

Chem 263 Spring 2019 Quantum Mechanics

Required Text: Quantum Mechanics for Scientists and Engineers (David A. B. Miller)

Supplemental Text: Quantum Chemistry (Ira Levine); Solid State Physics (Ashcroft/Mermin)

Instructor: Yuan Ping, 354 PSB, 459-1390 (o), yuanping@ucsc.edu

Class Meets: TuTh, 11:40am-1:15pm, Nat Sciences Annex 102

Office hours: Fri. 1:30-2:30 pm or by appointment (email or call).

Homework: Assigned every other Thursday and collected the following Thursday (usually)

Grades: Based on HW (4 times) (40%), one take home final (40%) and one report (20%)

Report instructions: The report contains two parts: part I, read a recent joint experimental-theory paper, and explain how theoretical results support experiments in terms of: a. theoretical methods, b. physical quantity they compute, c. supportive argument and connections to experiments; part II, propose an experimental-theory project from your own experiments: a. what observations experiments need theory to explain or what physical phenomena experiments need theory to predict, b. what physical quantity you think theory should compute (and what theoretical approach could be possibly used *e.g.* similar to the paper you read), c. what possible theoretical outcomes could support experiments or make useful predictions for experiments

General Plan: We will cover the fundamental principles and modern theoretical methods in quantum mechanics that are used to describe the structure and dynamics of many-electron atoms, molecules and solids. We will discuss how to derive and solve both the electronic and the nuclear Schrödinger equations analytically and numerically to calculate the eigenfunctions and eigenvalues (*e.g.* energies) for molecules/solids. Dirac notation will be introduced early and used throughout the course. A special emphasis on quantum theory of solids will be introduced in the later part of this course.

Specific Plan:

W1. Waves and quantum mechanics - Schrödinger's equation (chapter 1 and 2)

W2. The time-dependent Schrödinger equation (chapter 3)

W3. Functions and operators (chapter 4)

W4. Operators and quantum mechanics (chapter 5)

W5. Angular momentum (chapter 9)

W6. The hydrogen atom (chapter 10)

W7. Spin (chapter 12) and identical particles (chapter 13)

W8. Electronic structure methods

. Born-Oppenheimer approximation

. Basic electronic structure: Hartree Fock theory, Density Functional Theory and beyond

. Basis sets and pseudopotentials

. Orbital energies, total energy and force

W9. Quantum mechanics in crystalline materials (chapter 8) including computer labs

. Lattice structures, reciprocal lattices and homogenous electron gas

W10. Quantum mechanics in crystalline materials including computer labs

. Band structures, density of states, metal/semiconductors/insulators

. Applications for heterogeneous catalysis and excited state properties