Spring 2016  
CHEM 442  
Physical Chemistry I  
Quantum Chemistry & Spectroscopy  
University of Illinois at Urbana-Champaign

Room: 217 Noyes Laboratory  
Lecture period: January 20 – May 4, MWF 10:00 – 10:50 AM  
Final exam: May 12, 8–11 AM (217 Noyes Laboratory)

Instructor: So Hirata  
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Office hours: MWF 11:00 – 11:50 AM

Teaching assistant 1: Sean Carney  
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Office hours: T 3:30 – 4:30 PM @ Chem Library Group Study Room;  
R 4:30 – 5:30 PM @ Chem Library Conf. Room (except Feb 11)

Teaching assistant 2: Joseph Courtney  
Email: joseph.m.courtney@gmail.com  
Office hours: T 3:30 – 4:30 PM @ Chem Library Group Study Room;  
R 3:30 – 4:30 PM @ Chem Library Conf. Room (except Feb 11)

Required text: P. Atkins and J. de Paula, “Physical Chemistry,” 10th or earlier edition

Prerequisites: CHEM 204 or 222; MATH 225 or 415; PHYS 211, 212 or 214  
Recommended: MATH 285

Objectives: CHEM 442 is the first of the two-term sequence of Physical Chemistry, CHEM 442-444. It covers quantum mechanics in relation to atomic and molecular electronic structure and spectroscopy. The objective is the mastery of basic principles, numerical techniques, and applications of quantum chemistry, molecular point-group symmetry, and the theory of rotation, vibration, and electronic spectroscopies as well as electron spin and nuclear magnetic resonance spectroscopies.

This will be a problem course of instructions (or an inverted or flipped course). All lectures are recorded and made available online along with the power point presentations at http://butane.chem.illinois.edu/sohirata. Students are expected to view these at home and in advance. In each class, a set of problems on the day’s lecture topic (see below for the tentative schedule) is handed out to students, who solve them either individually or in teams. In the next class, randomly selected students are asked to present and explain their solutions and all must submit the written solutions. A next set of problems is given. This will be repeated throughout the course.
Exams: There will be **two (2) hourly examinations** (occurring during the normal class period in the normal classroom) and a **final examination**.

Attendance: Class attendance is essential and will be monitored through the submissions of written solutions in each class.

Grades: The participation in the problem course of instruction 50% + the final exam 20% + the hourly exams 30%. The total percentage score will be rounded to the nearest integer. Grade A (A+, A, and A−) will be given to a score 85 –100%; B (B+, B, and B−) to 75 – 84%; C (C+, C, and C−) to 65 – 74%; D (D+, D, and D−) to 50 – 64%.

Student code: Students’ rights and responsibilities are stipulated in the student code found at [http://admin.illinois.edu/policy/code](http://admin.illinois.edu/policy/code)

Tentative schedule: See [http://butane.chem.illinois.edu/sohirata](http://butane.chem.illinois.edu/sohirata)