Mechanical Engineering Dept. Department

Syllabus
ME 449: Introduction to Atomistic Simu (3-0-3)

Course Catalog Description:

Classical and quantum mechanics techniques for atomistic simulations, Essentials of statistical thermodynamics and quantum mechanics concepts, Classical molecular dynamics, Density functional theory. Materials properties: Band structure, elastic constant, thermal conductivity, Phonons and vibrational spectroscopies, free-energy calculations, diffusion coefficients, viscosity, surface chemistry, Transition State Theory.

Course Objectives:

1. Explain MD fundamentals including: Newton’s equation integration methods, interaction potentials, energy landscape, correlation functions etc
2. Explain how to apply MD to obtain materials properties and analysis the results
3. Introduce concepts and methods in modern electronic structure theory as applied to materials science
4. Describe how to perform first-principles calculations, modeling, and design of materials
5. Explain the numerical aspects of DFT in detail. Explain the two popular of basis sets, i.e., Gaussian basis and plane-wave basis, for performing DFT
6. Describe how to perform DFT calculations on small molecules and simple solids and calculate the properties of solids and free energies of molecules

Course Learning Outcomes:

CLO1. Explain the dependency of materials properties on the level of time and length scale and identify the best simulation technique for the given problem

CLO2. Explain the basics of molecular simulations and DFT calculations

CLO3. Apply MD and DFT to perform geometry optimization

CLO4. Calculate materials properties using molecular dynamics and DFT methods

CLO5. Analyze the results from MD and DFT calculation and evaluate the errors associated with the calculations

Learning Resources:

- • Understanding Molecular Simulation: from Algorithms to Applications., D. Frenkel, B. Smit, Academic Press, 2002. • Density Functional Theory: A Practical Introduction, D. S. Sholl, J. A. Steckel, WILEY, 2009.

- • Computer Simulation of Liquids, M.P. Allen, D.J. Tildesley, OXFORD, 1987(2009 reprint). • Materials Modelling using Density Functional Theory, F. Giustino, OXFORD, 2014.
- Other learning material such as computer-based software, professional standards or regulations and software. LAMMPS, GROMACS, OVITO, QE

Lecture Assessment Plan:

Assessment Task	Week Due	Weight
Term Project	14	25.0%
Midterm Exam	8	20.0%
Final Exam	as scheduled	25.0%
Quizzes	Every two weeks	10.0%
Assignments	Every week	20.0%

Lecture Weekly Schedule:

Week#	Topics
1	Introduction to computational methods for materials science
2	Shell scripting and HPC introduction
	Classical molecular dynamics
3	Classical molecular dynamics (Continue)
4	Classical molecular dynamics (Continue)
5	Classical molecular dynamics (Continue)
6	Classical molecular dynamics (Continue)
7	Classical molecular dynamics (Continue)
8	Classical molecular dynamics (Continue)
9	Classical molecular dynamics (Continue)
	Density Functional Theory
10	Density Functional Theory (Continue)
11	Density Functional Theory (Continue)
12	Density Functional Theory (Continue)
13	Density Functional Theory (Continue)
14	Density Functional Theory (Continue)
15	Density Functional Theory (Continue)