Course Number: 28187

Course Name: Molecular Dynamics

Course Type: Theory	Type & Max Unit: Constant 3
Prerequisite:	Corequisite: Nothing
Level: Graduate	First Presentation:
Group: Dynamics and Vibrations	Last Edition: 2018

Objectives:

This course teaches students fundamentals of simulations of atomistic systems. Also they will learn how to write codes and how to work with well-known software packages.

Topics:

1- Introduction to the Application of the Molecular Dynamics for Modeling of the Nano-scale Systems

2- Different Interatomic Potentials (Force Fields, Molecular Mechanics, Electrostatic Forces, van der Waals Forces, Potentials for Metals, Silicon, Carbon, …

3- Energy Minimization Methods (Steepest Descent, Conjugate Gradient, Newton, Simplex, …), and Related Methods for Exploring Energy Surfaces

4- Computer Simulation Techniques (Periodic Boundary Conditions, Cut-off Radius, Neighborhood List, Long Range Forces (Ewald Summation, Tree Method, …)

5- Molecular Dynamics Simulations Methods (Integration Methods: Velocity Verlet, Prediction-Correction, …, Suitable Time Step Selection, Equipartition Theorem, Constrained Dynamics, Rigid Molecules Simulations, Different Ensembles, Simulation in Constant Temperature: Different Thermostats, Virial Theorem, Simulation in Constant Pressure, Different Barostates, …)

6- Introduction to Coarse Graining Methods (General Particle, Residue Based CG, Martini CG, Shaped Based CG, …)

References:

1. A. R. Leach, Molecular Modelling: Principles and Applications, Prentice Hall, 2001.

2. J. M. Haile, Molecular Dynamics Simulation: Elementary Methods, Wiley-Interscience

3. D. C. Rapaport , “The Art of Molecular Dynamics Simulation”, Cambridge University Press, 2004.
4. W. Humphrey, A. Dalke, and K. Schulten, “VMD - Visual Molecular Dynamics”, Journal of Molecular Graphics, vol. 14, p. 33-38, 1996.
5. J. C. Phillips et al., “Scalable molecular dynamics with NAMD,” Journal of computational chemistry, vol. 26, no. 16, p. 1781, 2005. “NAMD A Parallel Object-Oriented Molecular Dynamics Program”
6. “LAMMPS Molecular Dynamics Simulator”. Sandia National Laboratories. Retrieved 2010-10-03.