Molecular Simulations in Chemical Engineering - Web course

COURSE OUTLINE

Molecular simulations of liquids, gases, metals, polymers, biological systems and other complex fluids combined with contemporary experiments promise to revolutionalize how we think of molecular world.

This course aims to provide student with an understanding of the methods, capabilities, and limitations of molecular simulation.

This should enable the student to make sound judgments regarding the quality of molecular simulation studies reported in the literature and decide whether molecular simulation is suited for application to their research, and if so, to know how to begin developing a simulation program applicable to their problems.

Further, it is expected that completion of this course will leave the student with a much deeper understanding of the molecular basis of physical behavior.

Contents:

Fundamentals of molecular simulations - Ab-initio Methods, Basis Sets, Hartree-Fock Theory, Density Functional Theory, Geometry Optimization, Vibrational Analysis.

Elementary, classical statistical mechanics, elementary concepts of temperature, ensembles and fluctuations, partition function, ensemble averaging, ergodicity.

Molecular Dynamics Methodology - Force Field, Integrating Algorithms, Periodic Box and Minimum Image Convention.

Long Range Forces, Non Bonded Interaction, Temperature Control, Pressure Control, Estimation of Pure Component Properties,Radial Distribution Function; Molecular Dynamics Packages.

Monte Carlo simulation - Monte Carlo integration, simple biasing methods, importance sampling, Markov chain, transition-probability matrix, detailed balance, Metropolis algorithm.

Monte Carlo simulation in different ensembles; Monte Carlo simulation for polymer; Advanced Topics.

COURSE DETAIL

S.No	Topics	No. of Hours
1	Fundamentals of molecular simulations -Ab-initio Methods, Basis Sets, Hartree-Fock Theory, Density Functional Theory, Geometry Optimization, Vibrational Analysis.	5
2	Classical statistical mechanics, elementary concepts of temperature, ensembles and fluctuations, partition function, ensemble averaging, ergodicity.	6
3	Molecular Dynamics Methodology - Force Field, Integrating Algorithms, Periodic Box and Minimum Image	4

NP-TEL

NPTEL

http://nptel.iitm.ac.in

Chemical Engineering

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	Convention, Long Range Forces, Non Bonded Interaction.	
4	Temperature Control, Pressure Control, Estimation of Pure Component Properties, Radial Distribution Function; Molecular Dynamics Packages.	5
5	Monte Carlo simulation - Monte Carlo integration, simple biasing methods, importance sampling, Markov chain, transition-probability matrix, detailed balance.	5
6	Metropolis algorithm.	6
7	Monte Carlo simulation in different ensembles.	4
8	Monte Carlo simulation for polymer; Advanced applications.	5
	Total	40

References:

Text Books:

1. Daan Frenkel and Berend Smit, Understanding Molecular Simulation: From Algorithms to Applications, 2e, Academic Press, New York, 2002.
2. M.P. Allen and D.J. Tildesley, Computer Simulation of Liquids, Clarendon Press, Oxford, 1987.

References:

1. K. Binder, The Monte-Carlo Method in Condensed Matter Physics, Berlin : Springer-verlag, 1992.
2. D. A. McQuarrie, Statistical Mechanics, Harper and Row, New York, 1976.
3. Andrew R. Leach, Molecular modelling: principles and applications, 2e, Pearson, New Delhi, 2001.