MRS MATERIALS RESEARCH SOCIETY®

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MRS Bulletin Webinar

NOVEMBER 2ND
11AM TO 12:30PM

FREE EVENT!

REGISTRATION REQUIRED!

https://mrs.digitellinc.com/mrs/

Host

Pratyush Tiwary
University of Maryland

Guest Speakers

Maria K. Chan
Argonne National Laboratory

Arun K. Mannodi Kankkithodi
Purdue University

Sapana Sarupria
University of Mineesota Twin Cities

The materials science community across academia and industry has long benefitted from and contributed to the development of quantitative methods to reveal predictive patterns in the triad of structure–property-function relationships across all branches of materials sciences and engineering. It is now possible to train artificial intelligence (AI) and machine learning (ML) models to make predictions or extract patterns at spatiotemporal scales that were previously impossible with conventional computational materials modeling. Powerful open-source toolkits for AI/ML model training and architecture selection have also made ML more accessible. As a result, in laboratories across the world, scientists and engineers are identifying ways in which they can incorporate AI and ML into their research.

The September and October issues of MRS Bulletin broadly review some of the critical, recent progress in the application of AI/ML to various aspects of materials science. These include AI/ML approaches for crystal structure prediction, high-throughput microscopy, designing energy materials, and describing force-fields governing material and molecular behavior. The talks in the webinar will cover and provide a flavor of some of these aspects.

TALK PRESENTATIONS

- **Theory-informed AI/ML for Microscopy & Spectroscopy**
  - Maria K. Chan
- **High-throughput Computations and Machine Learning for Halide Perovskite Discovery**
  - Arun K. Mannodi Kanakkithodi
- **Machine learning for molecular simulations of crystal nucleation and growth**
  - Sapna Sarupria