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TMS2025

154th Annual Meeting & Exhibition

March 23–27, 2025
MGM Grand Las Vegas
Hotel & Casino
Las Vegas, Nevada, USA
#TMSAnnualMeeting

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2025 SYMPOSIUM:

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Bridging Scale Gaps in Multiscale Materials Modeling in the Age of Artificial Intelligence

The connections between computational material tools at dierent length/time scales are long-existing problems. Many physical-based methods have difficulties constructing the quantitative governing equations based on lower-scale simulation data to achieve high accuracy and transferability in higher-scale simulations. Addressing these problems has become more urgent with increasing interest in chemically complex materials (including high entropy materials), materials under extreme conditions, and advanced materials processing. Fortunately, the growth of computational resources and materials data repositories is resulting in the availability of various types of training data sets for machine learning. Furthermore, the development of artificial intelligence (AI) techniques is also expanding the range of methods to utilize, analyze, and interpret these data.

The collective integration efforts through the computational material science community and the experimental collaborators enhance these practices. To echo this trend in the integration of computational material science and AI, this symposium is dedicated to topics that emphasize the applications of AI and machine learning methods to build quantitative and robust connections between computational material tools at different length/time scales to accurately explain and predict complex material behaviors observed in experiments.

Topics include, but are not limited to:

- Understanding and prediction of material properties using physics-informed and/or data-driven models based on training datasets from first-principles calculations and/or atomistic simulations.
- Construction of machine learning interatomic potentials based on training datasets from first-principles calculations.
- Mesoscale simulation methods (phase field, Monte Carlo, kinetic Monte Carlo, dislocation dynamics, etc.) based on governing equations fitted by physics-informed and/or data-driven models with training datasets from first-principles calculations and atomic simulations.
- Construction of continuous models based on discrete models using AI (such as discrete dislocation dynamics to density-based dislocation dynamics).
- Construction of phenomenological models aided by AI analyses of simulation and/or experimental results.
- Construction and tuning of governing equations of mesoscale simulations based on AI analysis of experimental results.

ORGANIZERS

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