. Additionally, a printed text for this course will be available on reserve at Millikan library (8th floor).
• **Collaboration Policy/Honor Code** We encourage collaboration on problem sets, but all students must write-up and hand-in their work separately. It is advised to spend at least an hour working on the problems yourself before collaborating with others. Exams will be take home and no collaboration will be allowed. Both problem sets and exams have an **open notes** policy only for notes taken **this year**. Your own notes from class, any materials downloaded from the class website **from this year**, and the printed class text are all free to be used for problem sets and exams. Notes from previous years, even if they are your own, are not allowed. No other textbooks or resources are permitted to be used to do problem sets or exams.
Please email a TA if you have questions regarding this policy.

Lecture Schedule

1	Review QM, role KE in stability of H and bonding in H2+
2	nodal thm, role of KE in bonding of H2, VB description H2
3	MO description bonding H2, symmetry theorem
4	Pauli Princ, spin, Slater det
5	Lack of bonding in He2, bonding in He2+
6	H atom excited states (1s,2p,3d etc),Li shielding,Aufbau principle
7	MO description Be, B, C,Hund's rule, N, O, F, Ne
8	Bonds to H: FH,OH,NH,BeH,BH,CH
9	CH vs SiH, CF vs CH use VB arguments
10	Symmetry Diatomics, Mulliken correlation Diagram
11	bonding Homonuclear diatomics (Ne2,F2,O2,N2,N2+,C2,B2,Li2, Li2+)
12	bonding in hydrocarbons (C2Hx, x=1,2,3; HC bond E)
13	semiconductors: Si,GaAs, GaN. Si(100) surface reconstruction
14	surface reconstruction GaAs(100) 2x4, Si(111) 7x7
15	Hydrocarbons: thermochem, resonance, strain
16	Woodward-Hoffmann Rules cycloaddition, electrocyclic, MO correlation diag
17	Pericyclic reactions, VB view
18	TM Atoms and bonding: reductive elimination, oxidatinve addition of Pt, Pd compounds
19	MH+ diatomics, Exchange, Periodic Trends
20	homogeneous catalysts:metallocene polymerization catalysts
21	homogeneous catalysts: ROMP, Periana CH4 activation
22	Bulk Metals: Structures, IEM, Binding H,C,O,N to Pt,Ru,Ni surfaces
23	HC reforming/Pt surfaces, fuel cell catalysts
24	Hemoglobin, c-P450
25	Ionic bonding molecules and crystals
26	Hypervalency (XeFn, ClFn, etc), IBX
27	Perovskites (catalyst, supercond., ferroelectric)
28	Fullerences, bucky tubes, etc
29	superconductors (BCD concept, explain High Tc cuprates)

TA Schedule

PS #1	Caitlin
PS #2	Fan
PS #3	Caitlin
PS #4	Hai
Midterm	Fan
PS #5	Hai
PS #6	Fan
PS #7	Hai
PS #8	Caitlin
Final	All