TMS2016
145th Annual Meeting & Exhibition

FEBRUARY 14-18 DOWNTOWN NASHVILLE, TENNESSEE MUSIC CITY CENTER

Connecting the Global Minerals, Metals, and Materials Community.

Computational Methods for Uncertainty Quantification, Model Validation, and Stochastic Predictions

Experimental measurements exhibit uncertainty that is described by their precision and accuracy. The same holds true for computational results, as, similarly to the limitation of measuring instruments, the models behind simulation methodologies and their numerical evaluations exhibit limitations. Moreover, in recent years, stochastic computational techniques and data analysis methods have advanced the study of materials in a wide variety of fields. To be interpreted correctly, results obtained using any of the above-mentioned methodologies, at any length scale, need a careful evaluation of their uncertainties. Moreover, a way to evaluate the predictability of simulation techniques is to validate their findings using other experimental or computational approaches. This symposium will focus on stochastic methods, computational methodology validation, as well as uncertainty evaluation for computational approaches at various length scales, including methodologies like density functional theory (DFT), empirical energy models, etc., whose results have traditionally been reported without error bars. The goal of the symposium is to cover these research topics in an interdisciplinary approach that connects theory and experiment with a view toward applications.

Four sessions are planned:

- Advancements in stochastic methodologies (for material discovery)
- Validation and uncertainty evaluation for DFT and other quantum-mechanical based methods
- Validation and uncertainty evaluation for empirical potential/force fields based simulation methodologies
- Validation and uncertainty evaluation for larger scale methodologies (finite element, mesoscale, etc.).

Organizers include:

Francesca Tavazza, National Institute of Standards and Technology (USA)
Richard Hennig, University of Florida (USA)
Mark A Tschopp, U.S. Army Research Laboratory (USA)
Li Ma, National Institute of Standards and Technology (USA)

Learn More at www.tms.org/TMS2016

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