Chmy 564: Advanced Quantum Chemistry

Preliminary Syllabus (29nov18)

Professor: Callis
Office: 55 CBB
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Time and place: MWF 1:10-2:00 in Gaines Hall 345
Text: Quantum Chemistry, 7th Edition by Ira N. Levine
Some other reading will be provided.
Prerequisite: Chmy 557 or 371 or equivalent or consent.
Undergraduates are welcome! (even without 557)
Webpage http://www.chemistry.montana.edu/callis/courses/chmy564.html

Note: A strong attempt will be made to build on previous courses students may have had, but at the same time be self-contained and complete. The aim is to impart a maximum of understanding and intuition, in addition to some new skills—all with a minimum of time-consuming homework.

Scope: Applications of quantum mechanics to many-electron atoms and molecules, concentrating on stationary and time-dependent electronic and vibrational states.

Course Outline:

Part I: Time Independent

1. Personalized review of philosophy and foundations, including:
    - Scope of theoretical chemistry (starting with the Big Bang)
    - Need for quantum mechanics
    - Quantum concepts and "understanding" quantum mechanics
    - Brief review of operators, wavefunctions, the virial theorem, and the Schrödinger equation with and without time,
    - Wavefunction "curvature": relation to kinetic energy and tunneling
    - Nodal properties of 3D wavefunctions for various shapes
    - Physical relevance and the Rules of Quantum Mechanics
    - Comments on Dirac notation

2. Variation principle, linear variation method, and perturbation limit
    - Theorem and its importance
    - Examples of non-linear variation
    - General equations for linear variation method
    - Diagonalizing the 2 x 2 orthonormal case "at a glance"
    - Larger matrices: use of simple programs
    - Non-orthogonal case

3. Born-Oppenheimer approximation,
Franck-Condon factors, and vibrational structure of molecular electronic transitions (including photoelectron spectra)

4. Integration of symmetry and group theory in the context of quantum mechanics

5. Quantum Chemistry, including hands-on ab initio, DFT, and quantum molecular dynamics computation

Part II: Time dependent quantum mechanics

1. Time dependent Schrödinger Equation
    - Behavior at a resonance, and non-resonance, weak and strong coupling limits.
    - General time dependent perturbation theory; "Femi golden rule" with application to absorption and emission of light, and electron transfer.

2. (a) Time Dependence of Probability Density (Liouville Eq.)
    - Feynman-Vernon-Hellwarth vector space in the two-state problem
    - Coherence, dephasing
    - Applications to magnetic resonance

(b) **A**tom-centered **D**ensity **M**atrix **P**ropagation (**ADMP**)
This is part of the Gaussian 09 package, remarkably easy to use, and provides insight into mechanisms of simple chemical processes with short computation times (usually several minutes on a desktop computer).