

SUBMIT AN ABSTRACT FOR THE FOLLOWING SYMPOSIUM

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

AI/ML/Data Informatics for Materials Discovery: Bridging Experiment, Theory, and Modeling

Artificial intelligence, machine learning, and data informatics (AI/ML/DI) are rapidly becoming prevalent in materials discovery, design, and application. The application of AI/ML/DI presents groundbreaking opportunities to efficiently address complex tasks, such as rapidly screening vast candidate material spaces and formulating new constitutive equations in significantly shorter timeframes than traditional methodologies. However, as AI/ML/DI technologies advance within the materials domain, it is increasingly important to recognize and address the limitations and challenges that must be overcome to facilitate broader adoption. This symposium will focus on the frontiers of the use AI/ML/DI in the modern materials laboratory including during physical and computational experimentation.

A key challenge for the use of these techniques is the collection, curation, and application of sufficient amounts of high-quality data needed for accurate AI/ML/DI use. The materials field has traditionally been data-starved, posing unique challenges in comparison to other scientific disciplines. A focus of this symposium is presenting research for approaches to address data challenges in the materials field. In addition, the materials field, and particularly metals and minerals, has developed a considerable knowledge base over hundreds of years. Leveraging existing traditional expertise in conjunction with AI/ML/DI is also of major interest. This symposium will cover these research topics, and others listed below, from a perspective that connects theory and experiment.

Topics addressed in this symposium will include (but not be limited to):

- Uncertainty quantification, verification and validation applications for materials science
- Hybrid AI/ML/DI and traditional approaches for materials science
- Large language and foundation models for material property prediction, inverse design of new materials, and service-life estimation
- Collaborative federated learning for collaborative materials research
- Transfer learning approaches in materials science
- FAIR (findability, accessibility, interoperability, and reusability) data principles in materials data informatics
- Novel and enhanced AI-driven data generation, extraction, cleaning, and curation
- Physics-informed, generative, and scientific machine learning for scarce, sparse, and multi-modal datasets and ICME model development

SPONSORED BY:

TMS Materials Processing & Manufacturing Division; TMS Structural Materials Division; TMS Computational Materials Science and Engineering Committee; TMS Mechanical Behavior of Materials Committee

ORGANIZED BY:

- Niaz Abdolrahim, University of Rochester
- Kamal Choudhary, National Institute of Standards and Technology
- Dehao Liu, Binghamton University
- Darren Pagan, Pennsylvania State University
- James Saal, Citrine Informatics
- Christopher Stiles, Johns Hopkins University Applied
 Physics Laboratory
- Anh Tran, Sandia National Laboratories
- **Daniel Wines**, National Institute of Standards and Technology

www.tms.org/TMS2026

QUESTIONS? Contact programming@tms.org