Algorithm Development in Materials Science and Engineering

As computational approaches to study the science and engineering of materials become more mature, it is critical to develop, improve, and validate techniques and algorithms that leverage ever-expanding computational resources. These algorithms can impact areas such as: data acquisition and analysis from sophisticated microscopes and state-of-the-art light source facilities, analysis and extraction of quantitative metrics from numerical simulations of materials behavior, and the ability to leverage specific computer architectures for revolutionary improvements in simulation analysis time, power, and capability.

This symposium solicits abstract submissions from researchers who are developing new algorithms and/or designing new methods for performing computational research in materials science and engineering. Validation studies and uncertainty quantification of computational methodologies are equally 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, and finite element analysis
- Advancements in semi-empirical models and machine learning algorithms for interatomic interactions
- New techniques for simulating the complex behavior of materials at different length and time scales
- Computational methods for analyzing results from simulations of materials phenomena
- Approaches for data mining, machine learning, image processing, high throughput databases, high throughput experiments, and extracting useful insights from large data sets of numerical and experimental results
- Uncertainty quantification, model comparisons and validation studies related to novel algorithms and/or methods in computational material science

ORGANIZERS
Mohsen Asle Zaeem, Colorado School of Mines, USA
Garritt Tucker, Colorado School of Mines, USA
Charudatta Phatak, Argonne National Laboratory, USA
Bryan Wong, University of California, Riverside, USA
Mikhail Mendelev, Ames Laboratory, USA
Bryce Meredig, Citrine Informatics, USA
Ebrahim Asadi, University of Memphis, USA
Francesca Tavazza, National Institute of Standards and Technology, USA

SYMPOSIUM SPONSORS
TMS Materials Processing & Manufacturing Division
TMS Integrated Computational Materials Engineering Committee
TMS Phase Transformations Committee
TMS Computational Materials Science and Engineering Committee