

CHEM 562, Section 1: Atomic and Molecular Quantum Mechanics

Spring 2021 MW 12.05-1.25 pm. GILMAN 2205

Topics:

Slater-Condon Rules

Hartree-Fock Approximation

LCAO Approximation and Basis Sets

Atomic Terms (L-S, j-j coupling), spin-orbit coupling

Born-Oppenheimer Approximation

Introduction to Diatomic Molecules

Origins of Chemical Bonding

Terms in Diatomic Molecules

Molecular Hartree-Fock, Approximate Methods

H₂ molecule and the Failure of Hartree-Fock Theory

Configuration Interaction, MCSCF

Perturbation Theory methods

Coupled Cluster methods

Introduction to Optical Spectroscopy

Instructor: Dr. Dipayan Datta (e-mail: ddatta@iastate.edu)

Office: 201 Spedding Hall

Office hours: Thursdays and Fridays between 2:00-4:00 pm or by appointment.

No cell phone calls or texting, etc. are allowed in class

Recommended books: Textbooks 1 and 2 are directly related to the content of this class. Books 3-5 will be used as additional references for certain topics.

1. Ira N. Levine

Quantum Chemistry, *7th Edition*

Prentice-Hall

2. Attila Szabo and Niel S. Ostlund,

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory

Dover Publications

3. Hans A. Bethe
Intermediate Quantum Mechanics
Taylor and Francis Group
4. E. U. Condon and G. H. Shortley
The Theory of Atomic Spectra
Cambridge University Press
5. Frank L. Piller
Elementary Quantum Chemistry
Dover Publications

Course grading:

All exams will be open book & open notes.

Midterm1: 25%
Midterm2: 25%
Final: 50%

Persons with disabilities: Please address any special needs and special accommodations with me at the beginning of the semester or as soon as you become aware of your needs. Those seeking accommodations based on disabilities should obtain a Student Academic Accommodation Request (SAAR) form from the Student Disability Resource (SDR) office (phone 515-294-7220). SDR is located on the main floor of the Student Services Building, Room 1076.