Class Syllabus
Ch120a: Nature of the Chemical Bond (Winter term 2023)

Instructor: William A. Goddard III (wagoddard3@gmail.com; wag@caltech.edu)

Teaching Assistants: : Charles Musgrave III (musgrave@caltech.edu)
Lectures: MWF 2-2:55 pm.
Room: Beckman Institute 115
Office hour: Monday 3-4 pm, Beckman Institute SB205E (Charles' office, subject to change)

Grading and Homework:

- There will be six problem sets, a midterm exam, and a final exam. The final exam counts for 48% of the total grade in the course. The midterm exam is 24% of the total grade, and the sum of the homeworks is 28% of the total grade.
- **Homeworks** will be assigned on Wednesdays and will be due back on the following Wednesday at 2pm. 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 consist of topics cumulative over all homeworks.

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 with 6 hour time limit; no collaboration 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 Alex if you have questions regarding this policy.

Prerequisites:
Some knowledge of quantum mechanics and chemistry. (It is sufficient to have learned the material in 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 inspired by Linus Pauling, who revolutionized the teaching of chemistry by including the concepts from quantum mechanics (QM), but not its equations. We now include the new understanding that has resulted from QM calculations over the last 60 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**, **bioengineering, 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, oxidative addition, and reductive elimination). *Examples*: the Grubbs ROMP catalysts and the Periana CH4 → CH3OH 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
- **Catalysts**: heterogeneous, homogeneous, electrocatalysis
- **Bioinorganics:** Electronic states in oxy-hemoglobin and cytochrome P-450
- **Hypervalent systems:** XeFn*,* ClFn, IBX chemistry
- **Superconductors:** Fundamental mechanisms, applications to organic and cuprate systems
- **Metals and metal alloys:** Bonding in bulk structures, chemisorption, and reaction on their surfaces

Tentative Lecture Schedule

Lecture #	Topic
1	Elements QM, role KE in stability of H and bonding in H2+ and H2
2	VB-MO H2-QMp2-4-Spin-PP-SlatDet
3	Energetics
4	H atom excited states (1s,2p,3d etc),Li shielding, Aufbau principle
5	MO description Be, B, C, Hund's rule, N, O, F, Ne
6	Bonds NeH, FH.OH,NH
7	BeBCHn-CH vs SiH, CF vs CH VB arguments
8	CC bonds, diamond-Si,Si(100) surface
9	Si(111) 7x7
10	GaAs(110),(100)reconstruction, bands
11	Symmetry
12	Mullikan correlation Diagram bonding Homonuclear diatomics
13	Reactions with O2, ozone, HO2, HOOH, VB vs MO,He2,He2+, vdw
14	Woodward-Hoffmann Rules cycloaddition, electrocyclic, MO correlation diag, VB view
15	Carbon, Hydrocarbons: thermochem, resonance, strain
16	Graphene, Fullerenes, bucky tubes, etc
17	Heme-O2,CO
18	TM Atoms and bonding: reductive elimination, oxidative addition Pt, Pd compounds
19	MH+ diatomics, Exchange, Periodic Trends
20	Ru Grubbs Metathesis
21	Homogeneous catalysts:CH4 to CH3OH, olefin metathesis
22	Heterogeneous catalysts: V2O5, VPO, BiMoOx, oxidation, ammoxidation
23	Electrocatalysis: water splitting, CO2 reduction
24	Pt surfaces, fuel cell catalysts
25	Ionic bonding molecules and crystals
26	Perovskites (catalysts, cuprates, ferroelectric)
27	Hypervalency (XeFn, ClFn, etc), IBX