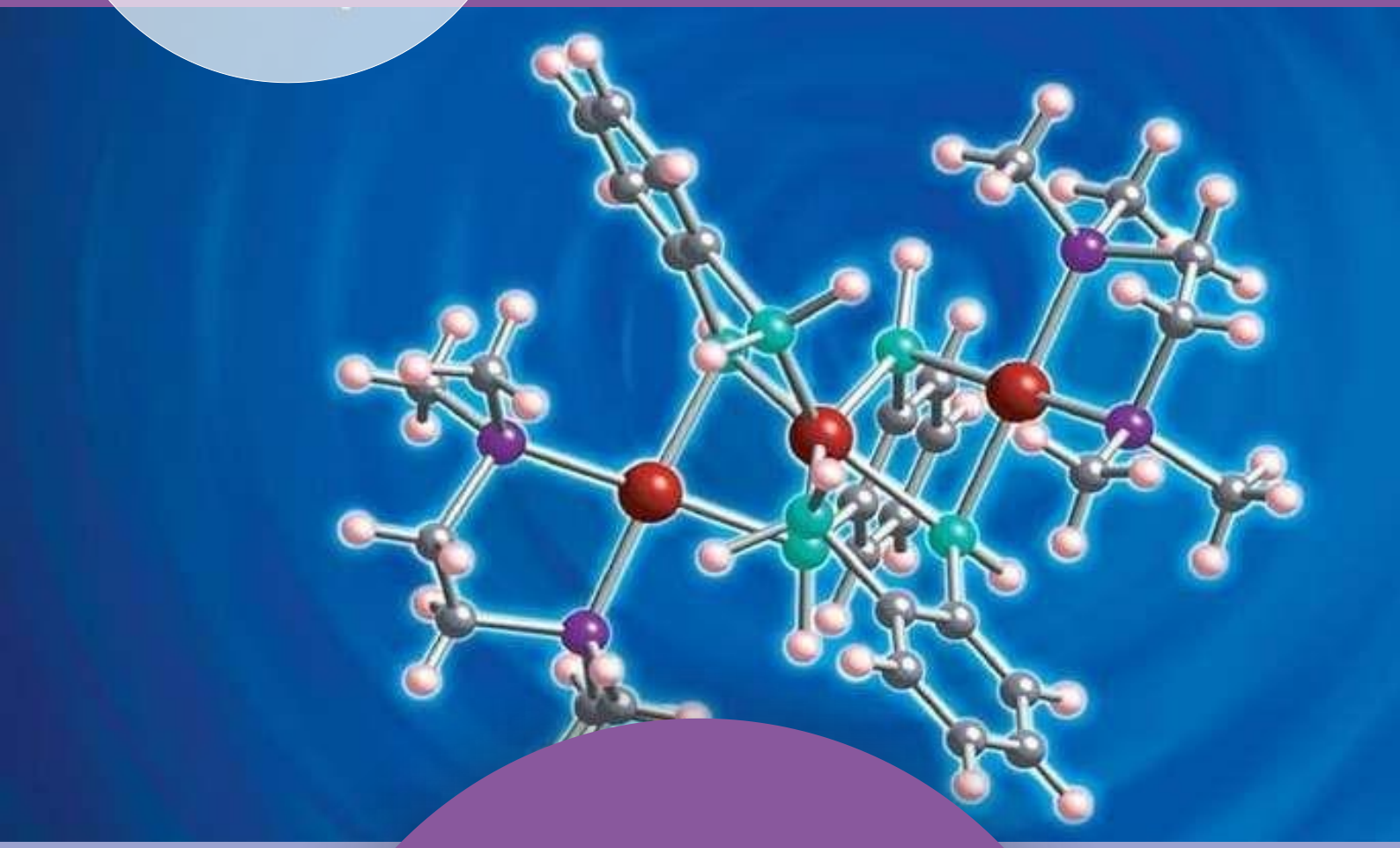
SHARDA UNIVERSITY
Beyond Boundaries

NAAC A+ ACCREDITED

SHARDA SCHOOL OF BASIC SCIENCES & RESEARCH

Department of Chemistry and Biochemistry



COURSE

Basics of Computational Chemistry

(NV33111)

VALUE ADDED COURSE BROCHURE

2024-25

SHARDA UNIVERSITY

Sharda University envisions to serve the society by being a global University of higher learning in pursuit of academic excellence, innovation and nurturing entrepreneurship. It has 13,000+ students from 95+ countries, 29 states, and Union Territories, providing cultural diversity and global exposure to students. It has 26000+ alumni who are today leaders in their realms. Sharda University is NAAC A+ University with Overall NIRF Rank of 87. Teaching Learning Center at Sharda University is to equip the faculty members with the expertise, skills and knowledge they need for capacity building of students. Teaching as a profession requires highly specialized skills and knowledge to impact significantly on student learning and therefore teachers must refine their conceptual and pedagogical skills.

