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TMS 2017
146th Annual Meeting & Exhibition

February 26 – March 2, 2017
San Diego, California, USA

COMPUTATIONAL MATERIALS DISCOVERY AND OPTIMIZATION – FROM BULK TO MATERIALS INTERFACES AND 2D MATERIALS

Advances in theoretical understanding, algorithms, and computational power are enabling computational tools to play an increasing role in materials discovery, development, and optimization. For example, recently developed data mining techniques, genetic algorithms, machine-learning approaches, and predictive empirical potentials enable the "virtual synthesis" of novel materials, with their properties being predicted on a computer before ever being synthesized in a laboratory. Stochastic computational techniques and data analysis methods play an increasing role in materials characterization, design, and optimization. Large-scale computations for complex materials, that are needed to guide and complement novel experiments benefit from reliable empirical energy models.

This symposium will cover recent applications and methodological developments at the frontier of computational materials science, 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 will include:

- First principles materials discovery
- Optimization algorithm to search the structure-composition design space
- Data mining techniques, genetic algorithms, neural networks, cluster expansions, and machine-learning algorithms for structures, properties, and processing
- Innovations that improve accuracy and efficiency of computational materials design
- Computational discovery and design of novel bulk materials, materials interfaces and 2D materials for energy technologies, electronic devices, and catalysis

ORGANIZERS

Richard Hennig, University of Florida, USA
Arunima Singh, National Institute of Standards and Technology, USA
Dallas Trinkle, University of Illinois, Urbana-Champaign, USA
Eric Homer, Brigham Young University, USA

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