

Bridging Experiments and Atomistic Modeling



DAE-BRNS Theme Meeting

Friday, November 4, 2022

Multipurpose Hall, TSH
Anushaktinagar, Mumbai - 400094

Organizer

Chemical Engineering Division
Chemical Engineering Group
Bhabha Atomic Research Centre
Trombay, Mumbai - 400085



Scope of the Theme Meeting

A one-day theme meeting on "Bridging Experiments and Atomistic Modeling (**BEAM-22**)" is being organized by Chemical Engineering Division, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai, India, on November 4, 2022. The meeting is supported by the Board of Research in Nuclear Sciences (BRNS), Department of Atomic Energy (DAE).

The power of atomistic modeling is growing rapidly with the continuing development of computer power, new and robust algorithms, and the availability of software. Today, molecular modeling can sometimes provide useful estimates of the properties and behavior of materials - even before they have been synthesized and useful estimates of the parameters and behavior needed to do traditional chemical engineering process development & design. The theme of the meeting is contemporary research on atomistic modeling for the development and design of chemical engineering systems and processes. The deliberations of the theme meeting will cover the atomistic modeling aided studies on following topics.

- A. Fundamental Studies on Structures, Thermodynamics and Transport Properties.
- B. Metal Ion and Isotope Separation.
- C. Nuclear Waste Processing and Water Purification.
- D. Reaction Mechanism, Catalysis and Gas Storage.
- E. Nanomaterials, Polymers and Amorphous Materials.
- F. ML/AI based Molecular Recognition.

Patron

Dr. A.K. Mohanty
Director, BARC

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Board of Research in Nuclear Sciences (BRNS) supports research and development activity in universities, institutes of higher learning and national laboratories in India in the fields relevant to the mandate of Department of Atomic Energy. BRNS also supports symposia, conferences, seminars and workshops in various areas of science and technology.

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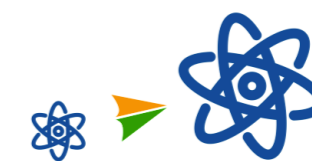
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No Registration Fee for Participants

Interested participants may please contact Secretary, Organizing Committee, through e-mail (Consent of Head of the Division is necessary). You may also reach us at daeccs2019@gmail.com

Last Date of Registration: October 20, 2022