CALL FOR ABSTRACTS

THE WORLD COMES HERE.

TMS 2018

147th Annual Meeting & Exhibition

MARCH 11 – 15, 2018
PHOENIX, ARIZONA

SUBMIT AN ABSTRACT TO:

MATERIALS DESIGN

COMPUTATIONAL METHOD AND EXPERIMENTAL APPROACHES FOR MODEL DEVELOPMENT AND VALIDATION, UNCERTAINTY QUANTIFICATION, AND STOCHASTIC PREDICTIONS

This symposium will focus on stochastic methods, computational methodology development, and validation, as well as uncertainty evaluation for experimental and computational approaches at various length scale. The goal is to cover these topics in an interdisciplinary approach, which connects theory and experiment, with a view towards materials applications. A focus will be the development and validation of interatomic potentials for materials research and design, as advances in classical molecular dynamics and Monte Carlo Simulations are now paving the way for the rational design and development of materials. The advances in the predictive capability of these modeling methods are attributed to the increases in computational resources and advanced algorithms that have enabled the continued development of interatomic potentials to model complex interactions (metallic, covalent, ionic, van der Waals, or mixed) and phenomena at the atomic scales. This symposium brings together materials scientists and engineers, physicists, chemists, biologists, mathematicians, and data management experts to discuss the current state of the capabilities of interatomic potentials and their role in accelerated materials design for metals and metallic alloys. There are five sessions planned:

- Validation and uncertainty evaluation for quantum-mechanical approaches
- Interatomic potential development
- Interatomic potential validation and uncertainty evaluation
- Validation and uncertainty evaluation for finite element and multiscale modeling (effect of chosen constitutive equations, meshing, element types, coupling methods etc.)
- Advancements in stochastic methodologies (for material discovery)

Topics addressed in this symposium will include:

- Evaluation of DFT exchange-correlation functional and pseudopotentials
- Development, validation and uncertainty quantification for interatomic potentials
- Metals and metallic alloys
- Reactive material systems
- Molecular, biomolecular and polymer systems
- Semiconductors and 2D materials
- Ceramics and ceramic composites
- Complex interfaces
- Phase transformation behavior at high temperatures and pressures
- Neural network and genetic algorithm approaches
- Advances in optimization algorithms and materials informatics
- Data mining
- Verification, validation, and uncertainty quantification for meso- and continuum scale modeling

ORGANIZERS

Francesca Tavazza, National Institute of Standards and Technology, USA
Mark Tschopp, Army Research Laboratory, USA
Richard Hennig, University of Florida, USA
Avinash Dongare, University of Connecticut, USA
Shawn Coleman, U.S. Army Research Laboratory, USA

SPONSORS

TMS Materials Processing & Manufacturing Division
TMS Computational Materials Science and Engineering Committee

ABSTRACT DEADLINE IS JULY 1, 2017. SUBMIT ONLINE AT www.programmaster.org/TMS2018.

QUESTIONS? CONTACT programming@tms.org