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TMS2024

153rd Annual Meeting & Exhibition

MARCH 3–7, 2024
HYATT REGENCY ORLANDO
ORLANDO, FLORIDA, USA
#TMSAnnualMeeting

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2024 SYMPOSIUM:

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

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

A critical component of the development and deployment of new technologies is the discovery, characterization, optimization, and transition of materials. Computational investigations at various spatio-temporal scales have proven to be effective tools for all components of this material design process.

Recently, both high-throughput computational and experimental approaches have facilitated characterization of selected incredibly large spaces of possible materials and contributed to the formation of large materials databases. Furthermore, text mining methods applied to vast sets of scientific literature are emerging for machine-learned synthesis methods. Finally, advanced scientific machine learning (SciML) approaches increasingly reveal their values for developing surrogate material models, and for improving predictive capabilities for material processing and performance. Thus, integrating computed data with experiments supports viewing artificial intelligence (AI) and data informatics to accelerate the search for new materials and advance engineered systems, as well as to understand and predict complex behavior of existing materials. However, all these computational frameworks, including those physics-based or data-driven methods, need a careful assessment of their uncertainties at different 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 methods for materials, AI-ready materials data issues, computational methodology validation, as well as uncertainty quantification, verification, and validation of computational materials models across various 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):

- Machine learning and artificial intelligence approaches applied to materials science: model development, applications, and validation
- Physics-based regularization of machine learning models
- Data mining: difficulties, techniques, and applications; including development of mineable data features
- Validation and uncertainty quantification
- Materials design under uncertainty

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