Fundamentals of Molecular Simulations (FunMolSim 2019)

Date & Day	Time	Session	Speaker	Topic	Venue
March 5, Day 1	8.30 - 9.00	Registration			PBCEC
	9.00 - 10.30	Lecture	Jayant Singh	Introduction to Molecular Simulations, Ensembles and Connection to Thermodynamics	PBCEC
	10.30 - 11.00	Tea Break			
	11.00 - 12.30	Lecture Tutorial	Jayant Singh	Computing Interaction Potential Forces	PBCEC
	12:30 -14.00	Lunch Break			
	14.00 - 15.00	Hands On		Linux Console and HPC basics	L2, CC
	15.00 - 16.00	Lecture	Pankaj Apte	Basics of Molecular Dynamics Simulation	L2, CC
	16.00 - 16.30	Tea Break			
	16.30 - 17.30	Tutorial	Pankaj Apte	Molecular Dynamics Simulations	L2, CC
March 6, Day 2	9.00 - 10.30	Lecture	Ganapathy Ayappa	Extended Systems Molecular Dynamics, NVT, NPT	PBCEC
	10.30 - 11.00	Tea Break			
	11.00 - 12.30	Tutorial	Ganapathy Ayappa	Tutorial on extended systems MD	PBCEC
	12.30 - 14.00	Lunch Break			

	14.00 - 15.30	Lab session	Debdip Bhandary	Hands on MD s/w	L2, CC
	15.30 - 16.00	Tea Break			
	16.00 - 17.30	Lab session	Praveen Sappidi	Hands on MD s/w	L2, CC

	9.00 - 10.30	Lecture	Jayant Singh	Monte Carlo Simulations: Importance Sampling – Metropolis Method	L2, CC
	10.30 - 11.00	Tea Break			
	11.00 - 13.00	Hands On	Sandip Khan Manish Maurya	Hands on MC coding and open s/w	L2, CC
March 7, Day 3	13.00 - 14.30	Lunch Break			
	14.30 - 15.30	Lecture	Jayant Singh	Monte Carlo -continued	PBCEC
	15.30 - 16.00	Tea Break			
	16.00 - 17.00	Lecture	Suresh Bhatia	Special Lecture on Adsorption	PBCEC

	9.00 - 10.30	Lecture	Jayant Singh	Free-energy methods (Parallel Tempering, Umbrella Sampling, Meta Dynamics)	PBCEC
	10.30 - 11.00	Tea Break			
	11.00 - 12.30	Lecture	Jhumpa Adhikari	Phase equilibria Calculations using molecular simulations	PBCEC
	12.30 - 14.00	Lunch Break			

March 8, Day 4	14.00 - 15.30	Tutorial	Jhumpa Adhikari	Tutorial: Phase diagram calculations via MC methods	L2, CC
	15.30 - 16.00	Tea Break			
	16.00 - 17.30	Tutorial	Praveen Sappidi Debdip Bhandary	Calculating free-energy: cases studies	L2, CC
	19.30 onwards	Course Dinner			VH

March 9, Day 5	9.00 - 10.30	Lecture	Ethaya Mani	Soft Matter Simulations-Monte Carlo and Kinetic Monte Carlo, Coarse-grain approaches	PBCEC
	10.30 - 11.00	Tea Break			
	11.00 - 12.30	Lecture	Indranil Saha Dalal	DPD/Brownian Simulations	PBCEC
	12.30 - 14.00	Lunch Break			
	14.00 - 15.30	Tutorial	Ethaya Mani	Hands on KMC simulations of Soft Matter	L2, CC
	15.30 - 16.00	Tea Break			
	16.00 - 17.30	Tutorial	Indranil Saha Dalal	Hands on DPD and Brownian simulations	L2, CC
	Distribution of Course Certificate				

CC = Computer Centre   **PBCEC is at Visitor's Hostel**