CHEM 3010: Physical Chemistry
Quantum Chemistry and Spectroscopy
Course Outline

Prerequisite: CHEM 2011 (CHEM 2000 is not required but highly desired).

Instructor: Toby Zeng, tzeng@yorku.ca

Textbook: Physical Chemistry (PC), by Thomas Engel and Philip Reid (Pearson Prentice Hall) 4th Edition. PC is also available as two "half-books": Quantum Chemistry and Spec- troscopy (QCS) and Thermodynamics, Statistical Thermodynamics, & Kinetics (TSTK). The half that you need for CHEM 3010 is QCS. As far as CHEM 3010 is concerned QCS has all the material from PC that we need and it is identical to PC. The required book for CHEM 2011 is PC, or the other half, TSTK. If you don't have PC but you have TSTK, you can buy the other half (QCS) and you will have everything. The chapter numbers I use are those of the half-book, QCS: just add 11 to get the corresponding chapter number in PC.

Lecture: MWF 10:30-11:30, MF at CB 129, W at CB 115

Tutorial: by appointment only, on ZOOM **(ID 931 936 6302)**

Office hour: CB208 or on ZOOM (ID: 931 936 6302), appointment by email (tzeng@yorku.ca).

Website: eclass.yorku.ca. All materials, including recordings of lectures, will be posted onto our eClass page.

Topics covered: Basic ideas of quantum mechanics; model systems (particle in box, rigid rotor, and harmonic oscillator) and their application in chemistry; hydrogen atom; basic atomic physics; molecular orbitals

Tentative **Grading scheme**: 20% for assignments, 30% for the two midterms, and 50% for the final exam. This scheme is **tentative** and subject to change.

Questions About Grading: If you have any questions about gradings of your assignments and midterms, please bring them up within **two** weeks after you get the graded sheet. **Please DO NOT wait until the end of the term.**

Learning Objectives (ideal):

By the end of the term you should be able to ...

1. Explain the differences between classical mechanics (CM) and quantum mechanics (QM).
2. Describe key experiments that led to QM: photoelectric effect, electron diffraction, the H atom spectrum, blackbody radiation.
3. Calculate the photonenergy, wavelength, and frequency associated with transitions between energy levels in atoms and molecules.
4. Compare the Bohr and Schrödinger descriptions of the H atom.
5. Identify situations where QM is needed using concepts like the De Broglie wavelength, the physical dimensions of a system, energy level separations and temperature.
6. Explain wave-particle duality and the Heisenberg uncertainty principle.
7. Carry out simple calculations with complex numbers.
8. Give a general discussion of the Schrödinger equation, its different terms, how it is solved, and what its solutions mean.
9. Explain the differences between the time-dependent and time-independent Schrödinger equations.
10. Carry out simple calculations with eigenvalue equations.
11. Discuss the physical meaning of eigenvalues and eigenfunctions associated with QM operators, in particular, how they are related to measurements.
12. Explain the meaning of “normalized”, “orthogonal”, “orthonormal” and “complete set” and their relevance for physical chemistry.
13. Discuss the postulates of QM.
14. Carry out simple calculations using the eigenvalues and/or eigenfunctions of model systems: the free particle (FP), the particle in a box (PIB), the particle on a ring (POR, also called rigid rotor), the particle on a sphere (POS), and the harmonic oscillator (HO)
15. Discuss the correspondence principle using the PIB.
16. Explain the technique of separation of variables using the 3-dimensional PIB.
17. Use the PIB model to describe qualitative aspects of atoms, chemical bonds, π conjugated systems, metals, and insulators.
18. Evaluate commutators of pairs of operators and explain their relevance for QM.

19. Explain the Stern-Gerlach experiment and discuss electron spin.
20. Describe qualitatively the different degrees of freedom in molecules: electronic, vibrational, rotational and translational.
21. Describe the harmonic oscillator (HO), its treatment in CM and QM, and key results about vibrations of diatomic molecules.
22. Describe the rigid rotor (or particle on a ring, POR), its treatment in QM, and key results about molecular rotations.
23. Explain how separation of variables is used to describe the motion of nuclei in QM as a product of a translational wavefunction, a rotational wavefunction, and a vibrational wavefunction.
24. Describe spherical harmonics and explain their role in the wavefunctions associated with molecular rotations and in orbitals (electronic wavefunctions).
25. Carry out simple calculations involving eigenfunctions, eigenvalues or quantum numbers of the POR, POS and HO models.
26. Discuss rotational and vibrational spectra in general and the relevant parts of the electromagnetic spectrum (microwave, infrared).
27. Discuss rotational and vibrational spectra in relation to energy levels and quantum numbers in the POR, POS and HO models.
28. Use selection rules, energy level expressions, and Planck's relation in simple spectroscopic calculations.
29. Use the Boltzmann relation for the population of energy levels in typical situations of physical chemistry.
30. Describe the H atom, the relevant Schrödinger equation, and orbitals obtained from it.
31. Discuss the orbital approximation, and orbitals, for many-electron atoms.
32. Discuss the symmetry of wavefunctions under exchange of identical particles, spin, the Pauli principle, and how they lead to singlet and triplet states.
33. Use the variational principle in simple situations.
34. Explain the SCF method and Slater determinants for many-electron atoms.
35. Discuss the electronic configurations of atoms.

36. Define and use ionization energy, electron affinity, Mulliken electronegativity, and Pearson-Parr hardness.