University of Wisconsin-Madison Spring 2020 Chemistry 562. Physical Chemistry

Instructor: Professor A. Yethiraj, 8305B Chemistry, 608 262 0258, Office hours: By

appointment

Teaching assistants: Mr. Inhyuk Jang (ijang5@wisc.edu) and Mr. Xinyi Li

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Canvas Course URL https://canvas.wisc.edu/courses/174914

Instructional mode: face-to-face

Course Description: Quantum theory, atomic structure, molecular structure and spectra, statistical mechanics, reaction dynamics

Requisite: Chem 561 or Chem 565 or Chemical & Biological Engineering 310 (formerly called CBE 211), AND Physics 202 or 208.

How Credit Hours are Met: This class meets for forty-one 50-minute lectures over the course of the semester. Students are expected to do at least 135 hours of learning activities, which includes class attendance, reading, studying, preparation, problem sets, and other learning activities.

Grading: Two mid-term exams (100 points each), 12 problem sets (10 points each), and one final exam (200 points). All exams are closed-book. Mid-term exams will be held in-class on February 21 and April 2.

Learning outcomes: This course discusses the microscopic view of matter and chemical phenomena using the tools of quantum mechanics and statistical thermodynamics. By the end of the semester, students should be able to

- 1. Describe fundamental quantum mechanics concepts, including operators, wave functions, and the uncertainty principle.
- 2. Use quantum chemistry models to describe the translational, rotational, and vibrational motion of particles, the microscopic details of atomic and molecular structures, and the basis of rotational, vibrational and electronic spectroscopies.
- 3. Apply quantum chemistry and statistical thermodynamic models to describe bulk thermodynamic properties, chemical equilibrium, and chemical reaction dynamics.

Textbook/Reference

Atkins, P., and J. de Paula. Physical Chemistry (9th edition), Recommended

Course Outline

- 1. Quantum Theory: Introduction and principles
- 2. Quantum Theory: Techniques and applications
- 3. Atomic Structure and Spectra
- 4. Molecular Structure
- 5. Molecular Spectroscopy
- 6. Statistical Thermodynamics: Concepts
- 7. Statistical Thermodynamics: Applications
- 8. Rates of Chemical Reactions
- 9. Reaction dynamics