

THE WORLD COMES HERE.
TMS 2025
154th Annual Meeting & Exhibition



March 23–27, 2025
MGM Grand Las Vegas
Hotel & Casino
Las Vegas, Nevada, USA
#TMSAnnualMeeting



SUBMIT AN ABSTRACT FOR THE FOLLOWING TMS2025 SYMPOSIUM:

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

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 across many scales, but also for the conceptual design and discovery of novel materials systems with controlled properties. In the recent past, the sophisticated interfaces of thermodynamic kinetic models, databases, computation techniques, and application programming has brought paradigm shift in our ability to predict composition-structure-property relationship in various material process.

This symposium will cover topics related to the stability, synthesis, properties, and materials discovery, based on computational methods, including data-based and high-throughput methods, and the integration of computational tools with experiments and processes.

Topics of interest include, but are not limited to:

- Advanced statistical and data-based methods (e.g., machine learning, uncertainty quantification) for CTK.
- Integration of CTK with experiments and computationally guided synthesis of materials.
- Phase prediction, equilibria, stability, transformations, electronic and photonic performance, and nano/micro-structural evolution,
- Innovative computational approaches for materials discovery and design,
- Alloy design, microstructure control, multi-phase/multi-component systems,
- Prediction of materials properties (mechanics, chemistry, electronic, transport, etc.),
- Effect of external and internal fields (mechanical, electric, magnetic, etc.) on the stability, microstructure, and materials properties,
- Computational studies of the role of phonons, magnons, and other excitations in the stabilization of phases and/or phase transformations
- Materials defects physics,
- Thermodynamic linear response theory for chemical short-range order.

ORGANIZERS

Prashant Singh, Ames National Laboratory; **Rodrigo Freitas**, Massachusetts Institute of Technology; **Nicolas Argibay**, Ames National Laboratory; **Raymundo Arroyave**, Texas A&M University; **James Morris**, Ames Laboratory

SYMPOSIUM SPONSORS

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QUESTIONS?

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