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TMS 2025

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

AI/Data Informatics: Computational Model Development, Verification, Validation, and Uncertainty Quantification

Materials discovery has traditionally been a slow, iterative process guided by intuition, insight, and trial-and-error. However, new advances in computation and experimentation are posed to radically alter this paradigm. High-throughput approaches have facilitated characterization of expansive design spaces of possible materials and contributed to the formation of large materials databases. Furthermore, text mining methods and large-language models applied to vast sets of scientific literature are emerging for machine-learned synthesis methods. Finally, supervised and self-supervised machine learning approaches increasingly reveal their value for building surrogate material models and improving predictive capabilities for material processing and performance. Enhancing the use of these 'big' data through decision making informed by artificial-intelligence (AI) and data informatics as a means to accelerate the discovery of superior materials and advanced engineered systems, as well as to understand and predict complex behavior of existing materials. Before this can happen though, all these computational frameworks, including physics-based or data-driven methods, need a careful assessment of their uncertainties at and across different time and length scales. Beyond uncertainty quantification, efficacy of any simulation method needs to be validated using experimental or other high-fidelity computational approaches. This symposium will focus on AI and data informatics methods for materials, AI-ready materials data issues, computational methodology validation, as well as uncertainty quantification, verification, and validation of computational materials models at all scales. The goal of the symposium is to cover these research topics from an interdisciplinary perspective that connects theory and experiment, having a view towards materials applications.

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

- Generative machine learning for developing new candidate material systems
- Optimization of high-throughput computational and experimental materials characterization and testing
- Artificial intelligence approaches applied to materials design and optimization: model development, applications, and validation
- Physics-based regularization of machine learning models
- Data mining and large language models: difficulties, techniques, and applications; including development of mineable data features
- Validation and uncertainty quantification
- Materials design incorporating uncertainty

ORGANIZERS

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