Submit an abstract by July 1

SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2022 SYMPOSIUM:

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics

This ongoing TMS symposium series focuses on Computational Thermodynamics and Kinetics (CTK) of materials over a broad range of scales covering from the atomic to macroscale, and including applications to materials design, synthesis, processing, and service. The ability to compute thermodynamic and kinetic properties and further utilization of these information on other CTK methods is rapidly transforming the field of materials science and engineering.

This year, we welcome submissions relating to novel developments and applications of CTK methods to explore new phenomena across different scales in novel materials. In addition to fundamental CTK methods, we encourage abstracts regarding uncertainty quantification and machine-learning assisted modeling of thermodynamics and kinetics properties of functional materials and recent advances in computational methods and algorithms for microstructure modeling. Submissions are welcome from all facets of CTK, such contributions dealing with fluids, interfaces, phase transformations (e.g., melting, solidification), and soft matter.

Topics of choice for this year include, but are not limited to:

- Computational approaches for materials discovery and design
- Computational models of phase prediction, equilibria, stability, and transformations
- Novel approaches to predict properties (mechanics, chemistry, transport, etc.) of materials
- Machine learning assisted computational modeling of materials behavior
- Uncertainty quantification for phase-equilibria and/or phase transition modeling
- The effect of external and internal constraints e.g., elastic/plastic/electric/magnetic/etc. fields and internal degree of freedoms on microstructure of materials
- Computational studies of the role of phonons, magnons, and other excitations in the stabilization of phases and/or phase transformations
- Experimental studies for validation of thermodynamic and kinetic modeling approaches

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