School of Interdisciplinary Engineering and Sciences (SINES)
National University of Sciences & Technology (NUST)

Title : Computational Modeling of Materials
Code : CSE-840
Credit Hours: 3-0

1. **Description:** This course uses the theory and application of computer simulations to model, understand, and predict the properties of real materials. Specific topics include: energy models from classical potentials to first-principles approaches; density functional theory and the total-energy pseudopotential method; errors and accuracy of quantitative predictions, thermodynamic ensembles, and transport properties. The course employs case studies from industrial applications of advanced materials to nanotechnology. Lab sessions will give students direct experience with simulations of classical force fields, electronic-structure approaches and molecular kinetics and dynamics.
2. **Educational Objectives**: The course aims to introduce students a variety of methods used in different fields of materials science. The course will comprise of lecture notes, lab exercises and assignments of electronic-structure calculations and materials modeling at the meso and nanoscale
3. **Course Outcomes**: By the end of the course, students are expected to be able to i) design, perform and analyze computer experiments using electronic and atomistic simulation techniques appropriate for the problem at hand, ii) be able to extract materials properties from the simulations; iii) recognize the approximations and estimate the level of accuracy to be expected from each modeling technique, and iv) be able to critically read the current scientific literature on computational modeling and simulation of materials.

Detailed Course Contents:

a. Introduction,
   1. Different types of materials
   2. Nanomaterials and their dimensionality
   3. Analysis of bonding in C60
   4. Composite materials

b. Self-Assembled Monolayers
   1. Structure of SAMs
   2. Design and preparation of SAMs
   3. Carbon Nanofoam and Graphene Nanosheets
   4. MXene

c. Energy Models
   1. Pair Potentials
   2. Lattice parameter and energy
   3. Potentials, Supercells, Relaxation methodology
   4. Linear Augmented Plane Wave Potential
   5. Energy Bands
   6. Application to Lattice Models, Sampling Errors, Metastability
   7. ReaxFF
   8. Energetics and Structure from Empirical Potentials
   9. Free Energies and Physical Coarse-Graining

d. Potentials for Organic Materials and Oxides; Quantum World

1. Model Hamiltonions
2. Thermodynamics and Structure Prediction
3. Thermodynamics and kinetics of adsorption

e. Modeling of nanomaterials and complex nano systems
1. Surface modeling of thin films
2. Surface modeling of thin films
3. Simulation of silicon nanowire transistors

Weekly Lecture Breakdown

Week	Topics
1	• Different types of materials • Nano-materials and their dimensionality
2	• Analysis of Bonding and characteristics in Nanoclusters
3	• Composite materials
4	Self-Assembled Monolayers, • Structure of SAMs • Design and preparation of SAMs
5	• Carbon Nanofoam and 2D materials • Graphene Nanosheets • MXene
6	Energy Models • Pair Potential
7	• Lattice parameter and energy • Lab Assignments
8	• Potentials, Supercells, Relaxation methodology • Linear Augmented Plane Wave Potential • Lab Assignments
9	**Midterm**
10	• Energy Bands Structure • DOS, Energy density • Application to Lattice Models, Sampling Errors, Metastability • Lab Assignment
11	• Energetics and Structure from Empirical Potentials
12	• Model Hamiltonians
13	• Thermodynamics and Structure Prediction
14	• Thermodynamics and kinetics of adsorption • Maxwell-Boltzmann distribution
15	• Modeling of nanomaterial and complex Nano systems
16	• Surface modeling of thin films, 2D Materials
17	• Simulation of nanowire transistors
18	**ESE**

5. Lab work:

Supercomputing lab at SINES will be used for exercises

6. Recommended / Reference Books:

1. Introduction to Computational Materials Science: Fundamentals to Applications by Richard LeSar, 1st edition (2013), Cambridge University Press

2. *Computational Materials Science, an Introduction* by June Gunn Lee, Second Edition (2017), CRC Press.

3. *Atomic and Electronic Structure of Solids* by Kaxiras, E (2003), Cambridge, UK: Cambridge University Press.
4. Electronic Structure: Basic Theory and Practical Methods *by* Martin, R, (2004), Cambridge, UK: Cambridge University Press,.
5. *Chemistry of Nanomaterials Fundamentals and Applications*, by Tahir Iqbal Awan, 1st Edition (2020), Elsevier.

Nature of Assessments

Homework/ Assignments:	5%
Quizzes:	5%
MSE:	30%
Final Exam:	40%
Project:	20%