Syllabus of MS131:
Instructor: Marco Bernardi (bmarco@caltech.edu)
TA: TBA

Lectures: Tuesday & Thursday, 2:30pm – 4pm.
Location: Watson 104
Recitations & TA office hours: to be announced by the TA
Check out **Moodle** for class materials

Policy – Contributions to the final grade:
Weekly problem sets: 30%. Problem sets are due in the box outside Steele 113.
Mid-term: 30%. Final: 40%.
Mid-term and Final are take-home, open book exams.

Prerequisites: Introductory quantum mechanics (e.g., Griffiths, or Chapter 2 of B&J).

Introduction:
1. Particles and forces. Origin of the elements. Nucleus, electrons, atoms, and solids.
Study: notes, handout.

Electronic structure of atoms:
2. Hydrogen atom: solution of Schrodinger's equation
3. Helium atom. Perturbative and variational approximations.
4. Exchange interaction. Many-electron atoms (qualitative) and Aufbau. Slater determinants.
5. Hartree-Fock.
This part of the course includes a brief review of spin, particle-exchange symmetry for the many-electron wavefunction, and the variational method.
Study: B&J chapter 2, parts of chapter 3, 4, 6, 7. Hartree-Fock is covered also in G&P.

Molecules and solids:
6. Born-Oppenheimer approximation. Electronic and vibrational hamiltonians. Examples. H_2^+ ion
7. Hydrogen molecule. Molecular orbitals. Huckel model.
8. Crystalline solids and translation symmetry. Bravais lattice and basis. Crystal structures.
9. Reciprocal lattice and Brillouin zone. Bloch states. Plane waves and pseudopotentials. Energy bands, and classification of semiconductors, metals, and insulators.
10. Bandstructures. Tight binding method. Examples.
11. Introduction to Density Functional Theory.
Study: Chapter 8 B&J and/or chapters 8–9 Atkins (molecules). Chapters 2–5 G&P (solids).

Bonding, structure, and electronic structure in specific material families:
12. Metals: Free-electron model, Jellium. Simple metals, *d* electrons, heavier metals.
13. Semiconductors (group IV, III-V, II-VI). Spin-orbit interaction.
14. Ionic crystals. Oxides. Transition metal oxides. Crystal field (ligand) theory.
15. Introduction to strongly correlated materials. Hubbard model. Mott insulators. Examples.
Study: G&P chapter 6. Notes.

Symmetry:
16. Introduction to symmetry and groups. Symmetry elements and operations in crystals.
17. Point groups in solids and molecules. Derivation of the 32 point groups.
18. Screw axes, glide planes. Introduction to space groups and international tables. Examples.
19–20. Tensor properties of crystals. How symmetry affects physical properties.
19–20. Beyond crystalline order: defects, dislocations, surfaces, amorphous materials.
Two options for lectures 19–20. Class to decide. **Study:** Buerger, plus notes and handouts.

Textbooks

Recommended books for atoms and molecules:
[B&J]: B.H. Bransden, C.J. Joachain, Physics of Atoms and Molecules. Addison-Wesley (2^{nd} ed.) Comprehensive treatment of atomic physics. Good introduction to molecular physics. Chapter 2 of this book is a great summary of basic QM. We will use this book for atoms and molecules. This book is referred above as B&J.

[Atkins]: P. Atkins, R. Friedman, Molecular Quantum Mechanics. Oxford (4^{th} ed. or 5^{th} ed.) Excellent treatment of molecular orbitals, theoretical quantum chemistry, and group theory. A must-have for quantum chemists.

Recommended books for solids:
[G&P] G. Grosso, G. Pastori Parravicini. Solid State Physics. Academic Press (2^{nd} ed.) A great book worth buying if you will be studying solid state physics beyond this class. Does not cover symmetry and groups. Referred above as G&P. This is a very good book on solids.
[Buerger] M. Buerger, Elementary Crystallography (Wiley 1963). We will use parts of this book for symmetry and point / space groups. You don't need to buy this book.

Optional (use from time to time for specific topics):
– P.A. Cox, Transition Metal Oxides. Oxford Press. Excellent resource on oxides.
– E. Kaxiras, Atomic and Electronic Structure of Solids. Cambridge.
Has a good collection of topics. It may not excel in any single topic, but it's a good starting point to study atoms and solids. The appendices are excellent. Good chapter on defects.
– N. Ashcroft, D. Mermin, Solid State Physics. Brooks/Cole. A timeless classic.

Useful textbooks:
It may be helpful to have introductory textbooks on quantum mechanics and electromagnetism handy. I like these two:
– D.J. Griffiths, Introduction to Quantum Mechanics. Pearson Prentice Hall (2^{nd} ed.)
– D.J. Griffiths, Introduction to Electrodynamics. Pearson Prentice Hall (3^{rd} ed.)