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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| --- | --- | --- | --- | --- | --- |
| W1  Ch. 1:  Quantum Theory | 9/8 D1  Introduction  1-1: BBR  1-2: Planck  1-3: Einstein | 9/9 | 9/10 D2  1-4: H-Atom Spectrum  1-5: Rydberg Const  1-6: de Broglie  1-7: de Broglie Wave | 9/11 | 9/12 D3  1-8: Bohr Theory  1-9: Heisenberg |
| W2  Ch. 2:  Classical Wave Eq. | 9/15 D4  Discussion  2-1: Vibrating String  2-2: Wave eq. | 9/16  5 pm: HW#1 Due | 9/17 D5  2-3: Differential Eq.  2-4: General Solution  2-5: 2-d wave eq. | 9/18 | 9/19 D6  3-1: Schrodinger eq  3-2: Operator  3-3: Eigenvalue |
| W3  Ch. 3:  Particle in a Box | 9/22 D7  Discussion  3-4: Wave function  3-5: Quantized Energy | 9/23  5 pm: HW#2 Due | 9/24 D8  3-6: Normalized Wave F  3-7: Average momentum  3-8: Uncertainty Prin.  3-9: 3-d particle in-a-box | 9/25 | 9/26 D9  No Class☺ |
| W4  Ch. 4:  Quantum Postulate | 9/29 D10  Discussion  4-1: State of a System  4-2: Q. Operator  4-3: Observable | 9/30  5 pm: HW#3 Due | 10/1 D11  4-4: Time-dependent  4-5: Orthogonality  4-6: Commutator | 10/2 | 10/3 D12  5-1: Hook's law  5-2: Reduced mass  5-3: Internuclear potential  5-4: Energy level of HO |
| W5  Ch. 5:  Harmonic Oscillator  Rigid Rotator | 10/6 D13  Discussion  5-5: IR  5-6: HO wave Func. | 10/7  5 pm: HW#4 Due | 10/8 D14  5-7: Hermite Polynom  5-8: Energy level of RR  5-9: Rot. Diatom | **10/9**  **7 pm**  **Exam I**  **Ch 1, 2, 3, 4** | 10/10 D15  6-1: Exact Soln of H atom  6-2: Spherical Harmonics |
| W6  Ch. 6:  Hydrogen Atom | 10/13  Mid-Term Recess | 10/14  Mid-Term Recess | 10/15 D16  Discussion  6-3: Angular Momentum | 10/16  5 pm:  HW#5 Due | 10/17 D17  6-4: Three Q. numbers  6-5: s Orbital |
| W6.5  W7  Ch. 7:  Approximate Methods | 10/20 D18  Discussion  6-6: p orbitals  6-7: He atom | 10/21 | 10/22 D19  7-1: Variation Method  7-2: Secular Determinant | 10/23 | 10/24 D20  7-3: Variation Parameters  7-4: Perturbation Theory  5 pm: HW#6 Due |
| W7.5  W8  Ch. 8:  Multielectron | 10/27 D21  Discussion  8-1: Atomic Unit  8-2: Helium  8-3: Hartree-Fock | 10/28  5 pm: HW#7 Due | 10/29 D22  8-4: Spin  8-5: Antisymmetric   8-6: Slater Determinant | 10/30 | 10/31 D23  8-7: HF and Exp.  8-8: Term Symbol  8-9: J |
| W8.5  W9  Ch. 9:  Chemical Bond:  Diatomic Molecules | 11/3 D24  Discussion  8-10: Hund's rule  8-11: Atomic Spectra | 11/4  5 pm: HW#8 Due | 11/5 D25  9-1: The Born-Oppenheimer Approx.  9-2:  9-3: Overlap Integral | **11/6**  **7 pm**  **2nd Exam**  **Ch 5, 6, 7, 8** | 11/7 D26  9-4: Stability of Bond  9-5: Bonding, Anti B.  9-6: H2 MO |
| W9.5  W10  Ch. 9:  Chemical Bond:  Diatomic Molecules | 11/10 D27  Discussion  9-7: Order  9-8: No He2 molecules  9-9: Pauli Exclusion  9-10: O2 | 11/11  5 pm: HW#9A-I Due | 11/12 D28  9-11: Photoelectron  9-12: Heteronuclear Di.  9-13: SCF-LCAO-MO | 11/13 | 11/14 D29  9-14: Molecular Term Sy.  9-15: Symmetry  9-16: Excited Electron St. |
| W10.5  W11  Ch. 10:  Polyatomic Mol. | 11/17 D30  Discussion  10-5: Aromatic  10-6: Butadiene | 11/18  5 pm: HW#9-II Due | 11/19 D31  13-1: EM spectrum  13-2: Rot-Vib  13-3: *P* and *R* branch  13-4: Pure Rot. Spec | 11/20 | 11/21 D32  13-5: Overtones  13-6: Electronic Spec.  13-7: Frank-Condon |
| W11.5  Ch. 13  Molecular Spectroscopy | 11/24 D33  Discussion  13-11: Selection Rules  13-12: RR  13-13: HO. | 11/25  5 pm: HW#10 Due | 11/26  Thanksgiving recess | 11/27  Thanksgiving Day | 11/28  Thanksgiving recess |
| W12  Ch. 14: NMR  Ch. 15: Laser | 12/1 D34  Discussion  14-1, 14-2, 14-3, etc. | 12/2  5 pm: HW#11  Due | 12/3 D35  15-1, 15-2, 15-3 | 12/4 | 12/5 D36  15-4 |
|  | 12/8 Exam Period Begins | 12/9 Final Exams | 12/10 | **12/11**  **3rd Exam**  **Ch 9, 10, 13, 14, 15** | 12/12 |