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FEBRUARY 27-MARCH 3, 2022
ANAHEIM CONVENTION CENTER & ANAHEIM MARRIOTT
ANAHEIM, CALIFORNIA, USA
#TMSAnnualMeeting

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2022 SYMPOSIUM:

MATERIALS DESIGN

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

Technological advances heavily rely on the discovery, characterization, development, and transition of materials. Computational investigations at different spatiotemporal levels are proven effective tools for characterizing, understanding, and predicting material-properties, and for proposing new material possibilities. Recently, both high-throughput computational and experimental approaches facilitated scans of incredibly large spaces of possible materials, especially functional materials, and contributed to the formation of large materials databases. Further, text mining methods applied to vast sets of scientific literature are leading to machine-learned synthesis methods. Additionally, advanced machine learning (ML) increasingly reveals their value for developing sophisticated material models, and for improving computational methods. Thus, the power of integrating computed data with experiments supports viewing artificial intelligence (AI) and data informatics as a possible way to accelerate the search for new materials. However, all of these computational frameworks, including those physics based-approaches or data-based methods, need a careful evaluation of their uncertainties at different scales. Furthermore, efficacy of any simulation method needs to be validated using experimental or other high fidelity computational approaches.

This symposium will focus on AI methods, big data issues, computational methodology validation, as well as uncertainty evaluation for computational approaches used at various length 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):

- Big data: issues, techniques, and applications
- Machine learning and other artificial intelligence approaches applied to material science: model developing, 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

Saurabh Puri, Microstructure Engineering
Dennis M. Dimiduk, BlueQuartz Software LLC
Darren C. Pagan, Pennsylvania State University
Anthony D. Rollett, Carnegie Mellon University
Francesca M. Tavazza, National Institute of Standards and Technology
Christopher F. Woodward, Air Force Research Laboratory

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