SS807 MOLECULAR MODELING AND SIMULATION 3-0-0-3

Definitions, Scope and Classifications: Minimization of functions; Statistics – Macroscopic properties from molecular Simulations: Representing molecules and Molecular interactions; Energy and Forces for molecular Interactions: Constraints: periodic Boundaries and Neighbor Lists: Monte Carlo Simulations: Algorithm, Detailed balance, Computing properties, Exercises: Molecular Dynamics: Initialization, force calculation, Algorithm, Computing Equilibrium and Dynamic properties, Exercises: Computational Chemistry: Atomistic and Coarse-grained Approaches: Advanced Energy Minimization Techniques : Softwares for Molecular Modeling.

TEXT BOOKS/REFERENCES:

1. K. I. Ramachandran, Deepa Gopakumar and Krishnan Namboori, "*Computational Chemistry and Molecular Modeling: Principles and Applications*", Springer, 2008.
2. D. Frenkel and B. Smit, "*Understanding Molecular Simulations: From Algorithams to Applications*", Second Edition, Academic press, 2002.
3. M. P. Allen and D. J. Tildesley, "*Computer Simulation of Liquids*", Clarendon Press, 1987.
4. Tamar Schlick, "*Molecular Modeling and Simulation: An Interdisciplinary Guide*", Springer, 2002.