NOC:Chemistry - I - Video course

COURSE OUTLINE

The Course is divided into two units, namely, Quantum Chemistry: Introduction and Introduction to Molecular Spectroscopy.

COURSE DETAIL

Unit	Unit Contents
1	**Quantum Chemistry: Introduction** To introduce the elements of quantum chemistry starting from Schrodinger equation and solve the following model problems to identify results that are unique to the study of matter at the microscopic level. The model problems that will be discussed here are: • particle in a one dimensional box with infinite barriers • particle in a two and three dimensional rectangular and square boxes also, with infinite barriers • particle confined to move on a ring and on a spherical surface • one dimensional harmonic oscillator model • non-technical account of the solution to electron in a hydrogen atom • visual representations and elementary calculations involving atomic orbitals of the hydrogen atom and • Heisenberg uncertainty principle with calculations of uncertainties of measurable quantities in the above models. The postulates of quantum mechanics with particular emphasis to calculating expectation values of measurable quantities will be presented and the models will be used to illustrate the postulates.
2	**Introduction to Molecular Spectroscopy**

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Chemistry and Biochemistry

Pre-requisites:

The following two books are recommended for students for supplementary reading and solving problems related to this course. Relevant sections of them will be indicated through mails and classroom interactions.

1. **Physical Chemistry, fourth edition**¸by Robert J. Silbey, Robert A. Alberty, Moungi. G. Bawendi, Wiley Interscience, 2005, New York. An Indian reprint is available from bookstores in India.
2. **Physical Chemistry: A Molecular Approach** ¸by Donald A. McQuarrie and John D. Simon, University Science Books, 1997. An Indian reprint by Viva Books, New Delhi is available from bookstores in India.

Coordinators:

To introduce molecular spectroscopy through an elementary account of the interaction of radiation with matter. A qualitative description of the semi-classical model for absorption, emission and stimulated emission of radiation in its interaction with matter will be given in the course. Beer-Lambert law and laboratory practices using the law for quantitative measurements in the lab will be described.
A brief account of molecular vibrations for diatomic and triatomic molecules will be given by relating the results of the harmonic oscillator model studied in Unit 1. The Franck-Condon principle and a few simple electronic spectra will be presented to provide elementary connections to electronic transitions and chemical processes.

Course Deliverables:

At the end of the modular study with two units, the student will be able to do the following:

Calculate the energy levels and transition frequencies for a one-dimensional system in which the particle is confined, using the Schrodinger equation.

Calculate expectation values and verify uncertainty principle for the models stated in the course.

Be able to visualize any spherical harmonics of order 3 or higher and perform calculations involving normalization and orthogonality between orbitals.

Calculate vibrational frequencies using harmonic approximation for simple diatomic molecules.
Calculate simple analytic values for concentrations of species that absorb visible light using Beer-Lambert law.
Define matrix elements of operators using harmonic oscillator basis functions.
Relate molecular transition probabilities between different energy levels to the molecular dipole moment matrix elements.

The student is expected to have sufficient background information to attempt the study of quantum mechanics of larger and other real systems. The solutions for the Schrodinger equation for the hydrogen molecule ion and hydrogen molecule will also help the student to study overlap, exchange and Coulomb contributions to chemical bonding in other larger systems.

Coordinators:

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