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TMS 2026

155th Annual Meeting & Exhibition

March 15–19, 2026
San Diego Convention Center
and Hilton San Diego Bayfront
San Diego, California, USA
#TMSAnnualMeeting

SUBMIT AN ABSTRACT FOR THE FOLLOWING SYMPOSIUM

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Foundations for Autonomous Materials Design

This symposium is concerned with understanding, constructing, and optimizing ML/AI tools for processing-structure-properties relationships in materials science and engineering, to autonomously develop materials. The intent here is to go beyond combinatorics for materials discovery (i.e. active learning over chemistries to optimize a small set of properties) and rather into maturing candidate materials into deployable materials, which requires an iterative design process in which new constraints often emerge.

There has been considerable effort to develop physics-based models that map between input domains (processing) and output domains (structure and/or properties). Modern machine learning algorithms, for the first time, allow for exploring not just point solutions, but the effects of whole processing paths on the final output. These paths, themselves, can be engineered and manipulated to achieved desired results. For example, in a complex processing path, a cooling stage can be modified to explore its effects on structures or properties. If regions can be mapped out where small changes in the process results in a small perturbation of the structure/property – navigability - this allows for autonomous iterative design.

This symposium aims to bring together researchers interested in the various components of autonomous materials design. For this symposium, relevant contributions can include:

- Integrated Computational Materials Engineering models for mapping process-structure or structure-process and inversion of these models
- Generative AI for microstructure prediction
- Control theory and feedback design for process optimization
- Latent space representations of multi-dimensional (hierarchical and/or multi-modal) materials information
- Manifold hypothesis for data representation
- Generation of paired datasets for model training
- Stochastic models of microstructure and their representation
- Metric space and topological space representations of materials data
- Disentanglement and identification of latent space dimension in terms of materials relevant features
- Novel approaches for autonomous search for solutions with multiple objectives and constraints

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