

PHYSICAL METALLURGY

Computational Thermodynamics and Kinetics

The Computational Thermodynamics and Kinetics (CTK) symposium, held yearly for over 20 years, highlights the latest advances in computational tools and techniques that broaden our understanding of the thermodynamics and kinetics of materials. Advanced CTK methods play an ever-increasing role, not only in bringing new insight in the fundamental behavior of materials, but also for the conceptual design and discovery of novel materials systems with outstanding properties.

This symposium will cover topics related to the stability, synthesis, properties, and discovery of new materials, based on computational methods, including data-based and highthroughput methods, and the integration of computational tools with experiments and processes. Topics of interest include, but are not limited to:

- Phase prediction, equilibria, stability, transformations, electronic and photonic performance, and nano/microstructural evolution, including the influence of defects and interfaces
- Innovative computational approaches for materials discovery and design
- Alloy design, microstructure control, multi-phase/multicomponent systems
- Prediction of materials properties (mechanics, chemistry, electronic, transport, etc.)
- Effect of external and internal constraints (elastic, plastic, electric, magnetic, etc.) on the stability, microstructure, and properties of materials
- Integration of CTK with experiments and computationallyguided synthesis of materials
- Advanced statistical and data-based methods (e.g. machine learning, uncertainty quantification) for CTK

ORGANIZERS

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