Approval: 8th Senate Meeting

Course Name: Computational Chemistry

Course Number: CY522

Credits: 3-0-0-3

Prerequisites: CY 521 Mathematics for Chemistry & CY 512 Advanced Quantum Chemistry

Intended for: UG/PG

Distribution: Core.

Semester: Odd.

Course Preamble: The objective of this course is to develop basic understanding among students on chemical structure and transformation of organic molecules and also to develop critical thinking skills. The course will provide an overview of the fundamental concepts of electronic structure, molecular arrangements, substitution effects, stereochemistry and common organic reactions. Students will be provided with in-depth information on the above areas.

Course Outline:

Unit 1: Introduction to Computational Chemistry [16 Lectures]

Scope of computational chemistry, Numerical Methods (algorithms), Molecular Mechanics / Force Field Methods, molecular dynamics, Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states.

Unit 2: Basics of Approximate methods. [6 Lectures]

Variational method, Hartree-Fock methid. Molecular orbital theory, Slaterdeterminants, anti-symmetry principle, restricted and unrestricted references, self-consistent-field (SCF) procedure.

Unit 3: Use of Approximate methods [6 lectures]

Basis sets, Hartree-Fock algorithm, Electronic spin degeneracy, evaluating the spin of Slater determinants, computational simplification using Group Theory, Semi-empirical methods, Geometry optimization.

Unit 4: Thermodynamic Properties [8 Lectures]

Intrinsic reaction coordinate (IRC) analysis, Introduction to analytic gradient theory, Transition state theory, statistical mechanics, and thermodynamic properties.

Unit 5: Advanced Methods [6 Lectures]

Electron correlation, Configuration interaction, Many-body perturbation theory. Comparing the performance of electronic structure theories.

Unit 6: Hands on experience [0 Lecture]

Hands on experience on the use of computational chemistry packages & understanding of experiments done in Laboratory courses

Textbooks

1. F. Jensen, Introduction to Computational Chemistry, John Wiley & Sons, 2nd Edition, West Sussex, England (2007).

2. A. Szabo and N. S. Ostlund, Modern Quantum Chemistry, McGraw-Hill Inc., 2nd edition, New York, USA (1989).

Reference Books

1. D. A. McQuarrie, Quantum Chemistry, Viva Books, New Delhi, India (2011).

1. Ira N. Levine, Quantum Chemistry, Prentice-Hall: Englewood Cliffs, NJ, USA (1991).

2. F. A. Cotton, Chemical Applications of Group Theory, Wiley-Interscience; 3rd Edition, New York, USA (1990).

3. C. J. Cramer, Essentials of Computational Chemistry, John Wiley & Sons, 2nd edition, West Sussex, England (2004).

4. A. R. Leach, Molecular Modelling: Principle and Applications, Prentice-Hall, Englewood Cliffs, NJ, USA (2001).

5. D. Young, Computational Chemistry, John Wiley & Sons, New York, USA (2001).

6. E. G. Lewar, Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer; Berlin, Germany (2003).