Approved in 44th BoA Meeting (24-11-2021)

Course number : EN 511
Course Name : Computational Methods in Material Science
Credit Distribution : *1-0-6-4*
Intended for : UG/PG (Compulsory for MTech. in Materials and EnergyEngineering, and Elective for others)
Prerequisite : Instructor's consent
Mutual Exclusion : None

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1. Preamble:

This course is designed keeping the students coming from diverse fields in mind. It assumes a initial knowledge of physics, chemistry and mathematics at undergraduate level. It will provide a solid conceptual background necessary for calculating the various physical properties of (especially energy based) materials mentioned below using standard first principle-based codes. Finally, the students will use ABINIT, AFLOW and JARVIS codes to calculate these properties with reasonable accuracy.

2. Course Modules with quantitative lecture hours:

Theory: Density functional theory, Pseudo potentials, Plane wave and Projector augmented wave methods, Exchange-correlation functionals, Self-consistent solutions, Density of states, Band structures, Optical properties, Electrical & thermal conductivities, Seebeck coefficient, Polarization, Piezoelectric tensor, Specific heat, Entropy, Free energy, Elastic tensors, Moduli of elasticity, phonon dispersion, and Machine learning. [14 Hours]

Laboratory/practical/tutorial Modules: [84 Hours]

Part-1: Introduction to the various features of ABINIT code. Calculations of properties related to (i) Photovoltaic materials: Density of states, Band structures, & Optical properties; (ii) Thermoelectric materials: Electrical conductivity, thermal conductivity, Seebeck coefficient, Specific heat, Entropy, Free energy; and (iii) Piezoelectric materials: Polarization, Piezoelectric tensor, Elastic tensors & Moduli of elasticity. [48 Hours]

Part-2: Introduction to the various features of AFLOW and JARVIS codes. Search of new materials with better (i) Electronic, (ii) Optical, (iii) Thermoelectric, and (iv) Piezoelectric properties. [20 Hours]

Project: Proposing and demonstrating various scenarios for improving the properties of the existing state-of-the-art Photovoltaic, Thermoelectric, and Piezoelectric materials. [16 Hours]

3. Text books:

1. Electronic Structure: Basic Theory and Practical Method, Volume 2 by Richard M. Martin, Cambridge University Press, 2020.
2. Machine Learning in Materials Science: Recent Progress and Emerging Applications by Tim Mueller, Aaron Gilad Kusne and Rampi Ramprasad; A Chapter in Reviews in Computational Chemistry, Volume 29, Editors: Abby L. Parrill and Kenny B. Lipkowitz, John Wiley & Sons, Inc., 2016

References:

1. Burke, Kieron. "The abc of dft." Department of Chemistry, University of California 40 (2007).

4. Similarity with the existing courses: NA

(Similarity content is declared as per the number of lecture hours on similar topics)

S. No.		Course Code	Similarity Content	Approx. % of Content

3. **Justification of new course proposal if cumulative similarity content is >30%:**