

KU8DSECHE402: COMPUTATIONAL CHEMISTRY

Semester	Course Type	Course Level	Course Code	Credits	Total Hours
VIII	DSE	400	KU8DSECHE402	4	60

Learning Approach (Hours/ Week)		Marks Distribution			Duration of ESE (Hours)
Lecture/ Tutorial	Practical/ Internship	CE	ESE	Total	
4	0	30	70	100	2

Course Description: Computational Chemistry is an interdisciplinary course that merges principles of chemistry, physics, and computer science to understand and predict the behaviour of chemical systems using computational techniques. This course is designed for students with a background in chemistry and an interest in applying computational methods to solve chemical problems.

Course Prerequisite: General Chemistry, Physical Chemistry, Basic programming skills

Course Outcomes:

CO No.	Expected Outcome	Learning Domains
1	Understand the theoretical foundations of computational chemistry. Classify and analyze the importance of quantum mechanics in understanding molecular behaviour.	U
2	Demonstrate proficiency in the use of basis sets and molecular orbitals in computational chemistry	An
3	Understand the foundations of Understand the foundations of DFT and utilize it to study the properties of molecular systems	U
4	Conduct computational spectroscopy to predict vibrational, electronic, and NMR spectra.	C

5	Prepare input programs in Gaussian / GAMESS / ORCA or other format for various calculations	A
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**Remember (R), Understand (U), Apply (A), Analyse (An), Evaluate (E), Create (C)*

Mapping of Course Outcomes to PSOs

	PSO 1	PSO 2	PSO 3	PSO 4	PSO 5	PSO 6	PSO 7
CO 1	3	0	3	1	0	3	0
CO 2	3	3	0	2	2	0	3
CO 3	3	2	3	0	0	3	0
CO 4	3	1	3	1	1	3	0
CO 5	3	3	0	0	1	0	3

Course Contents for Classroom Transaction:

M O D U L E	U N I T	DESCRIPTION	HOURS
1	COMPUTATIONAL CHEMISTRY – I		16
	1	Theoretical foundations of computational chemistry – Historical development and role in modern chemistry	
	2	Theory, computation & modelling – Definition of terms – Need of approximate methods in quantum mechanics	
	3	Computable quantities – Structure, potential energy surfaces and chemical properties – Cost and Efficiency	
	4	Classification of computational methods- Hartree – Fock Method-Ab initio methods	

	5	Hartree – Fock method- Self Consistent Field (SCF) treatment of polyatomic molecules– Closed shell systems– restricted HF calculations– Open shell systems– ROHF and UHF calculations– The Roothan– Hall equations– Koopmans theorem– HF limit and electron correlation	
	6	Introduction to post-HF methods	

	COMPUTATIONAL CHEMISTRY – II		6
2	1	Semiempirical methods- the basic principle of SCF-SE methods – Neglect of diatomic differential overlap approximation (NDDO) – intermediate Neglect of differential overlap approximation (INDO) – complete Neglect of differential overlap	
	2	Approximation (CNDO) – parameterization – modified intermediate Neglect of differential overlap (MINDO) – modified NDDO and MNDO models – Austin model 1(AM1)	

	COMPUTATIONAL CHEMISTRY – III		10
3	1	Density Functional Theory (DFT) - Introduction – Representability problems – Hohenberg-Kohn theorems – Kohn-Sham theory – reduced density matrix methods – local density approximation application – generalized gradient approximation	
	2	Hybrid functionals – performance and properties of density functional methods. Comparison between DFT and HF	

	COMPUTATIONAL CHEMISTRY – IV		16
4	1	Basis sets: Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets – contracted basis sets,	

		Pople-style basis sets: Nomenclature, calculation of number of basis functions and primitives used in a given basis set – correlation consistent basis sets, basis set superposition errors (BSSE).	
	2	Molecular Mechanics: Basic principles – developing force field – the stretch energy – the bending energy – torsional energy – the Van der Waals energy – the electrostatic energy – cross terms – parameterizing the force field – geometries and frequencies calculated by MM – strength and weakness of MM – Force fields in molecular docking.	

	TEACHER SPECIFIC MODULE- COMPUTATIONAL CHEMISTRY – V		12
	Directions: Molecular dynamics or any other topic relevant to the course according to teacher's choice can be included.		
5	Molecular Dynamics (MD): Basic principles – Calculation of simple thermodynamic properties–energy, heat capacity, pressure and temperature, phase space, periodic boundary conditions, monitoring the equilibration, analyzing the results of a simulation, error estimation – MD using simple models – continuous potentials, finite difference methods, choosing the time step Applications - Prediction of molecular properties using computational chemistry – Equilibrium molecular geometry – Applications in vibrational spectroscopy: calculating IR and Raman frequencies of molecules – Applications in UV and NMR spectroscopy – Applications in chemical thermodynamics Understanding molecular geometry input (Z-matrix input) – Writing Z-matrix input of simple molecules with <i>Natom</i> < 12 – Preparing computational chemistry input program in Gaussian / GAMESS/ ORCA or other format to calculate various molecular properties such as single point energy, geometry optimization, frequency calculation, etc.		

Essential Readings:

1. Leach AR. Molecular Modelling: Principles and Applications. 2nd ed. Harlow England: Prentice Hall.
2. Cramer CJ. Essentials of Computational Chemistry: Theories and Models. 3rd ed. Somerset: Wiley.
3. Frank Jensen, Introduction to Computational Chemistry, John Wiley & Sons Ltd.
4. David Young, Computational Chemistry- A Practical Guide for Applying Techniques to Real World Problems, Wiley -Interscience
5. Tamás Veszprémi and MiklósFehér, Quantum Chemistry: Fundamental and applications, Springer-India
6. Errol G. Lewars, Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics, 2nd edn., Springer
7. I.N. Levine, Quantum Chemistry, 6th Edition, Pearson Education Inc
8. Szabo A Ostlund NS. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory. Mineola NY: Dover Publications.
9. W. Koch, M.C. Holthausen, A Chemist's Guide to Density Functional Theory, Wiley-VCH Verlag.
10. David B Cook, Handbook of computational quantum chemistry, Oxford University

Assessment Rubrics:

Evaluation Type		Marks
End Semester Evaluation		70
Continuous Evaluation		30
a)	Test Paper*	12
b)	Assignment	6
c)	Seminar	6
d)	Viva-Voce	6
Total		100

*Average mark of the best two written tests may be considered for internal mark.