PH442: Theory and Simulation of Nanostructures 3 0 0 6

Interatomic Potentials: Potential energy Surface, pair potential approximation; advantages and limitations, Phenomenological potentials; Buckingham, Morse, Lennard-Jones and Berker, Pseudo potentials, Many-Body potentials.

Molecular Dynamics(MD): Models for MD calculations; initial value, Isothermal equilibrium, boundaries, Nano-design and Nano-construction, solution of the equation of motion; Verlet, Gear-Predictor, and other methods, Efficient Force Field Computation; Forcederivation, List method, Cell algorithm, Scalable parallel procedure.

Characterization: Thermal stability, Material properties, wear at the Nanometer level, Mean Values and correlation functions.

Nano-Engineering: Functional Nanostructures, Nano-Machines, Nano-clusters; influence of initial conditions, temperature, crystalline structure, etc. Simulated Nano-structure transformations.

Texts/References:

1. M. Rieth, *Nano-Engineering in Science and Technology: An Introduction to the World of Nano-Design*, World Scientific, (2003).
2. M. A. Ratner and D. Ratner, *Nanotechnology: A Gentle Introduction to the next Big Idea*, Pearson (2002).
3. J. M. Haile, *Molecular Dynamics Simulation*, John Wiley & sons (1992).