

# Modeling and Simulation in Energy Storage

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## Overview

Energy storage is a key enabler in the energy sustainability eco-system. Lithium-ion batteries have transformed the modern rechargeable world with footprint in the portable electronics, vehicle electrification and grid-scale storage. The importance of modeling and simulation in accelerating innovation and design toward improved performance (energy/power), safety and life of lithium-ion batteries is critical. These are complex, dynamical systems, which include coupled physical and electrochemical processes encompassing electronic, ionic, diffusive transport in solid/electrolyte phases, electrochemical and phase change reactions and stress generation in porous electrodes. The performance, thermal safety, and lifetime of Li-ion batteries are predicated on fundamental understanding of the underlying reaction and transport processes. This course will lay out the details of a comprehensive computational modeling framework of thermo-electrochemical interactions in lithium-ion batteries toward predicting performance life and safety.

Course participants will learn these topics through lectures. Also case studies and assignments will be shared to stimulate research motivation of participants.

<b>Modules</b>	<b>A: Modeling and Simulation in Energy Storage: 11-17 December 2021 (7:30 - 9:30 PM, IST)</b> <b>(In Virtual Mode)</b>
<b>You Should Attend If...</b>	<ul style="list-style-type: none"><li>• Executives, engineers and researchers from manufacturing, service and government organizations including R&amp;D laboratories.</li><li>• Student students at all levels (BTech/MSc/MTech/PhD) or Faculty from reputed academic institutions and technical institutions.</li></ul>
<b>Fees</b>	The participation fees for taking the course is as follows: <b>Participants from abroad : US \$100</b> <b>Industry/ Research Organizations: Rs. 4000</b> <b>Academic Institutions:</b> <b>Student Participants: Rs. 200</b> <b>Faculty Participants: Rs. 2000</b>

# The Faculty



Partha P. Mukherjee is a Professor of Mechanical Engineering at Purdue University. His prior appointments include Assistant Professor and Morris E. Foster Faculty Fellow of Mechanical Engineering at Texas A&M University (2012-2017), Staff Scientist at Oak Ridge National Laboratory (2009-2011), Director's Research Fellow at Los Alamos National Laboratory (2008-2009), and Engineer at Fluent India (subsidiary of Fluent Inc., currently Ansys Inc., 1999-2003). He received his Ph.D. degree in Mechanical Engineering from The Pennsylvania State University in 2007. His awards include Scialog Fellows' recognition for advanced energy storage, University Faculty Scholar and Faculty Excellence for Early Career Research awards from Purdue University, The Minerals, Metals & Materials Society Young Leaders Award, to name a few. His research interests are focused on mesoscale physics and stochastics of transport, chemistry, and materials interactions, including an emphasis in the broad spectrum of energy storage and conversion. (Email: [pmukherjee@purdue.edu](mailto:pmukherjee@purdue.edu); Research Group: <https://engineering.purdue.edu/ETSL/>)



**Dr. Amaresh Dalal** is currently Professor of Mechanical Engineering at Indian Institute of Technology, Guwahati. He received his Ph.D. degree from Indian Institute of Technology Kanpur in 2009 and he was Post-doctoral Research Associate at Purdue University from Sep 2008 - Dec 2009. He has research interests in the area of Computational Fluid Dynamics and Heat Transfer, Finite Volume Methods and Unstructured Grid Techniques, Multiphase Flows, Natural and Mixed Convection Flows. Dr. Dalal is now deeply involved in developing a general purpose, versatile and robust computational fluid dynamics solver over hybrid unstructured grid which can solve a wide range of real-life fluid flow, heat transfer, and problems involving transport phenomena over complex geometries. He received Prof KN Seetharamu Medal and Prize for the Best Young Researcher in Heat Transfer-2017 from Indian Society of Heat and Mass Transfer.

## Course Co-ordinator

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<http://www.gian.iitkgp.ac.in/GREGN>

# Schedule: Modeling and Simulation in Energy Storage

**Dates:** December 11-17, 2021 in Virtual Mode

**Time:** 7:30 - 9:30 PM IST (9:00 - 11:00 AM, US EST)

## **Day 1: Dec. 11**

Lecture 1: 1 hr

Introduction to the fundamentals of electrochemical and transport mechanisms in lithium-ion batteries

Lecture 2: 1 hr

Basics of how the underlying transport and electrochemical mechanisms affect performance, life, and safety of lithium-ion batteries

## **Day 2: Dec. 12**

Lecture 3: 1 hr

Coupled governing differential equations that characterize the electrochemical and transport processes in Li-ion batteries

Lecture 4: 1 hr

Thermo-electrochemical coupled modeling framework for Li-ion battery performance, safety, and degradation

## **Day 3: Dec. 13**

Lecture 5: 1 hr

Computational modeling and analysis for Li-ion battery performance prediction

Lecture 6: 1 hr

Computational modeling and analysis of coupled thermo-electrochemical interaction

## **Day 4: Dec. 14**

Lecture 7: 1 hr

Computational modeling of Li-ion battery thermal safety

Lecture 8: 1 hr

Analysis of Li-ion battery thermal safety under abuse conditions of thermal and electrochemical extremes

## **Day 5: Dec. 15**

Lecture 9: 1 hr

Computational modeling of Li-ion battery degradation due to lithium plating

Lecture 10: 1 hr

Analysis of lithium plating under operational extremes for Li-ion batteries

## **Day 6: Dec. 16**

**Tutorial 1:** 2 hrs

Modeling and analysis of Li-ion battery performance

## **Day 7: Dec. 17**

**Tutorial 2:** 2 hrs

Modeling and analysis of Li-ion battery thermal safety