



**SUBMIT AN ABSTRACT BY JULY 1**

**FEBRUARY 27-MARCH 3, 2022**  
**ANAHEIM CONVENTION CENTER & ANAHEIM MARRIOTT**  
**ANAHEIM, CALIFORNIA, USA**  
**#TMSAnnualMeeting**

**SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2022 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, improve, and validate techniques and algorithms that leverage ever-expanding computational resources. These physical-based and data-intensive 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 implementation on novel peta- and exascale 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
- 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, model comparisons, and validation studies related to novel algorithms and/or methods in computational material science

#### **ORGANIZERS**

**Mohsen Asle Zaeem**, Colorado School of Mines

**Mikhail Mendeleev**, KBR

**Garritt J. Tucker**, Colorado School of Mines

**Ebrahim Asadi**, University of Memphis

**Bryan M. Wong**, University of California, Riverside

**Samuel T. Reeve**, Oak Ridge National Laboratory

**Enrique Martinez Saez**, Clemson University

**Adrian S. Sabau**, Oak Ridge National Laboratory

#### **SYMPOSIUM SPONSORS**

TMS Computational Materials Science and Engineering Committee

TMS Integrated Computational Materials Engineering Committee

TMS Phase Transformations Committee

TMS Solidification Committee

[www.tms.org/TMS2022](http://www.tms.org/TMS2022)

**QUESTIONS?**  
Contact [programming@tms.org](mailto:programming@tms.org)