**Chemistry 646/464**: Theoretical Chemistry (Spring 2016)

Time and Place:  M, W 12:00-12:50 PM, LaT 201 or otherwise arranged, and F 12:00-12:50 PM FR205 or otherwise arrange

Textbook:  *Quantum Chemistry & Spectroscopy,*  by Thomas Engel

Instructor:  Tao Xu, Office: LaT 326, Phone: 753-6357, e-mail: xu@niu.edu

Office Hour:  M, W 1:00-2:00 PM or by appointment

| Date | Tentative Topic | Reading |
|---|---|---|
| Jan. 19 | **Martin Luther King, Jr. Birthday (University Closed)** | |
| Jan. 20, 22 | From Classical to Quantum Mechanics | Ch. 1 |
| Jan. 25, 27, 29 | The Schrödinger Equation | Ch. 2 |
| Feb. 1, 3, 5,8 | The Quantum Mechanical Postulates | |
| Feb. 10, 12, 15 | Using Quantum Mechanics on Simple Systems | Ch. 3-4 |
| Feb. 17, 19,22 | The Particle in the Box and the Real World | Ch. 5 |
| Feb. 24, 26, 29 | Commuting and Noncommuting Operators and | |
| | the Surprising Consequences of Entanglement | Ch. 6 |
| Mar. 2 | **First Mid Term Exam: 12:00-12:50 P.M.,** | |
| Mar. 4, 7, 9 | A Quantum Mechanical Model for the Vibration and | |
| | Rotation of Molecules | Ch. 7 |
| Mar. 11, | The Vibrational and Rotational Spectroscopy of Diatomic Molecules | Ch. 8 |
| March 13-20 | **Spring Break** | |
| Mar. 21, 23 | The Vibrational and Rotational Spectroscopy of Diatomic Molecules | Ch. 8 |
| March 25, 28, 30 | The Hydrogen Atom | Ch. 9 |
| April 1, 4, 6 | Many-Electron Atoms | Ch. 10 |
| April 8, 11 | Examples of Spectroscopy Involving Atoms | Ch. 11 |
| April 13 | **Second Mid Term Exam: 12:00-12:50 P.M.,** | |
| April 15, 18 | Chemical Bonding in $H_2^+$ and $H_2$ | Ch. 12 |
| April 20, 22, 25 | Chemical Bonding in Diatomic Molecules | Ch. 13 |
| April 27, 29, May | Molecular Structure and Energy Levels for Polyatomic Molecules | Ch. 14 |
| May 4, | Reading day | |
| May 5 | **Final Exam: 12:00-1:50 P.M., Monday** | |

Grading:   There are weekly homework problems (10 points each), two mid-term exams and one final exam (100 points each).  In addition, the students will carry out two computational projects (50 points each) in the second half of the semester.  The total points are weighted as

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|---|---|
| Weekly  homework problems: | 30% |
| Two mid-term exams | 40% (20% each) |
| Final exam: | 30% |

Student's grade is based on the percent finish of the total available points as weighted above:
A: %100-90     B: %89-80     C: %79-70     D: %69-60     F: < %60