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# **SUBMIT AN ABSTRACT TO:**

### **PHYSICAL METALLURGY**

# **COMPUTATIONAL THERMODYNAMICS AND KINETICS**

The ability to compute thermodynamic and kinetic properties and their effect on material response is rapidly transforming the field of materials science and engineering. Since 2001, this ongoing TMS symposium has highlighted advances in the tools and applications of computational thermodynamics and kinetics, from the atomic to macroscale, and including applications to materials design, synthesis, processing, and service. This year, we continue to welcome submissions relating to novel developments and applications of computational thermodynamics and kinetics and kinetics methods, as well as the use of established computational thermodynamics, to explore new phenomenon and materials.

This symposium will cover topics that provide new insights into the properties of materials; expand our understanding of materials design, processing, and optimization; or guide the discovery of fundamentally new materials. Topics of choice for this year include:

- Computational modeling exploring the thermodynamics and kinetics of heterogenous chemical reactions at surfaces and interfaces, with a focus on electrochemistry and catalysis
- Computational techniques to model extended timescales to understand the kinetics of microstructure evolution and secondary phase transitions.
- Developments in computational techniques for the thermodynamics and kinetics of diffusion, defect properties, and phase transformations in materials
- Thermodynamic and kinetic modeling approaches for materials discovery and design

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