1. Smith, B. C. *Infrared Spectral Interpretation: A Systematic Approach*, CRC Press.
2. Silverstein, R. M., et al. *Spectrometric Identification of Organic Compounds*, Wiley
3. Speyer, R. F. *Thermal Analysis of Materials*, Marcel Dekker, 1994.
4. Hatakeyama, H. & Hatakeyama, T. *Thermal Analysis: Fundamentals and Applications to Polymer Science*, Springer.
5. Goldstein, J. I., et al. *Scanning Electron Microscopy and X-ray Microanalysis*, Springer.
6. Skoog, D. A., Holler, F. J., & Crouch, S. R. *Principles of Instrumental Analysis*, Cengage Learning.
7. Sparks, D. L. *Environmental Soil Chemistry*, Academic Press. (For leaching relevance).
8. Callister, W. D., & Rethwisch, D. G. *Materials Science and Engineering Laboratory Manual*, Wiley.

Suggested readings:

1. Ratner, B. D., Hoffman, A. S., Schoen, F. J., & Lemons, J. E. Biomaterials Science: An Introduction to Materials in Medicine (3rd Edition) - Academic Press
2. Park, J., & Lakes, R. S. Biomaterials: An Introduction (3rd Edition) - Springer
3. Williams, D. F. The Biomaterials: Silver Jubilee Compendium - Elsevier
4. Ong, K. L. Orthopedic Biomaterials in Research and Practice - Springer
5. How, T. V., & Black, R. A. Biomaterials and Devices for the Circulatory System – Woodhead
6. Lanza, R., Langer, R., & Vacanti, J. Principles of Tissue Engineering (5th Edition) - Academic Press
7. Al-Shibouri, A. M., & Nimesh, S. Engineering Drug Delivery Systems - Elsevier

Online Resources:

1. National Institute of Biomedical Imaging and Bioengineering: https://www.nibib.nih.gov
2. Materials Today Biomaterials https://www.materialstoday.com/biomaterials

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.

DISCIPLINE SPECIFIC ELECTIVE 7

CREDIT DISTRIBUTION, ELIGIBILITY, AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
COMPUTATIONAL METHODS AND MOLECULAR MODELLING	**4**	**2**	**0**	**2**	**12th Class: Physics, Chemistry, Mathematics**	**-**

Course Objectives:

- To make students learn the theoretical background of computational techniques in molecular modelling.
- To give the different flavours of computational chemistry by the end of this course.
- To provide hands-on experience in molecular modelling on various software

Learning Outcomes:

Students will be able to:

- Explain the theoretical background of computational techniques and selective application to various molecular systems
- Compare computational and experimental results and explain deviations.
- Perform Optimization of geometry parameters of a molecule (such as shape, bondlength and bond angle) through the use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.
- Perform analysis of molecular properties using various software

UNIT 1: Introduction **(6 hours)**

Introduction to computational chemistry: Overview of Classical and Quantum Mechanical Methods (Ab initio, DFT, Semi-empirical, Molecular Mechanics, Molecular Dynamics, and Monte Carlo)

UNIT 2: Potential Energy Surfaces **(6 hours)**

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, Geometry optimization and energy minimization, the concept of transition state with examples, Hessian matrix

UNIT 3: Molecular Mechanics & Molecular Dynamics **(6 hours)**

Molecular Mechanics:

Force Fields (A brief explanation of all the terms of a basic force field), parametrising a force field, the basic idea of MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.

Molecular Dynamics:

The concept of the periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), steps in a typical MD simulation.

UNIT 4: Huckel Molecular Orbital Theory **(12 hours)**

Huckel MO with examples: ethene and propenyl systems, Properties calculated – energy, charges, bond order, electronic energies, resonance energies.

Ab-Initio Methods

Antisymmetry principle, Slater determinants, SCF method, Hartree-Fock method.

Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets

Practicals **(60 hours)**

Any 8 -10 Problems

1. Write the Z-Matrix of a given set of molecules.
2. Carry out geometry optimisation on H_2O, H_2S, H_2Se molecules compare the optimized bond angles and dipole moments from the results obtained. Obtain the ESP-mapped density surfaces and interpret the results obtained with reference to bonding in these molecules.
3. Calculate the energy of the following chemical species and arrange them in order of increasing stability:

   1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3- dimethyl-2-butene in order of increasing stability.

4. Carry out geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules:

   1-pentanol, 2-pentanol, 3-pentanol, 2-methyl butan-1-ol, 3-methyl butan-1-ol, 2-methyl butan-2-ol, 2-methyl butan-3-ol and 2,2-dimethyl propanol.

5. Based on the implicit electronic structure calculations, determine the heat of hydrogenation of Propylene.
6. Based on the calculations of enthalapies of the participating chemical species on the optimized geometry of the molecules, calculate the reaction enthalpy at 298K of (a) Steam reforming of methane (b) Haber-Bosch Process
7. Carry out geometry optimisation & Energy calculations on Benzene, Naphthalene, and Anthracene. Obtain Frontier Molecular Orbitals, visualise the Molecular Orbitals of these species, and interpret the results for bonding in these molecules.
8. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

   $BH^+ + NH_3 \rightarrow B + NH_4^+$

   Where $B = CH_3NH_2$, $(CH_3)_2NH$, $(CH_3)_3N$

9. Based on the results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis and trans 2-butene.
10. Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.
11. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
12. Calculate the electronic UV/Visible absorption spectrum of Benzene.
13. Calculate the electronic absorption spectra of formaldehyde.
14. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dime.

RECOMMENDED/ESSENTIAL TEXTBOOKS AND REFERENCES

Theory:

- Lewars, E. (2003), Computational Chemistry, Kluwer academic Publisher.
- Cramer, C.J. (2004), Essentials of Computational Chemistry, John Wiley & Sons.
- Hinchcliffe, A. (1996), Modelling Molecular Structures, John Wiley & Sons.
- Leach, A.R. (2001), Molecular Modelling, Prentice-Hall.
- House, J.E. (2004), Fundamentals of Quantum Chemistry, 2nd Edition, Elsevier.
- McQuarrie, D.A. (2016), Quantum Chemistry, Viva Books.
- Levine, I. N.; Physical Chemistry, 5th Edition, McGraw –Hill.

Practicals

- https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf
- https://dasher.wustl.edu/chem430/software/avogadro/learning-avogadro.pdf
- http://www.arguslab.com/arguslab.com/ArgusLab.html
- https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf
- https://gaussian.com/techsupport/
- https://gaussian.com/man/
- https://gaussian.com/wp-content/uploads/dl/gv6.pdf
- https://dasher.wustl.edu/chem478/software/spartan-manual.pdf
- http://www.mdtutorials.com/gmx/
- https://vina.scripps.edu/manual/

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.