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TMS 2023

152nd Annual Meeting & Exhibition

MARCH 19–23, 2023
SAN DIEGO CONVENTION CENTER &
HILTON SAN DIEGO BAYFRONT
SAN DIEGO, CALIFORNIA, USA
#TMSANNUALMEETING

SUBMIT AN ABSTRACT BY JULY 1 FOR THE FOLLOWING TMS2023 SYMPOSIUM:

MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering

As computational methodologies in the materials science and engineering become more mature, it is critical to develop and validate numerical techniques and algorithms that employ ever-expanding computational resources. The algorithms for either physics-based models or data-based models can impact critical materials science areas such as: data acquisition and analysis from microscopy, atomic force microscopy (AFM), state-of-the-art light source facilities, and analysis/extraction of quantitative metrics from numerical simulations of materials behavior. This symposium seeks abstract submissions for developing new algorithms and/or designing new methods for performing computational research in materials science and engineering. One symposium thrust is on implementation on the novel peta/exascale supercomputer architectures for revolutionary improvements in simulation analysis time, power, and capability. Another symposium thrust is for employing widely available state-of-the art cloud and clusters computing systems. Validation studies and uncertainty quantification of computational methodologies are also of interest.

Session topics include, but are not limited to:

- Advancements that enhance modeling and simulation techniques such as density functional theory, molecular dynamics, Monte Carlo simulation, dislocation dynamics, electronic-excited states, phase-field modeling, CALPHAD, crystal plasticity, and finite element analysis
- Advancements in semi-empirical models and machine learning algorithms for interatomic interactions, microstructure evolution, and meso/continuum models
- New techniques for physics-based, multi-scale, multi-physics materials modeling
- Computational methods for analyzing results and development of reduced models from high fidelity simulations data of materials phenomena
- Approaches for data mining, machine learning, image processing, image based microstructure generation, synthetic microstructure generation, high throughput databases, high throughput experiments, surrogate modeling, and extracting useful insights from large data sets of numerical and experimental results
- Approaches for improving performance and/or scalability, particularly on new and emerging hardware (e.g., GPUs), and other high-performance computing (HPC) efforts; and • Uncertainty quantification, statistical metrics from image-based synthetic microstructure generation, model comparisons, and validation studies related to novel algorithms and/or methods in computational material science

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