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 TIMES 2018
 March 11 – 15, 2018

 147th Annual Meeting & Exhibition
 March 11 – 15, 2018

SUBMIT AN ABSTRACT TO:

MATERIALS DESIGN

COMPUTATIONAL MATERIALS DISCOVERY AND OPTIMIZATION

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:

- Optimization algorithm to search the structure-composition design space
- 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
- Methods and applications for electrochemical interfaces
- Computational discovery and design of novel materials, such as 2D materials and materials for energy technologies

Six sessions are planned:

- Materials informatics methods
- Computational methods for materials discovery, characterization, and optimization
- 2D materials and materials epitaxy
- Materials Surfaces, interfaces, and electrochemistry
- Materials for energy technologies
- Materials for electronic device applications and energy technologies

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