FCH3 course outline

Quantum mechanics

1. Principles of QM
2. Schrödinger equation
3. Hamiltonian of a molecule
4. Born-Oppenheimer approximation
5. Atomic orbitals, quantum numbers, Pauli exclusion principle
6. Molecular orbitals, origins of chemical bond

Molecular vibrations

1. Separation of translational, rotational and vibrational degrees of freedom
2. QM formulation - Schrödinger equation for nuclei
3. Potential energy operator
4. Harmonic approximation, solution of Schrödinger equation for harmonic oscillator
5. Energy levels, zero point energy, shape of the wavefunction
6. Selection rules for vibrational transitions in IR spectrum
7. Anharmonicity, Morse potential
8. Polyatomic molecule: normal modes and normal coordinates

Computational chemistry

1. MO-LCAO approximation, Slater determinant
2. Variational principle
3. One-electron approximation, principles of Hartree-fock method
4. Correlation energy and methods for its calculation
5. DFT basics - Hohenberg-Kohn theorem
6. Computable properties - gradient, Hessian, electrostatic properties etc.
7. MM forcefield - form of the potential

Noncovalent interactions

1. Physical principles and distance dependence
    a. Coulombic interaction, dipole-dipole interaction
    b. Polarization(induction)
    c. London dispersion
    d. Pauli repulsion
2. Specific interaction motifs
    a. Hydrogen bond - changes in electronic structure, signature in IR spectrum
    b. Halogen bond, sigma-hole
3. NCI in thermodynamics - connection with van der Waals equation
4. Example in biochemistry - NCI in DNA double helix

Statistical thermodynamics

1. Temperature in classical thermodynamics
2. Boltzmann distribution - configurations and their weights, derivation of B.d.

3. Partition function and its interpretation
4. Molecular partition function, separation of degrees of freedom
5. Canonical ensemble, partition function of a system of non-interacting molecules
6. Input variables for a rigid-rotor / harmonic oscillator calculation
7. Entropy in statistical thermodynamics
8. Brief overview on quantities that can be derived from partition function
9. Interacting particles - numerical methods based on sampling (MD, MC)

Photochemistry

1. Electronic excitations, Frank-Condon principle
2. Probability of the transition, overlap of vibrational wavefunction, absorption spectrum
3. Non-radiating processes
    a. Vibrational relaxation
    b. Intersystem crossing
    c. Photodissociation
    d. Reactions in excited states, avoided crossing/conical intersection
4. Radiating processes - fluorescence, phosphorescence, Jablonski diagram
5. Quantum yield, photo-initiation of chain reactions
6. Stimulated emission, principles of laser

Nuclear magnetic resonance

1. Spin and its quantum numbers
2. Spin of a nucleus
3. Energy of a nucleus in magnetic field, Zeeman effect, Larmor frequency
4. NMR apparatus, importance of separation of the spin states
5. Shielding and chemical shift
6. Fine structure, splitting of lines, chemical equivalence of atoms