THE WORLD COMES HERE. TMS 2024 153rd Annual Meeting & Exhibition

MARCH 3–7, 2024 HYATT REGENCY ORLANDO ORLANDO, FLORIDA, USA #TMSAnnualMeeting



SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2024 SYMPOSIUM:

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Algorithm Development in Materials Science and Engineering

As computational methodologies in materials science and engineering are widely used, it is critical to develop and validate numerical techniques and algorithms that employ ever-expanding computational resources. Algorithms for physics and data-based models impact many critical materials science areas, e.g., data acquisition and analysis from microscopy and synchrotron facilities, data mining, and materials simulations. This symposium invites abstracts for developing new algorithms and designing new methods for computational research in materials science and engineering. This year's symposium focuses on three areas:

- Algorithms for exascale supercomputers that efficiently utilize GPU architectures to improve simulation and analysis time, power, and capability
- Algorithms for cloud and cluster computing systems
- Validation studies and uncertainty quantification of computational methodologies

Session topics include, but are not limited to:

- Enhanced techniques for density functional theory, molecular dynamics, Monte Carlo simulation, dislocation dynamics, electronic-excited states, phase-field modeling, CALPHAD, crystal plasticity, and finite element analysis
- Advances in semi-empirical models and machine learning algorithms for interatomic potentials, microstructure evolution, and meso/continuum models
- New techniques for physics-based, multi-scale, multiphysics materials modeling
- Computational methods for analyzing results and development of reduced models from high fidelity simulations data of materials phenomena
- Algorithms for data mining, machine learning, image processing, microstructure generation, high-throughput databases and 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

- Uncertainty quantification, statistical metrics from imagebased synthetic microstructure generation, model comparisons and validation studies related to novel algorithms and/or methods in computational material science
- Best practices for source-code development addressing computational efficiency, reproducibility, testing, commenting, maintenance (e.g., version control)

Selected presentations will be invited to submit full papers for a *JOM* issue.

ORGANIZERS

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