Fall 2023
CHEM 442 Section B
Physical Chemistry I
Quantum Chemistry & Spectroscopy
University of Illinois at Urbana-Champaign

Room:	Noyes 161
Lecture period:	August 21 – December 6, MWF 10:00 – 10:50 AM
Final exam:	December 14, 8:00 – 11:00 AM @ Noyes 161
Moodle:	https://learn.illinois.edu/ (for announcements and grades dissemination only)
Instructor:	So Hirata Email: sohirata@illinois.edu Phone: 217-244-0629 (for receiving messages only) Office hours: MWF 11:00 AM – 12:00 PM @ Noyes 355F
Teaching assistant 1:	Daniel McIntosh Email: daniel57@illinois.edu Office hours: R 11:00 AM – 1:00 PM @ Noyes 355A (tentative)
Teaching assistant 1:	Rapti Pal Email: raptip2@illinois.edu Office hours: T 2:00 PM – 4:00 PM @ Noyes 355A (tentative)
Required text:	None
Recommended text:	P. Atkins and J. de Paula, "Physical Chemistry," any edition
Prerequisites: Recommended:	CHEM 204 or 222; MATH 225 or 415; PHYS 211, 212 or 214 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 ***an inverted (or flipped) course***. All lectures are recorded and made available online along with the powerpoint 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. See more on this below.

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 attendance 37% + the participation 18% + the final exam 15% + the two hourly exams 2 x 15%. Grade A (A+, A, and A–) will be given to a score 85 –100%; B (B+, B, and B–) to 75 – 84.99%; C (C+, C, and C–) to 65 – 74.99%; D (D+, D, and D–) to 50 – 64.99%.
Student code:	Students' rights and responsibilities are stipulated in the student code found at http://admin.illinois.edu/policy/code
Tentative schedule:	See http://butane.chem.illinois.edu/sohirata
Inverted course:	(1) All lectures are recorded and made available online along with PowerPoint files. Watch one at home and solve the matching problem set before class. Note that some lectures are divided into 2 video files. (2) During class, as many students as there are problems in the problem set are randomly selected and asked to write down the solutions on the blackboard and explain them to the class. The score of +1 is recorded to each presenting student (regardless of the accuracy of the solution), –1 to absence, 0 to a pass, and +2 to volunteering for a difficult problem. These scores become the basis of the ***participation score*** of the final grade. (3) At the end of class, all students are asked to submit the written solutions. They are not graded but recorded as attendance and become the basis of the ***attendance score*** of the final grade. No early or late submission is accepted.