

INDIAN INSTITUTE OF TECHNOLOGY INDORE

Discipline of Mechanical Engineering

Organizes

5-Days Active Learning Course on

Atomistic Modelling of Solids: Theory & Applications

December 21-25, 2020

Sponsored by Technical Education Quality Improvement Programme (TEQIP)-III, MED



TEQIP-3
Technical Education Quality Improvement Programme

NEED AND NOVELTY OF COURSE:

This is a first of its kind course and its novelty lies in the following in view of incorporation of nanotechnology related topics in various disciplines/centers, advent of nanotechnology research in Indian educational systems and R&D sectors, and availability of computational facilities. Materials exhibit dramatically altered properties and physical mechanisms when they have characteristic dimensions below ~ 100 nanometers. This is attributed to the enhanced role of lattice defects, surfaces and interfaces, and quantum effects. This course will provide a single window and platform for participants to comprehend the wide range of topics for studying the behavior/properties of nanomaterials, especially 21st centuries wonder carbon- and boron nitride-based materials which are widely used in multifarious nanotechnology applications. The great disparity in scales of materials and the evolved size-scale effects essentially require atomistic modelling as it serves as a complement to costlier and time-consuming conventional experiments; therefore, atomistic simulations and their use/applications at continuum level is exciting and stimulating students/researchers from all disciplines and scientific fields. Keeping the interest of participants from various backgrounds in mind, the contents of the course were developed which will be covered by the experts with interdisciplinary expertise and multi-institutional experience as well as from industry.

COURSE SYLLABUS

Purpose and need of this course! Advantages and limitations of continuum modelling/mechanics; Basics of nanomechanics, principles of molecular mechanics and dynamics, potentials, ensembles, potential field and Virial stress; Atomic/molecular structure of nanomaterials, intermolecular forces, atomistic elasticity, functionalization and lattice defects; Multiscale modeling, Bohr's correspondence principle, linking atoms and continuum, and mechanics and modeling of nanocomposites; Application/use of atomistic results at bulk level (macro- and micro-meter levels); Lab modules on modeling of thermomechanical properties of carbon- and boron nitride-based nanostructures; A number of basic research studies from advanced materials and nanotechnology; Case studies and applications of atomistic modelling of solids in multidisciplinary areas.

COURSE FACULTY

- Dr. Shakti S. Gupta, IIT Kanpur
- Dr. Chandra Veer Singh, University of Toronto, Canada
- Dr. Priyal Shah, Advanced Micro Devices, California, USA
- Dr. Srimanta Pakhira, IIT Indore
- Dr. Sumanta Samal, IIT Indore
- Dr. Shailesh I. Kundalwal, IIT Indore (*Lead Expert & Coordinator*)

COURSE OBJECTIVES

- To provide the participants with a theoretical and fundamental understanding of nanomechanics and atomistic modelling.
- To provide the participants with a working knowledge of nanostructure-property relations and modeling of nanostructures.
- To provide the participants with a training of use of GNU General Public License-based simulation tools needed for quantitative characterization/visualization of nanostructures.
- To introduce the participants into practical problems of nanomechanics, and their solutions, through case studies in multidisciplinary areas.
- To demonstrate the application of this course in the modeling of bulk properties of advanced materials on varied lengths from millimeter to micrometer.

COURSE MODULE

This is an active learning-based course and comprised of lectures, labs, and hand-on training/demonstrations via the use of **GPL-based software** which will tremendously help participants to immediately kick-start application of atomistic modelling with available & minimum resources.

CERTIFICATE

Participants who successfully complete the course will be awarded with a certificate.

TARGET PARTICIPANTS

This course is a tailor made for the students, engineers, researchers, and faculty members from diverse fields of study/research. Number of participants are limited to 50 on first come first basis.

REGISTRATION PROCESS

Online Mode: Registration using link "[Atomistic Modelling of Solids](#)"
Via E-mail: The below particulars can be sent to kundalwal@iiti.ac.in along with a scanned copy of your institute/organization identity card.

Name:

Designation:

Institution/Organization:

Address of Institution/Organization:

Academic qualification:

Are you a faculty member from TEQIP Institute? (**Yes or No**):

E-mail id:

Phone/Mobile No.:

(Payment details for all others except "faculty" participants from TEQIP institutes. Only "faculty" participants from TEQIP institutes are exempted from the registration fees)

Bank name:

Payment reference No.

Amount transferred:

Date of transaction:

Any other relevant information:

REGISTRATION FEE

- **No fee for faculty participants from TEQIP Institutes.**
- The fee is **₹ 6000 for students/postdocs** from TEQIP/Non-TEQIP Institutes and **₹ 8000 for faculty/Scientist** from Non-TEQIP Institutes and other universities/organization.
- For industry personnel, the fee is **₹ 10000**.

Note: The fees includes service tax.

For TEQIP Faculty Participants: The nomination along with the registration form must be sent through their TEQIP coordinator to the e-mail of course coordinator: kundalwal@iiti.ac.in. Email confirmation in advance is suggested.

Online Registration Link: "[Atomistic Modelling of Solids](#)"

Registration Deadline: December 14, 2020

Notification of Acceptance: By December 15, 2020

Note: Technically the course will be started from **Dec 16, 2020** by providing systematic instructions to the registered participants on installing free and open source software such as LAMMPS, NanoEngineering-1, VMD, etc. in their laptops/computers (any version). It is expected that the essential software required for the course are running in their systems by the start of course.

MODE OF CONDUCT OF COURSE: ONLINE

Mode of payment (for other than TEQIP Faculty participants)

Online Payment: Please click or copy & paste below link.

<https://forms.eduqfix.com/indoreiit/add?formType=9263526567614218>

Bank Transfer: Registration fee can be paid through NEFT/IMPS to the below A/c number:

Name of the Beneficiary: Registrar, IIT Indore

Name of Bank: Canara Bank

Branch: Simrol, Indore

Account No. 1476101027440

IFSC Code: CNRB0006223

COURSE COORDINATOR:

Dr. Shailesh I. Kundalwal

Associate Professor of Mechanical Engineering, IIT Indore

Founding In-charge, Applied & Theoretical Mechanics (ATOM) Lab

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