Online Workshop on

ICME READINESS OF DIGITAL PLATFORMS

An Invited Technical Presentation Series: July-August, 2021

Organized by
ICME National Hub
in association with
Indian National Academy of Engineering

DIGITAL SCIENTIFIC PLATFORM FOR MATERIALS INNOVATION

By

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Date and Time

August 31, 2021 (Tuesday), 06:00 PM IST

Zoom link for the event

https://iitk-ac-in.zoom.us/j/95710536859?pwd=M3BzSXJJZzlHY1kxNWd4TEk1YkdMZz09

Meeting ID: 957 1053 6859

Passcode: 534631

About the Workshop

Integrated Computational Materials Engineering (ICME) is an emerging and transformative discipline with a huge potential to accelerate materials discovery, product design and process optimization. The Indian National Academy of Engineering (INAE) is engaged in developing a technology roadmap for "Accelerated Materials Discovery, Scale-up and Exploitation Strategy for Strategic Materials Needs of India". The compilation and integration capabilities of various digital platforms that can assist the ICME community is one of the essential parts of this effort. Therefore, the ICME National Hub at IIT Kanpur, in association with INAE, is organizing a "Workshop on ICME Readiness of Digital Platforms" – a technical presentation series about the capabilities of important digital platforms vis-à-vis accelerated development, production and exploitation of materials and products.

For more details please visit: https://www.iitk.ac.in/ICME/INAE-Workshop/

ICME National Hub Website: https://www.iitk.ac.in/ICME/

INAE Website: https://www.inae.in/

Abstract

Convenient access to a wide range of simulation methods has provided researchers across the world with the capability to gain unique insights into behavior of various classes of materials, as evidenced by more than 25,000 references in scientific literature. As computing resources (hardware and software) commoditize and the methods mature, two key challenges emerge;

1) to connect the hierarchy of methods available from electronic structure level through to macroscopic/engineering scales, and

2) to maximize the utility of the data arising from these simulations and experiments through careful automation, knowledge management and application of machine learning.

In this talk, we will highlight the capability of our scientific platform with reference to development of battery materials, composites and metal alloys in particular, and look forward to upcoming integrations that are poised to meet the challenges of both multi-scale modelling and closer integration with data science.

About the Speaker

Dr. Abhijit Chattopadhyay obtained his Ph. D. from Burdwan University India in Physical Analytical Chemistry in 1992. He joined National Chemical Laboratory, Pune, India after completing post-doctoral collaboration with UCSB, Santa Barbara and CNRS Montpelier. He then moved to Japan as Visiting Associate Professor in Tohoku University, Sendai, Japan in 1995 and then worked as Senior Researcher in National Advanced Industrial Institute (AIST), Sendai, Japan until 2004 before joining Dassault Systemes. Currently he is working as a Senior Manager of the Technical Team for the ASIA Pacific with a global role.

Dr. Chattopadhyay has published around 125 research papers in peer reviewed journals and has written several book chapters. He has been involved in various government projects and worked as project lead with different commercial companies to develop new functional materials in combination with multi-scale modeling and data science using scientifically aware enterprise platform.

Conveners

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