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TMS 2023

152nd Annual Meeting & Exhibition

MARCH 19–23, 2023
SAN DIEGO CONVENTION CENTER &
HILTON SAN DIEGO BAYFRONT
SAN DIEGO, CALIFORNIA, USA
#TMSANNUALMEETING

SUBMIT AN ABSTRACT BY JULY 1 FOR THE FOLLOWING TMS2023 SYMPOSIUM:

MATERIALS DESIGN

AI/Data Informatics: Computational Model Development, 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 spatiotemporal 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 machine learning (ML) approaches increasingly reveal their value 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 as a means 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-based 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 evaluation for computational materials modeling 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 are not 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 minable data features
- Validation and uncertainty quantification

ORGANIZERS

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