MATERIALS DESIGN

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 and improve 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.

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, phase-field modeling, CALPHAD, and finite element analysis
- 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, high-throughput databases, high throughput experiments, and extracting useful insights from large data sets of numerical and experimental results

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