(04-01-2021 to 10-01-2021)

Module I: COSMO based models and calculation of phase behaviour and thermodynamic properties

Conductor like Screening Models abbreviated as COSMO based models are quantum chemically derived excess Gibbs energy models that are used in thermodynamic calculations. One of the variant of COSMO based models is COSMO-SAC which is used to calculate the activity coefficients. The activity coefficients are subsequently used to calculate phase compositions. Apart from that, COSMO based models are used to calculate various other thermodynamic property and various descriptors of solvent such as hydrogen bond acidity and basicity

Learning Objectives:

At the end of this session participants will:

- ✓ Learn the theoretical background of COSMO based models and Basics of Quantum Chemical (QC) calculation.
- ✓ How to construct the COSMO code.
- ✓ Calculation of complex phase behaviour.
- ✓ Thermodynamic properties.
- ✓ Thermochemistry calculation.
- ✓ Calculation of Interaction energies.
- ✓ Calculation of Natural Bond Orbital.

Day-1	10:00-1:00	**Introduction to Conductor like Screening Models (COSMO)** ✓ Introduction to COSMO-RS and COSMO-SAC and its applications ✓ Details about COSMO theory ✓ Determination of activity coefficient and sigma profile ✓ Screening charge density calculation
Day-1	2:00-5:00	**Hands-on session 1:** In this session, participant will learn to construct the COSMO code and details input commands for running a simple molecule COSMO calculation. • Cosmo file generation • Sigma profile generation from cosmos file
Day-2	10:00-1:00	**Introduction to Quantum Chemical (QC) calculation**

		✓ Introduction to Quantum chemistry ✓ Geometry optimizations of molecules ✓ HF and DFT theory ✓ Natural Bond Orbital analysis
Day-2	2:00-5:00	**Hands-on session 2:** In this session, participants will be demonstrated different aspect of Quantum Chemical (QC) calculation such as: • Calculation of complex phase behaviour of molecules • Thermochemistry calculation • Calculation of Interaction energies • Calculation of Natural Bond Orbital
Day-2	5:00-6:00	**Miscellaneous session:** In this hand-on session, participants will be given a specific task to perform COSMO and quantum calculations (QC) using Gaussian 09. Doubt clarification session.

Module II: Introduction to Advanced Molecular Dynamics Simulation and Density Functional Theory

Molecular Dynamics (MD) simulation and Density Functional Theory (DFT) are advanced computational methods and their applications to solve various multiscale and multidisciplinary research problems. The aim of the event is to bring together researchers and scientists working in various computational methods to exchange ideas in state-of-the-art methods in electronic and atomic structure. MD simulations can also be used to calculate the thermodynamic and transport properties of a variety of systems. A wide class of scientific phenomena can be explored and understood from a molecular level. The advances in computing technology have also enabled us to solve a range of complex problems.

Learning Objectives:

At the end of this session participants will:

- ✓ Learn the theory behind Molecular Dynamics (MD) simulations.
- ✓ Learn use of NAMD software package.
- ✓ Learn use of VMD software package to analyse the trajectory file.
- ✓ Understand about Density Functional Theory (DFT) calculations that cover the basic principles and advance simulations.

Day-3	10:00-1:00	**Introduction to classical Molecular Dynamics (MD) simulations** ✓ Introduction to Nanoscale Molecular Dynamics (NAMD) and its applications ✓ Details about Force field equations (AMBER, CHARMS) ✓ NPT, NVT and NVE Ensembles ✓ Periodic Boundary Conditions (PBC) and PACKMOL ✓ Radial distribution function (RDF)
Day-3	2:00-5:00	**Hands-on session 1:** In this session, participant will learn about geometry optimizations of molecules and set up the input force field parameter file for NAMD. One simulation box will be demonstrated for the complex molecules such as ionic liquids. • Energy Minimization • Molecular Dynamics Simulation of Simple System (e.g. pure gas or liquid)

