

## PHYSICAL METALLURGY

## COMPUTATIONAL THERMODYNAMICS AND KINETICS

Computational thermodynamics and kinetics (CTK) has long been a significant symposium at TMS. It has been used to highlight the advances in tools, techniques and our understanding across the spectrum of scales in materials science. In this, its 20th year, we continue this ongoing tradition. This year, we continue to welcome submissions related to novel developments and applications of CTK techniques to explore and understand new phenomena and materials.

This symposium will cover topics that provide new insights into the properties of materials, expand our understanding of materials design, synthesis, processing, and optimization, or guide the discovery of fundamentally new materials. The materials science landscape has changed much in recent years. We also welcome submissions in the area of big data, data science and high throughput as it is applied to this evolving area in materials science and technology.

This year, topics of interest include but are not limited to:

- Computational models of phase equilibria, stability, transformations and microstructural evolution, including the effect of defects.
- Computational techniques for the calculation of diffusion, transport, and thermally activated processes for a wide range of applications, such as alloy design, microstructure control, multi-phase/multi-component systems.
- Computational modeling using modern data methods, machine learning, and inference that advances our understanding of materials and/or introduces new tools.
- Computational modeling of rare events, systems out of equilibrium, and materials at extremes.
- Computational studies of the role of phonons, magnons, and other excitations, including interactions between them, in the stabilization of phases and/or phase transformations.
- Computational thermodynamics and kinetic modeling approaches for materials discovery and design

## ORGANI7FRS

Nana Ofori-Opoku, Canadian Nuclear Laboratories, Canada Eva Zarkadoula, Oak Ridge National Laboratory, USA Enrique Martinez Saez, Los Alamos National Laboratory, USA Vahid Attari, Texas A&M University, USA

## SYMPOSIUM SPONSORS

TMS Materials Processing & Manufacturing Division
TMS Computational Materials Science and Engineering Committee

**Questions?**Contact programming@tms.org