MSE 831 Modeling of Material Processes

CHs: **3**

Pre-requisites: **Nil**

Course Objectives:

- To understand computer simulation modeling approaches to optimize required materials properties.
- Some basic introduction to molecular dynamic modeling.-

Course contents:

- Theory and application of atomistic computer simulations to model,
- Understand, and predict the properties of real materials.
- Energy models: from classical potentials to first-principles approaches.
- Density-functional theory and the total-energy pseudo-potential method.
- Errors and accuracy of quantitative predictions.
- Thermodynamic ensembles: Monte Carlo sampling and molecular dynamics simulations.
- Free energies and phase transitions. Fluctuations and transport properties.
- Coarse-graining approaches and meso-scale models.

Course Outcomes:

- Application of computer modeling software to optimize materials desired properties and overcoming different constraints expected in a given material development process.

Recommended Text / Reference Books:

- Molecular Modeling Techniques in Material Science (JorgRudiger)
- Topics in Computational Materials Science (C Y Fong)
- Computational Studies of New Materials (Daniel A Jelski, Thomas F George)