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

Room: 112 Transportation Building
Lecture period: August 27 – December 12, MWF 9:00 – 9:50 AM
Final exam: December 19, W 7:00 – 10:00 PM (the location to be announced)

Instructor: So Hirata
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Phone: 214-277-0629
Office: CLSL A206
Office hours: MWF 10:00 – 10:50 AM

Teaching assistant 1: TBA
Email: TBA
Office: TBA
Office hours: TBA

Teaching assistant 2: TBA
Email: TBA
Office: TBA
Office hours: TBA

Required text: P. Atkins and J. de Paula, “Physical Chemistry,” 9th or earlier edition

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

Objectives: CHEM 442 is the first of the two-term sequence of Physical Chemistry, CHEM 442-444, covering 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. All lectures are recorded and made available online along with the power point presentations, which students are expected to view 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 an hourly examination (occurring during the normal class period at the normal class room) 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 30% + the hourly exam 20%. 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

Tentative schedule:

<table>
<thead>
<tr>
<th>Date</th>
<th>Topics</th>
<th>Chapter**</th>
</tr>
</thead>
<tbody>
<tr>
<td>8/27, 29, 31, 9/5*, 7*, 10*, 12*, 14*</td>
<td>Quantum theory: introduction &amp; principles</td>
<td>7</td>
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<tr>
<td>9/17*, 19*, 21, 24, 26, 28, 10/1, 3</td>
<td>Quantum theory: techniques &amp; applications</td>
<td>8</td>
</tr>
<tr>
<td>10/5, 8, 12, 15, 17, 19, 22</td>
<td>Atomic structure &amp; spectra</td>
<td>9</td>
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<tr>
<td>10/24</td>
<td>Hourly exam</td>
<td>7, 8, &amp; 9</td>
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<tr>
<td>10/26, 29, 31, 11/2, 5, 7, 9</td>
<td>Molecular structure</td>
<td>10</td>
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<tr>
<td>11/12, 14, 16</td>
<td>Molecular symmetry</td>
<td>11</td>
</tr>
<tr>
<td>11/26, 28, 30, 12/3, 5, 7, 10, 12</td>
<td>Molecular spectroscopy</td>
<td>12, 13, &amp; 14</td>
</tr>
<tr>
<td>12/19</td>
<td>Final exam</td>
<td>7 – 14</td>
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</tbody>
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* Substitute instructor: TBD.
** In the 9th edition.