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TMS 2019

148th Annual Meeting & Exhibition

CALL FOR ABSTRACTS

March 10–14, 2019
San Antonio, Texas, USA

SUBMIT AN ABSTRACT TO:

MATERIALS DESIGN

Computational Approaches for Big Data, Artificial Intelligence and Uncertainty Quantification in Computational Materials Science

Technological advances heavily rely on the discovery, characterization, and development of materials. Computational investigations, at the continuum, classical, and quantum level, have proven to be extremely effective tools in both characterizing material properties and identifying new material possibilities. High-throughput approaches have recently helped scanning the incredibly large space of possible materials, and contributed to the formation of large databases. Artificial intelligence techniques are seen as a reliable way to further accelerate such search for new materials. All these computational approaches are only as good as the quality of data they are trained on and results at any length scale need a careful evaluation of their uncertainties. Furthermore, a way to evaluate the predictability of simulation techniques is to validate their findings using other, experimental or computational, approaches.

This symposium will focus on artificial intelligence methods, big data issues, computational methodology validation, as well as uncertainty evaluation for computational approaches at various length scale. The goal of the symposium is to cover these research topics in an interdisciplinary approach, which connects theory and experiment, with a view towards materials applications.

Topics addressed in this symposium will include:

- Big data: issues, techniques and applications
- Machine learning and other artificial intelligence approaches applied to material science: model developing, applications and validation
- Data mining: difficulties, techniques and applications
- Validation and uncertainty quantification for:
  - atomistic modeling (DFT and classical force fields)
  - meso- and continuum scale modeling
  - multi scale modeling

ORGANIZERS

Francesca Tavazza, National Institute of Standards and Technology, USA
Liang Qi, University of Michigan, USA
Christopher Woodward, Air Force Research Laboratory, USA
Adrian Sabau, Oak Ridge National Laboratory, USA
Houlong Zhuang, Arizona State University, USA
Sugata Chowdhury, National Institute of Standards and Technology, USA

Abstract Deadline is July 1, 2018.
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Questions?
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