26SC802 Applied Computational Chemistry 3 1 2 5

CO1: Understand various computational chemistry tools
CO2: Exposure to the theoretical background in computational chemistry
CO3: Acquire knowledge on wave function analysis
CO4: Applications of computational chemistry in computing molecular properties
CO5: Understand the novices of computational materials science

CO-PO Mapping

	PO							PSO		
	1	2	3	4	5	6	7	1	2	3
CO1	3	3	3	3	-	-	2	3	-	2
CO2	3	3	3	3	-	-	2	3	2	3
CO3	3	2	3	3	-	-	2	3	2	2
CO4	3	3	3	3	-	-	3	3	3	3
CO5	2	3	2	3	-	-	3	3	3	3

Evaluation Pattern

Component	Nature of Assessment	Marks
Internal	Continuous Assessment (Presentations / Assignments)	20
	Mid-Term Exam	30
External	End-Sem Exam	50
Total Marks		100

Unit I – Computational Tools for Electronic Structure Calculations
Potential Energy Surfaces - Basis Sets – STOs and GTOs – Contracted Basis Sets – Polarized and Diffused functions – Plane wave basis functions – Effective Core Potential (ECP) – Basis set superposition Error (BSSE) – Coulomb Integrals, Exchange Integrals - Importance of symmetry – Molecular Simulations – Force Field Method

Unit II - Computational Quantum Chemistry of Molecules
HF, UHF, ROHF, Broken Symmetry solutions, Post Hartree Fock, DFT, Geometry optimization, Hellmann-Feynmann Theorem, Properties (time dependent and independent), Semi-empirical methods, Solvent Models)

Unit III - Computational Analysis of Wave functions
Population Analysis – Mulliken, Hamilton, Lowdin and other schemes – NBO analysis – Localization of Bonds and lone-pairs – Energy partitioning Schemes – EDA and Morokuma Partitioning – Electron Density based Bonding analysis – Atoms in Molecules theory – Bond and Ring critical points – Role of Kinetic energy in bonding – Electron localization Functions

Unit IV - Computations of Molecular Properties

Normal modes - Vibrational Analysis and Characterization of Stationary Points – Atomic Charges – Overlap Population – Mulliken's partitioning scheme - Electrical Properties (dipole moments)– Magnetic Properties (NMR chemical shifts) – Thermodynamic properties – IRC and excited state studies – Solvent Models

Unit IV – Computational Quantum Chemistry of Materials

Orbitals in Periodic Potential – Bloch-functions and k-space – Energy Bands – Avoided Crossing – Folding of Bands – Pierls Distortion – Density of States (DOS) – projected DOS – Crystal Orbital Overlap Population – Fermi Energy – Electronic Structure of Solids – Band Gap Engineering – Surface Bonding – Phonon calculations.

Lab

Expt 1. Introduction to molecular and materials design software (Gaussview, Spartan, Materials Studio etc.)

Expt 2. Visualization of molecules/Solid-State Structures

Expt 3. Designing molecules/materials and assigning symmetry

Expt 4. Geometry Optimization and Vibrational Analysis (Gaussian)

Expt 5. Analysis and Visualization of computed output (Gaussview)

Expt 6. Interaction and correlation Diagrams from Extended Huckel calculations (CACAO/YaeHMOP/Avogadro)

Expt 7. Geometry Optimization and phonon calculations of Periodic Networks (Materials Studio)

Expt 8. Analysis of Bands, DOS and COOP (YaeHMOP/Avogadro)

Expt 9. Molecular Dynamics Simulations

Expt 10. Docking Studies

TextBooks:

1.Ira N. Levine, 'Quantum Chemistry', 6th Edition, Prentice-Hall, 2008

2. Frank Jensen, 'Introduction to Computational Chemistry', 2nd edition, Wiley, 2013

3. John P. Lowe, K. Peterson, 'Quantum Chemistry', 3rd edition, Elsevier Science, 2011

4. F. Albert Cotton, 'Chemical Applications of Group Theory', 3rd Edition, John Wiley, 1990.

5. Peter Atkins, Ronald Friedman, 'Molecular Quantum Mechanics', 4th edition, Oxford university press

6. R K Prasad, 'Quantum Chemistry', New Age International (P) LTD publishers

REFERENCES

1. Thomas A. Albright, Jeremy K. Burdett, M, -H Whangbo, 'Orbital Interactions in Chemistry', Wiley, 2013

2. Hoffmann, R. "Solids and Surfaces: A Chemist's View of Bonding in Extended Structures' Wiley, 2021

3. Michael Glazer, Gerald Burns. 'Space Groups for Solid State Scientists' Academic Press, 2013

4. David C. Young, 'Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems' John Wiley & Sons, Inc.2001.

Program Outcome (POs):

1. **Disciplinary knowledge:** Capable of demonstrating comprehensive knowledge and understanding of one or more disciplines that form a part of the current program.
2. **Problem-solving skills:** Develop problem-solving skills in familiar and non-familiar contexts and apply one's learning to real-life situations.
3. **Critical and Analytical thinking:** Inculcate critical and analytical thinking to analyze and evaluate the reliability and relevance of evidence, scientific arguments, draw valid conclusions, and support them with examples.
4. **Scientific reasoning and Research-related skills:** Ability to apply scientific reasoning in designing research-related problems, analyze, interpret, and draw conclusions from quantitative/qualitative data. Critically evaluate ideas, evidence, and report the results of an experiment or investigation.
5. **Communication Skills and Team work:** Develop the individual ability to express thoughts and ideas effectively in writing and orally; and also to communicate with members of diverse teams to work effectively and respectfully.
6. **Moral and ethical awareness:** Capable of recognizing ethical issues, understanding intellectual property rights, promoting ethical practices in all tasks, and considering environmental and sustainability concerns.
7. **Lifelong learning:** Ability to acquire knowledge and skills, including self-directed learning, for lifelong learning, personal development, and adapting to evolving workplace demands through continuous skill development and reskilling to meet economic, social, and cultural goals.

Program Specific Outcome (PSOs):

i. **PSO 1: Foundation in Chemical Principles and Interdisciplinary Applications:** Develop a strong foundation in chemical principles, practical skills, and the ability to apply knowledge to allied areas.

ii. **PSO 2: Experimental Design, Professional Skills, and Sustainable Applications:** Design experiments, interpret results, and demonstrate professional skills relevant to industry and research settings to address real-world challenges with a focus on sustainability, environmental stewardship, and alternate energy solutions.

iii. **PSO 3: Integration of Chemistry, Laboratory, and Computational Skills for Multifaceted Career Options:** Apply basic theoretical, laboratory, and programming knowledge in chemistry to pursue careers in interdisciplinary fields like drug design, analytical chemistry, pharmaceutical industries, polymer chemistry, energy materials.