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SUBMIT AN ABSTRACT BY JULY 1

MARCH 14-18, 2021 • ORLANDO WORLD CENTER MARRIOTT
ORLANDO, FLORIDA, USA
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SUBMIT AN ABSTRACT TO:

MATERIALS DESIGN

AI/DATA INFORMATICS: APPLICATIONS AND UNCERTAINTY QUANTIFICATION AT ATOMISTICS AND MESOSCALES

Technological advances rely on the discovery, characterization, and development of materials with novel properties. Computational investigations at the continuum, mesoscopic, and quantum level, have proven to be effective for both characterizing properties and identifying new material systems of interest. High-throughput approaches have recently helped in scanning the vast space of possible materials and contributed to the formation of large, public databases, enabling a cascade of research efforts branching from the original work. Artificial intelligence (automation, classification, regression) techniques are seen as a reliable way to further accelerate such searches for new materials. Special care is needed to ensure uniformity and quality of generated databases, but possibly even more importantly, to quantify and expose uncertainties in the data to provide accurate predictions. Furthermore, a way to validate the accuracy of simulation techniques, comparisons with experimental and other computational approaches are necessary.

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

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

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

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Abstract Deadline is July 1, 2020. Submit online at
www.programmaster.org/TMS2021.

Questions?
Contact programming@tms.org