Day-4	10:00-1:00	**Introduction to Density Functional Theory (DFT)** ✓ Introduction to GaussView 5 and Gaussian 09 ✓ Geometry optimizations of molecules with different level theory and basis set ✓ Calculations binding energy of solutes in solvents and free energies in solution
Day-4	2:00-5:00	**Hands-on session 2:** In this session, participants will be demonstrated how to carry analyse the output trajectory file of the MD simulation. Interaction Energy, Hydrogen bonding, Radial distribution function, MSD etc. using VMD. • Molecular Dynamics Simulation of Mixed System (e.g. two or more immiscible liquids and solutes) • Explicit and Implicit solvation model
Day-4	5:00-6:00	**Miscellaneous session:** In this hand-on session, participants will be given a specific task to perform both MD simulations and quantum calculations (QC) using NAMD and Gaussian 09 for calculating properties of interest using VMD. Any question relating to the MD simulation will be welcome and discuss.

Module III: Introduction to Monte Carlo Simulation using MCCCS Towhee: Theory and Practice

Monte Carlo for Complex Chemical Systems (MCCCS) Towhee is an open source atomistic Monte Carlo software package that is effective in predicting the thermodynamic properties of fluids and computing phase equilibria. This software is capable of simulating any type of molecule (rings, chains), supports simulations in a range of ensembles, supports a large number of force fields and contains a wide range of advanced sampling techniques.

Learning Objectives:

At the end of this session participants will:

- ✓ Learn the theoretical background of Monte Carlo Simulation.
- ✓ Learn capabilities of Towhee and how to use it.
- ✓ Run Towhee software correctly.
- ✓ Figure out how to use Towhee in their research.

Day-5	10:00-1:00	**Introduction to Monte Carlo Simulations and MCCCS Towhee:** This session is divided in two parts: In first part, following will be covered: ✓ Introduction to Monte Carlo Simulations and its applications in Chemical, Biochemical and Environmental Engineering. ✓ Force fields. ✓ Ensembles in Monte Carlo Simulations: Isothermal-isobaric ensemble (NPT), Canonical Ensemble (NVT), Gibbs Ensemble Monte Carlo Simulation (GEMC), Grand Canonical Monte Carlo Simulations (GCMC). ✓ Structural Information from MC Simulations (Radial distribution function - RDF). In second part, following will be covered: ✓ A brief introduction on MCCCS Towhee. ✓ Ensembles available in Towhee. ✓ Force fields and what is available in Towhee. ✓ Monte Carlo "moves" in Towhee. ✓ Sampling techniques available in Towhee. ✓ Basic structure of Towhee, required input files and generated output files.

Day-5	2:00-5:00	**Hands-on session 1 (NPT):** In this hands-on session, instructor will show how to carry out a single box Monte Carlo simulation to compute liquid density of simple molecule in isothermal-isobaric (NPT) ensemble and the same will be repeated by participants. This will include how to set up the input files and force field file and how to analyse the generated data. **Hands-on session 2 (NPT):** In this hands-on session, a single box simulation will be demonstrated for the computation of liquid density of complex molecules such as ionic liquids and deep eutectic solvents. Participants will also be demonstrated how to calculate the radial distribution function (RDF).
Day-6	10:00-1:00	In this session, two important files (towhee input and towhee_ff) which will be used in running Monte Carlo Simulations will be discussed in detail. Towhee input is the main input file for Towhee simulation which contains all information regarding the simulation and molecules. Variables defined in the file and format which should be used for running the simulation will be discussed. Towhee_ff is the force field file which follows a strict format and is the most important file. Participants will be demonstrated how to create a force field file.
Day-6	2:00-5:00	**Hands-on session 3 (GEMC):** In this session, participants will be demonstrated how to carry out a two box NVT Gibbs ensemble Monte Carlo simulation for determining single-component vapor-liquid coexistence. **Hands-on session 4 (GEMC):** In this session, participants will be demonstrated how to carry out a three box Gibbs ensemble Monte Carlo simulation for predicting the ternary diagram of a multicomponent system.
Day-6	5:00-6:00	**Miscellaneous session:** In this hand-on session, participants will be given a specific task to perform GEMC using Towhee. Doubt clarification session.