TMS2016
145th Annual Meeting & Exhibition

FEBRUARY 14-18 DOWNTOWN NASHVILLE, TENNESSEE MUSIC CITY CENTER

Connecting the Global Minerals, Metals, and Materials Community.

Computational Materials Discovery and Optimization: From 2D to Bulk 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.

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 with an interdisciplinary approach that 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:

- 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 materials, such as 2D materials and materials for energy technologies

Organizers include:

Richard Hennig, University of Florida (USA)
Houlong Zhuang, Oak-Ridge National Laboratory (USA)
Dallas R. Trinkle, University of Illinois, Urbana-Champaign (USA)

Learn More at www.tms.org/TMS2016

Join us at TMS2016 in Downtown Nashville, Tennessee, February 14-18!