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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 Materials Discovery and Design

Advances in theoretical understanding, algorithms, and computational power are enabling computational tools to play an increasing role in materials discovery, development, and optimization. Recently, application of data mining techniques, genetic algorithms, machine learning approaches, and predictive empirical potentials have demonstrated the "virtual synthesis" of novel materials, with their properties being predicted on a computer before ever being synthesized in a laboratory. This symposium will cover recent methodological developments and applications at the frontier of computational materials science and materials informatics, ranging from quantum-level prediction to macro-scale property optimization. The goal is to cover basic research topics in an interdisciplinary approach, which connects theory and experiment, with a view towards materials applications. Of particular interest is computational and theoretical work that features a strong connection to experiment.

Topics Include:
- Application of materials informatics approaches such as data mining, genetic algorithms, cluster expansions, and machine-learning for structures, properties, and processing
- Innovations that improve accuracy and efficiency of computational materials design
- Computational discovery and design of novel materials, such as 2D materials and materials for energy technologies
- Semi-empirical models of interatomic interaction

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