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TMS 2020

149th Annual Meeting & Exhibition

February 23-27, 2020 • San Diego, California, USA

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Materials Design

Computational Discovery and Design of Emerging Materials

Recent advancements in computational methods, computing power and materials informatics present us with an exciting opportunity to predictively discover and design materials for a variety of technologically relevant applications. In particular, quantum mechanical ab-initio methods such as density-functional theory simulations, dynamical mean-field theory, quantum Monte-Carlo simulations and time-dependent density functional theory have been pivotal in developing an atomistic-scale fundamental understanding of complex phenomena, and in the discovery and the design of several emerging materials, such as superconductors, topological insulators, magnetic materials, photocatalysts, battery materials, and most recently, quantum materials.

This symposium will cover the state-of-the art in the application as well as the integration of computational methods, particularly ab-initio simulation methods, with experiments and materials informatics applied to the discovery and design of emerging materials.

Topics include:
- Computational discovery and design of correlated electron materials, quantum materials, and superconductors
- Computational discovery and design of magnetic materials and topological insulators
- Application of computational methods for photocatalytic and battery materials discovery and design
- Computational discovery and design of materials for nanoelectronics
- Application of materials informatics approaches such as machine learning, genetic algorithms, and cluster expansion for an accelerated discovery and design of materials

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