ABOUT THE SCHOOL

Sharda School of Basic Sciences and Research (SSBSR) boasts of providing an interdisciplinary approach, exposure to different disciplines in science including Chemistry, Bio-Chemistry, Physics, Mathematics, Life Sciences, and Environmental Sciences. The Sharda School of Basic Sciences and Research is unique from other institutions of higher learning as it is committed to imparting knowledge in pure and applied sciences, which not only forms the foundation for further academic pursuits in science and technology but also acts as the foundation for students to pursue a career in multi facet directions. The academic programs are designed to meet the requirement of the latest technological developments and envisages to become a state-of-the-art department that cater the students at Graduate, Post- Graduate and Research level along with providing high- quality education and cutting-edge interdisciplinary research in sciences. SSBSR has well-equipped laboratories for Physics, MATLAB, Microbiology, Molecular Biology, Cell Culture, Virology, Biochemistry, Physical, Organic and Inorganic chemistry for Graduate and Post-Graduate Programs. In addition, there are Central Instrumentation Facility (CIF) and other advance research labs to promote research culture.

DEPARTMENT OF CHEMISTRY & BIOCHEMISTRY

The Department of Chemistry & Biochemistry endeavors to be nationally recognized model for nurturing students who can contribute to the ever changing technology of 21st century. The Department is committed to provide an excellent teaching & learning atmosphere for Undergraduate as well as post graduate students.

RESOURCE PERSON

Dr. Mridula Guin

Dr. Mridula Guin is presently working as Assistant Professor in the Department of Chemistry and Biochemistry, Sharda University. Previously she was associated with Maharaja Sayaji Rao University, Vadodara and Pooja Bhagavat Memorial Mahajana Education Centre, Mysore (Affiliated to University of Mysore) as Assistant Professor in chemistry. She received her Ph.D. from IIT Bombay in 2011. Dr. Mridula is a keen researcher and passionate teacher. She has published many research articles in reputed international journals. Her research area is computational investigations of weak interactions, transition metal complexes, high energy density materials (HEDMs) and photovoltaic materials. She has guided many students for their UG and PG dissertation work.

MODULE

School: SSBSR	**Batch : 2024-26**
Program: M.Sc.	**Current Academic Year: 2024-25**
Branch: Chemistry/Biochemistry	**Term : Even(2402), Semester : II**

1. Course Code	**NV33111**	
2. Course Title	**Basics of Computational Chemistry**	
3. Credits	**0**	
4. LTPC	**(30 Hours)**	
Course Type	**Value added course**	
5. Course Objective	1. To provide the understanding and hands on training of Molecular Mechanics and Quantum Mechanics 2. To understand the calculations of various semi-empirical methods 3. To extend the concept of basis sets, geometry optimization and frequency calculations through computational chemistry software 4. To provide the understanding of ab-initio theory and hands on experience of ab initio calculation 5. To provide the understanding of mathematical modeling of Density Functional Theory (DFT) through hands on experience	
6. Course Outcomes	CO1: The student will be able to get an idea of Molecular Mechanics and Quantum mechanics methods and its real field applications. CO2: The student will be able to get an idea of various semi-empirical methods and its calculations. CO3: The student will be able to understand basis sets, geometry optimization and frequency calculations through computational chemistry software. CO4: The student will be able to understand basic idea of ab initio theory and its applications through hands on training. CO5: The student will be able to apply computational chemistry software to study different properties of molecular systems using computational modelling. CO6: The student will be able to gain in depth knowledge of computational chemistry in terms of molecular mechanics, semi-empirical methods, basis sets, geometry optimization, electron correlation methods, Density Functional Theory and applications of Computational Chemistry.	
7. Course Description	This course will emphasize on the basic principles and fundamentals of computational chemistry and it applications, particularly focusing on hands on training to familiarize with computational chemistry software and calculations.	
8. Outline syllabus		CO Mapping
Unit 1	**Molecular Mechanics and Semi-Empirical Methods**	
A	Molecular mechanics / force field methods, the force field energy, advantages and limitations of methods of molecular mechanics.	CO1/CO6
B	The Schrödinger equation, molecular Hamiltonian, Born-Oppenheimer approximation.	CO1/CO6
C	Semi-empirical methods: CNDO, MNDO, AM1, MNDO-PM3, limits and advantages of semi-empirical methods.	CO1/CO6
Unit 2	**Basis Sets**	
A	Slater and gaussian type orbitals, polarization and diffuse functions,	CO2/CO6
B	Split-valence sets, classification of basis sets,	CO2/CO6
C	Dunning-Huzinga basis sets, correlation consistent basis sets, effective core potential basis sets.	CO2/CO6
Unit 3	**Geometry Optimization and Frequency Calculations**	
A	Introduction to Potential Energy Surface(PES), local minimum, global minimum, and saddle point	CO3/CO6
B	Frequency calculations, zero-point corrections, Intrinsic Reaction Coordinate (IRC) analysis	CO3/CO6
C	Computations HOMO, LUMO and band gap and generation of surfaces, reactivity descriptors	CO3/CO6
Unit 4	**Ab initio theory**	
A	Self-consistent field theory, Koopmans' theorem, Hartee-Fock theory, restricted and unrestricted Hartree-Fock,	CO4/CO6
B	Ab-initio calculations, Gaussian implementations	CO4/CO6
C	Comparison of ab-initio, semi empirical and DFT methods	CO4/CO6
Unit 5	**Density Functional Theory**	
A	Concept of Density Functional Theory and its applications	CO5/CO6
B	DFT for larger molecules	CO5/CO6
C	Computer aided assignments/mini projects with software.	CO5/CO6
Mode of examination	Assignments, Quizzes & Viva	