Indian Institute of Technology Kanpur

Proposal for a New Course

1. **Course No:** MSE6XX
2. **Course Title:** Materials from Atomistic Perspective
3. **Per Week Lectures:** 3 (L), Tutorial: 0 (T), Laboratory: 0 (P), Additional Hours [0-2]: 0 (A),
   Credits (3-0-0-0): **Duration of Course:** Full semester
4. **Proposing Department:** Department of Materials Science and Engineering

   Other Departments/IDPs which may be interested in the proposed course: ME, CHE, AE, MSP

   Other faculty members interested in teaching the proposed course: Somnath Bhowmick
5. **Proposing Instructor(s):** Shivam Tripathi (shivamt@iitk.ac.in)
6. **Course Description:**

   A) **Objectives:** Students will develop an understanding of how the behavior and interactions of atoms and electrons determine the structure, stability, and properties of materials. The course will combine fundamental concepts with hands-on computational simulations, nanoHUB-based interactive activities, and practical examples to help students explore materials at the atomic scale and connect simulation results with experimentally observable macroscopic properties.

   B) Contents (preferably in the form of 5 to 10 broad titles):

   Lecture-wise break-up (considering the duration of each lecture is 50 minutes)

S. No.	Broad Title	Topics	No. of Lectures
1.	Quantum mechanics and electronic structure	Introduction to the fundamental principles of quantum mechanics and their application to electrons in atoms and materials. Topics include wave functions, energy levels, atomic orbitals, quantum states, and electronic configurations.	5
2.	Electronic structure and chemical bonding	Fundamentals of electronic interactions responsible for bonding between atoms and molecules. Topic includes ionic, covalent, metallic, and van der Waals bonding and their connection to material structure and properties.	4
3.	Electronic structure of crystal	Electronic behavior in periodic crystalline materials, including formation of energy bands and electronic states. Topics include band gaps, metals, semiconductors, insulators, reciprocal space, and Brillouin zones.	4
4.	Density functional theory (DFT)	Introduction to density functional theory as a first-principles approach for predicting electronic structure and material properties. The computational workflow includes structural relaxation, energy calculations, electronic band structure, and density of states.	5

5.	Optical and dielectric properties	Interaction of electrons and atoms with electromagnetic fields and the resulting material response. Topics include polarization, dielectric properties, electronic transitions, optical response, and related microscopic mechanisms.	3
6.	Classical mechanics and molecular dynamics	Application of classical mechanics and molecular dynamics to describe atomic motion, interactions, and evolution of materials at the atomic scale. Topics include forces, potential energy, interatomic potentials, equilibrium configurations, atomic trajectories, temperature effects, diffusion, structural transformations, and hands-on molecular dynamics simulations.	5
7.	Statistical mechanics, vibration and phonons	Connection between microscopic atomic configurations, thermal motion, and macroscopic thermodynamic properties. Topics include probability distributions, temperature, entropy, ensembles, statistical averages, atomic vibrations, harmonic motion, normal modes, phonons, vibrational density of states, and phonon dispersion.	5
8.	Thermal and mechanical properties	Atomic-scale origins of thermal and mechanical behavior in materials. Topics include heat capacity, thermal expansion, thermal conductivity, elastic properties, stress, strain, and deformation.	3
9.	Connecting atoms to materials	Integration of atomistic, electronic, and statistical approaches to establish the connection between microscopic phenomena and measurable material properties. The emphasis is on understanding how atomic structure, electronic interactions, atomic dynamics, and statistical behavior collectively determine material properties**.**	2
10.	Case studies and applications	Application of computational methods and hands-on simulations to representative materials-science problems. Case studies will demonstrate how atomistic and electronic-structure simulations can be used to understand, predict, and analyse real material behavior.	4
Total			40

C) **Recommended pre-requisites, if any (examples: a- PSO201A, or b- PSO201A or equivalent):** None

D) **Short summary for including in the Courses of Study Booklet:** This course provides an integrated introduction to the computational study of materials, connecting atomic and electronic structure with macroscopic material properties. It combines fundamental concepts in quantum mechanics, electronic structure, DFT, molecular dynamics, statistical mechanics,

and material properties with hands-on nanoHUB-based simulations and real-world materials applications.

7. Recommended text/reference books:
   A) Ashcroft, N.W. and Mermin, N.D. (1976) "*Solid State Physics"*. Saunders College, Philadelphia, 116, 217.
   B) Martin, Richard M. "*Electronic structure: basic theory and practical methods"*. Cambridge university press, 2020.
   C) Frenkel, Daan, and Berend Smit. "*Molecular simulation: from algorithms to applications." Florida* (2000).
   D) Griffiths, David J., and Darrell F. Schroeter. "*Introduction to quantum mechanics"*. Cambridge university press, 2018
   E) Strachan, A., "*From Atoms to Materials: Predictive Theory and Simulations"*, nanoHUB, Purdue University.
8.
9. Any other remarks: None

Dated: 26/08/2026 Proposer: Shivam Tripathi

Dated: DPGC Convener:

The course is approved / not approved

Chairman, SUGC

Dated: