INSTITUTE	**FACULTY OF SCIENCE**
PROGRAM	**MASTER OF SCIENCE (CHEMISTRY)**
SEMESTER	**1**
COURSE TITLE	**PHYSICAL CHEMISTRY-I**
COURSE CODE	**02CY1401**
COURSE CREDITS	**6**

Course Outcomes: After completion of this course, student will be able to:

1. Identify, select and explain which concepts are involved and the way of theoretical framework of quantum mechanics.
2. Identify, describe and explain the quantum mechanical behaviour of simple systems, such as the harmonic oscillator and the rigid rotor.
3. Understand the application of molecular spectroscopy to different areas of science.
4. Solve problems related to physical and chemical aspects of solid surfaces.

Pre-requisite of course: Before learning Physical chemistry, student should aware about basic principles and theories of physical chemistry, thermodynamics, electrode potential, chemical reactions and other UG level chemistry

Teaching and Examination Scheme

Theory Hours	Tutorial Hours	Practical Hours	ESE	IA	CSE	Viva	Term Work
5	0	2	50	30	20	25	25

Contents : Unit	Topics	Contact Hours
1	**Quantum mechanics** Time independent Schrödinger equation. Properties of the Hermitian operator, canonical commutation relations, Ehrenfest theorem. Applications: Particle-in-a-box (1-, 2-, 3- dimensional), different potential functions and barrier problems, degeneracy, density of states. Simple harmonic oscillator: Ladder operator, properties of the eigenfunctions. Rigid rotor: Angular momentum operator, spherical harmonics. Hydrogen atom: Details of the solution, shapes of the orbitals.	20
2	**Molecular spectroscopy** Region of spectra, microwave spectroscopy, rigid rotor, selection rule, non-rigid rotor, Infrared spectroscopy, harmonic and anharmonicossilator, selection rule, Diatomic vibrating rotor, Electronic spectroscopy, Frank-Condon principle, Raman spectroscopy, condition of Raman activity, Vibrational Raman spectra of A-B2 type molecule.	20

Contents : Unit	Topics	Contact Hours
3	**Surface phenomena** Thermodynamics of surfaces, adsorption phenomena (mono- and multi layer). Langmuir and B.E.T. isotherms. Classification and properties of surfactants. Hydrophobic interactions. Micellization. Thermodynamics of micellization, 'phase separation' and 'mass action' models. Emulsion and 'reverse micelles'. Effect of micellization on the rate of chemical reactions. Characterization of the surface of a solid by different experimental techniques, including spectroscopy. Langmuir-Blodgett films.	20
Total Hours		**60**

Suggested List of Experiments:

Contents : Unit	Topics	Contact Hours
1	**Experiments** Experiment-1, Experiment-2, Experiment-3, Experiment-4, Experiment-5, Experiment-6, Experiment-7, Experiment-8	
Total Hours		

References:

1 Quantum Chemistry, Quantum Chemistry, Levine, Pearson , 2016

2 Introduction to. Quantum Mechanics, Introduction to. Quantum Mechanics, Griffith, Pearson , 2005

3 Introduction to Molecular Spectroscopy, Introduction to Molecular Spectroscopy, Barrow, McGraw-Hill , 1962

4 Physical Chemistry: A Molecular Approach, Physical Chemistry: A Molecular Approach, Donald A. McQuarrie, University Science Books,U.S., 1997

5 A Textbook of Physical Chemistry, A Textbook of Physical Chemistry, K L Kapoor , McGraw Hill , 2022

6 Atkins' Physical Chemistry, Atkins' Physical Chemistry, Peter Atkins, Oxford University Press, 2022

Suggested Theory Distribution:

The suggested theory distribution as per Bloom's taxonomy is as follows. This distribution serves as guidelines for teachers and students to achieve effective teaching-learning process

Distribution of Theory for course delivery and evaluation					
Remember / Knowledge	**Understand**	**Apply**	**Analyze**	**Evaluate**	**Higher order Thinking**
10.00	20.00	25.00	25.00	10.00	10.00

Instructional Method:

1. The course delivery method will depend upon the requirement of content and need of students. The teacher in addition to conventional teaching method by black board, may also use any of tools such as demonstration, role play, Quiz, brainstorming, MOOCs etc.
2. The internal evaluation will be done on the basis of continuous evaluation of students in the laboratory and class-room.
3. Practical examination will be conducted at the end of semester for evaluation of performance of students in laboratory
4. Students will use supplementary resources such as online videos, NPTEL videos, e-courses, Virtual Laboratory.
5. Use of hazardous/toxic chemicals should be avoided as far as possible in laboratory.
6. All students in the laboratory must wear safety goggles and lab coats during lab session.

Supplementary Resources:

1. http://www.nptel.ac.in/courses/104103069/#
2. http://ocw.mit.edu/courses/chemistry/
3. http://vlab.amrita.edu/index.php?sub=2
4. http://www.vlab.co.in/ba_labs_all.php?id=9