CHEM 0351

Quantum Chemistry and Spectroscopy

Fall, 2014

Instructor: Professor Sunhee Choi (Office BIH 544, Tel. ext. 5716, choi@middlebury.edu)

 Office Hour: MTWH 11 - 12:30

goals in this course: To understand atomic structure, molecular bonding, and spectroscopy

 using quantum theory.

Text Book: *Physical Chemistry A Molecular Approach* by McQuarrie and Simon,

University Science Books, 1997.

Meeting Times: MWF 8:40 - 9:55 (MBH 411)

Required activities:

**Reading and Participation**: Critically read the corresponding subject in the textbook (high light, make notes, Do Examples and Self-test, etc.) before you come to the class.

**Rewrite of Your Notes after the lecture**: Review your class notes as soon as possible after class. You can refer to your textbook or come to me to clarify confusing concepts. And rewrite your notes completely now that you have the organization of the total lecture in your mind. A summary of its main points can be also added.

**Homework problem sets**: You should make a habit of doing homework all by yourself. The main purpose of doing homework is for you to be able to learn independently and solve the problem independently. You should try to solve the problem for yourself for at least one solid hour before asking for help. This practice will eventually give you confidence in your ability in solving problems and enable you to do well in the exam.

**Exams**: Three Exams.

**Portfolio**: Make your portfolio as a written proof of your effort containing the following items:

* Rewrite of class material,
* Corrected HW problem solutions,

 If your portfolio shows your effort is outstanding, you will have opportunity to correct your exam and improve your grade. For example, if you got 80 points out of 100 for the first exam and you show me your Gold effort along with the corrected problems, your new grade for the first exam will be 90 points [80 + (100 - 80) x 0.5 = 90].

Determination of Final Grades

HW 25%

1st Exam 25%

2nd Exam 25%

3rd Exam 25%

Tentative Class Schedule

Chapter 1 The Dawn of the Quantum Theory (3 days)

Chapter 2 The Classical Wave Equation (2 days)

Chapter 3 The Schrödinger Equation and a Particle In a Box (4 days)

Chapter 4 Some Postulates and General Principles of Quantum Mechanics (2 days)

Chapter 5 The Harmonic Oscillator and the Rigid Rotator: Two Spectroscopic Models (3 days)

Chapter 6 The Hydrogen Atom (4 days)

Chapter 7 Approximate Methods (2 days)

Chapter 8 Multielectron Atoms (4 days)

Chapter 9 The Chemical Bond: Diatomic Molecules (5 days)

Chapter 10 Bonding in Polyatomic Molecules (1 day)

Chapter 13 Molecular Spectroscopy (3 days)

Chapter 14 Nuclear Magnetic Resonance Spectroscopy (1 day)

Chapter 15 Laser Spectroscopy (2 days)

