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TMS2017
146th Annual Meeting & Exhibition

February 26 – March 2, 2017
San Diego, California, USA

COMPUTATIONAL METHODS AND EXPERIMENTAL APPROACHES FOR UNCERTAINTY QUANTIFICATION AND PROPAGATION, MODEL VALIDATION, AND STOCHASTIC PREDICTIONS

Experimental measurements exhibit a certain degree of uncertainty that is described by their precision and accuracy. The same holds true for computational results; because, similarly to the limitation of measuring instruments, all models behind simulation methodologies have limitations. Traditionally, computational approaches, like density functional theory (DFT), empirical energy models, phase field, finite element, etc., have not focused attention to uncertainty, and thus report results without error bars. However 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, simulation results obtained using computational methodologies at any length scale need a careful evaluation of their uncertainties. Furthermore, 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 advances in stochastic methods, computational methodology validation, and uncertainty evaluation for both experimental and computational approaches at various length scales. The goal of the symposium is to cover these research topics in an interdisciplinary approach, which connects theory and experiment, with a view towards materials applications.

There are four sessions planned, covering:

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

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