CY704 Introduction to Theoretical Chemistry

Credit: 3-0-0-3 Approval: Approved in 2nd Senate

Elective or core: Elective

Students intended for: Ph.D.

Prerequisite: M.Sc. Semester: Odd

Course objective:

Theoretical chemistry lies at the interfaces among chemistry, physics and mathematics. It is likely to have major impacts over the next few years within the disciplines of materials chemistry and biological chemistry which currently are two of the most important research areas in chemical science.

The primary goals of the present course are to provide an overview of the roles that theory plays within the science of chemistry and to introduce the students to the modern day components of theoretical chemistry.

Course content:

- The Basics of Quantum Mechanics, Model Problems, Exact Solution. [6 hrs]
- Understanding Energy surfaces, beyond model problems, normal modes, local modes, transition states, symmetry. [6 hrs]
- An overview of theoretical chemistry: Structure, bonding, rate of changes,Molecular spectroscopy. [6 hrs]
- Electronic structure: atomic and molecular orbitals, Experimental Probes of Electronic Structure. [6 hrs]
- Statistical Mechanics: Collections of Molecules at or Near Equilibrium,Monte Carlo Evaluation of Properties, Molecular Dynamics Simulations, applications. [10 hrs]
- Chemical Dynamics: Theoretical Treatment of Chemical Change and Dynamics, Experimental Probes of Reaction Dynamics . [8 hrs]

Text & Reference Books:

An Introduction to Theoretical Chemistry, Jack Simons, Cambridge University Press, 2003.

Essentials of Computational Chemistry, C. J. Cramer, Wiley, 2002.

Molecular Reaction Dynamics and Chemical Reactivity, R. D. Levine and R. B. Bernstein, Oxford University Press, 1997.

Molecular Modeling, 2nd ed., A. R. Leach, Prentice Hall, 2001.