

CHM 6470: Chemical Bonding and Spectra I
Fall 2012.

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Book
Quantum Chemistry. Ira Levine. 6th edition

Class Times
T, R Period 2-3 (8:30 – 10:25 am) @ CLB 313

Office hours
T 3 → 4 PM, Leigh Hall 440

Course Outline

Homework:..... 25%
Midterms:.....50%
Final:..... 25%

Homework:

Homework due date is posted on the class calendar. Late homework (**if** it is turned in on the same day, but after deadline) will have a **20% deduction on the grade**. No more homework will be accepted for grading after that. Each homework problem has to show the **full derivation**. The homework answers should be present in a professional manner, with all steps explained. **No points will be given for a final result without justification.**

Exams and quizzes:

There will be 2 progress exams with dates to be announced soon.

There will be no make-up exams.

Cheating on an exam will result in a grade of zero for that case. If any homework or quiz assignment is suspect, a grade of zero will also be given for that assignment. If cheating is suspected, it will be reported to the university as such.

Honor Code:

The student honor code can be found at
<http://www.registrar.ufl.edu/catalog/policies/students.html>

The students and instructor are honor bound to comply with the Honors Pledge:

We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

Class schedule:

This is a ***tentative*** schedule for the course.

Topics:

1. Schrödinger Equation.
2. Particle in a box and particle in a finite well
3. Operators and bra-ket notation.
4. Hermitian operator and physical observable
5. Harmonic oscillator and lowering raising operator
6. Normal mode analysis
7. Uncertainty principle
8. Angular momentum
9. Spin and Pauli matrices
10. One particle central force problem
11. Hydrogen atom
12. Quantum mechanical Virial Theorem
13. Perturbation theory
14. Degenerate perturbation theory
15. Stark effect
16. Variational method and basis set
17. Huckel method and tight binding theory
18. Interaction between two states and avoided crossing
19. Hartree-Fock
20. Configuration Interaction and other correlated methods