CHEM 0351 (F '14) Tentative Schedule

 M T W Th F

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| --- | --- | --- | --- | --- | --- |
| W1Ch. 1:Quantum Theory | 9/8 D1Introduction1-1: BBR1-2: Planck1-3: Einstein | 9/9 | 9/10 D21-4: H-Atom Spectrum1-5: Rydberg Const1-6: de Broglie1-7: de Broglie Wave | 9/11 | 9/12 D31-8: Bohr Theory1-9: Heisenberg  |
| W2Ch. 2:Classical Wave Eq. | 9/15 D4 Discussion2-1: Vibrating String2-2: Wave eq. | 9/165 pm: HW#1 Due | 9/17 D52-3: Differential Eq.2-4: General Solution2-5: 2-d wave eq. | 9/18 | 9/19 D63-1: Schrodinger eq3-2: Operator3-3: Eigenvalue |
| W3Ch. 3:Particle in a Box | 9/22 D7 Discussion3-4: Wave function 3-5: Quantized Energy | 9/235 pm: HW#2 Due | 9/24 D83-6: Normalized Wave F3-7: Average momentum3-8: Uncertainty Prin.3-9: 3-d particle in-a-box | 9/25  | 9/26 D9No Class☺ |
| W4Ch. 4:Quantum Postulate | 9/29 D10 Discussion4-1: State of a System4-2: Q. Operator4-3: Observable | 9/305 pm: HW#3 Due | 10/1 D114-4: Time-dependent 4-5: Orthogonality4-6: Commutator | 10/2 | 10/3 D125-1: Hook's law5-2: Reduced mass5-3: Internuclear potential5-4: Energy level of HO |
| W5Ch. 5:Harmonic OscillatorRigid Rotator | 10/6 D13 Discussion5-5: IR5-6: HO wave Func. | 10/75 pm: HW#4 Due | 10/8 D145-7: Hermite Polynom5-8: Energy level of RR5-9: Rot. Diatom | **10/9****7 pm****Exam I****Ch 1, 2, 3, 4** | 10/10 D156-1: Exact Soln of H atom6-2: Spherical Harmonics |
| W6Ch. 6:Hydrogen Atom | 10/13 Mid-Term Recess | 10/14Mid-Term Recess | 10/15 D16Discussion6-3: Angular Momentum | 10/16 5 pm: HW#5 Due | 10/17 D176-4: Three Q. numbers6-5: s Orbital |
| W6.5W7Ch. 7:Approximate Methods | 10/20 D18Discussion6-6: p orbitals6-7: He atom | 10/21 | 10/22 D197-1: Variation Method7-2: Secular Determinant | 10/23 | 10/24 D207-3: Variation Parameters7-4: Perturbation Theory5 pm: HW#6 Due |
| W7.5W8Ch. 8:Multielectron  | 10/27 D21Discussion8-1: Atomic Unit8-2: Helium8-3: Hartree-Fock | 10/285 pm: HW#7 Due | 10/29 D228-4: Spin 8-5: Antisymmetric 8-6: Slater Determinant | 10/30 | 10/31 D238-7: HF and Exp.8-8: Term Symbol8-9: J  |
| W8.5W9Ch. 9:Chemical Bond:Diatomic Molecules | 11/3 D24Discussion8-10: Hund's rule8-11: Atomic Spectra | 11/4 5 pm: HW#8 Due | 11/5 D259-1: The Born-Oppenheimer Approx.9-2: 9-3: Overlap Integral | **11/6****7 pm****2nd Exam****Ch 5, 6, 7, 8** | 11/7 D269-4: Stability of Bond9-5: Bonding, Anti B.9-6: H2 MO |
| W9.5W10Ch. 9:Chemical Bond:Diatomic Molecules | 11/10 D27Discussion9-7: Order9-8: No He2 molecules9-9: Pauli Exclusion 9-10: O2 | 11/115 pm: HW#9A-I Due | 11/12 D289-11: Photoelectron 9-12: Heteronuclear Di.9-13: SCF-LCAO-MO | 11/13 | 11/14 D299-14: Molecular Term Sy.9-15: Symmetry9-16: Excited Electron St. |
| W10.5W11Ch. 10:Polyatomic Mol. | 11/17 D30Discussion10-5: Aromatic10-6: Butadiene | 11/185 pm: HW#9-II Due | 11/19 D3113-1: EM spectrum13-2: Rot-Vib13-3: *P* and *R* branch13-4: Pure Rot. Spec | 11/20 | 11/21 D3213-5: Overtones13-6: Electronic Spec.13-7: Frank-Condon |
| W11.5Ch. 13Molecular Spectroscopy | 11/24 D33Discussion13-11: Selection Rules13-12: RR13-13: HO. | 11/255 pm: HW#10 Due | 11/26 Thanksgiving recess  | 11/27Thanksgiving Day | 11/28Thanksgiving recess |
| W12Ch. 14: NMRCh. 15: Laser | 12/1 D34Discussion14-1, 14-2, 14-3, etc. | 12/25 pm: HW#11Due | 12/3 D3515-1, 15-2, 15-3 | 12/4 | 12/5 D3615-4 |
|  | 12/8 Exam Period Begins | 12/9 Final Exams | 12/10 | **12/11** **3rd Exam****Ch 9, 10, 13, 14, 15** | 12/12 |