Chemistry 2284B

PHYSICAL CHEMISTRY II: QUANTUM THEORY

[This is a tentative outline of a new course]

Prerequisite(s): Chemistry 1301A/B, Chemistry 1302A/B, 0.5 course from Calculus 1000 A/B, Calculus 1500A/B, Numerical and Mathematical Methods 1412A/B, and any other 0.5 course at the 1000-level from Calculus, Applied Mathematics, Mathematics, or Numerical and Mathematical Methods. Integrated Science 1001X may be used as a substitute for the combination of Chemistry 1302A/B and Calculus 1301A/B.

Antirequisite(s): Chemistry 2214A/B, former Chemistry 2384B, Chemistry 3374A

Calendar Description: Foundations of the quantum theory of chemical structure and bonding. Topics include chemically relevant model problems of quantum mechanics, elements of atomic and molecular spectroscopy, relationship between classical and statistical thermodynamics.

Course structure: 3 lecture hours, 1 tutorial hour.

Course Topics

1. Wave-particle duality of matter. The wavefunction and its interpretation.
2. The Schrödinger equation for the wavefunction. The formalism of quantum mechanics: operators, eigenfunctions and eigenvalues.
3. Conceptually important model problems of quantum mechanics: particles in potential wells of various shapes. Quantum tunneling.
4. Quantum-mechanical description of translational, rotational, and vibrational motion.
5. Elements of statistical mechanics. The Boltzmann distribution, molecular partition functions, calculations of thermodynamic state functions from partition functions.
6. Atomic orbitals, orbital energies, quantum numbers. Many-electron atoms. How quantum mechanics describes the electronic structure of molecules and solids.
7. Applications of quantum theory to molecular spectroscopy: Selection rules, lasers, elements of photochemistry.

Course Learning Outcomes

1. Scientific principles: Recognition that quantum mechanics provides a theoretical basis for all of chemistry, materials science, and spectroscopy.

2. Theoretical knowledge: Understanding of the key ideas and principle of quantum mechanics such as wave-particle duality, operators, wavefunctions, uncertainty principle, orbitals, etc.

3. Practical knowledge: Problem-solving skills in applying the key principles of quantum mechanics to simple problems in chemistry and spectroscopy.

4. Awareness of the limitations of the discipline: Recognize the limitations of the models and assumptions used in quantum mechanics as applied to chemistry, being able to illustrate these limitations with specific examples.

5. Autonomy and impact: Develop the ability to work productively, being able to illustrate the relevance of the discipline to chemical research and society as a whole.