The Chemical Bond (new syllabus)

Grading:
Final Test: 70 %
Middle term quiz: 10%
Final project: 20 %

Syllabus:

1. Review:
   - 1.1. de Broglie waves, wavelength, momentum, Planck constant, wave-particle duality.
   - 1.2. Bohr's complementarity and correspondence principles, quantization.
   - 1.3. Quantum mechanics postulates.
   - 1.4. Heisenberg uncertainty principle.
   - 1.5. Copenhagen interpretation (and others).
   - 1.6. Schrödinger equation (time dependent and independent).
   - 1.7. Wave function. Born's probability amplitude and probability density function of a particle.
   - 1.8. Quantum operators, Hermitian operators, Dirac notation.
   - 1.9. Angular momentum
   - 1.10. Atomic units.
   - 1.11. Particle in a Box (uni and multidimensional) and particle in a ring.
   - 1.12. Rigid rotor and harmonic oscillator.
   - 1.13. Hydrogen atom, quantum numbers, hydrogen-like orbitals.
   - 1.14. Born-Oppenheimer Approximation
2. Slater determinant. Hartree-Fock.
   - 2.1. Single determinant systems
   - 2.2. Spin orbitals and spatial orbitals.
   - 2.3. Pauli exclusion principle, indistinguishability, fermions and bosons.
   - 2.4. Open shell singlet and triplet, multi-determinantal systems.
   - 2.5. Kinetic and potential energy.
   - 2.6. Coulomb, exchange and Fock operators.
   - 2.7. Restricted and unrestricted HF.
   - 2.8. Multi-electron atoms.
   - 2.9. Molecules.
   - 2.10. Electron correlation ~~(dynamic and static).~~
   - 2.11. Hückel approximation.
3. Basis sets
   - 3.1. Minimal and multi-ζ basis sets
   - 3.2. Polarization and dispersion functions
4. MO-LCAO, Interaction diagrams
   - 4.1. H_2
   - 4.2. Diatomic molecules
   - 4.3. σ, π, δ bonds
   - 4.4. Hybrid orbitals
5. Vibrations
   - 5.1. Morse potential
   - 5.2. Harmonic oscillator
6. Non-covalent interactions
   - 6.1. Ionic
   - 6.2. Charge transfer
   - 6.3. Electrostatic
   - 6.4. Polarization
   - 6.5. London dispersion forces
   - 6.6. H bond
   - 6.7. Halogen bond
   - 6.8. Metallic bond
7. Molecular Symmetry
   - 7.1. Elements, operations, point groups.
   - 7.2. Symmetry and orbitals.
8. Thermodynamic properties
   - 8.1. Internal energy
   - 8.2. ZPE
   - 8.3. Entropy (rotational, translational, vibrational)
   - 8.4. Gibbs energy
9. Molecular geometry.
   - 9.1. Potential energy surface.
   - 9.2. Geometry optimization.
   - 9.3. Local and global minimums, transition states and higher order saddle points.
   - 9.4. Bond lengths, angles and dihedral angles.
   - 9.5. Hammond's postulate.
   - 9.6. Conformations.
10. Introduction to computational methods
    - 10.1. Electron correlation
    - 10.2. CI
    - 10.3. VB
    - 10.4. DFT
    - 10.5. MM