

*Connecting the global minerals, metals, and materials community.*



## **Plan Now to Attend:**

### **Computational Modeling and Stochastic Methods for Materials Discovery and Properties**

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, to stochastic methods for materials optimization and analysis. 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:

- 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
- Bayesian statistics based systems analysis
- Development of empirical and semi-empirical energy models
- Innovations that improve accuracy and efficiency of computational materials design

#### **Sponsored by:**

- TMS Functional Materials Division (formerly EMPMD); TMS Materials Processing & Manufacturing Division; TMS Structural Materials Division
- Chemistry and Physics of Materials Committee; Computational Materials Science and Engineering Committee

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