



## SUBMIT AN ABSTRACT FOR THE FOLLOWING SYMPOSIUM

### DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

## Local Chemical Ordering and Its Impact on Mechanical Behaviors, Radiation Damage, and Corrosion

Recent developments in the field of compositionally complex materials have sparked thought-provoking speculations regarding the role of local chemical ordering (LCO) in various chemistry–microstructure relationships. The practical motivation is clear: LCO could present a new dimension for tuning and designing the behavior of structural and functional materials. Meanwhile, from a fundamental perspective, the ubiquity of LCO suggests that it might become an indispensable component towards predictive physical modeling of compositionally complex materials.

A comprehensive thermodynamic and kinetic framework of LCO and its connections to microstructural evolution and phase stability are still lacking. This absence demonstrates the considerable challenge in working with the staggering chemical complexity of LCO, which lies just beyond the capability of current experimental and computational approaches. In this symposium we will explore emerging trends on computational and experimental efforts in understanding LCO and its impact on materials properties. Our goal is to deepen our understanding of novel concepts and highlight methodological challenges hindering the quantitative characterization of LCO.

Specific topics include:

- LCO impact on defects and microstructural evolution, from the atomistic to the mesoscale.
- Non-equilibrium dynamics and kinetics under extreme driving conditions, including high/cryogenic temperature, radiation, and corrosion
- Experimental characterizations and in-situ techniques, including S/TEM, 4D STEM, SEM, in situ TEM, X-Ray
- Simulation and modeling approaches, including first-principles methods, atomistic simulations, thermodynamic modeling, machine learning, and data-science approaches.

#### SPONSORED BY:

TMS Structural Materials Division; TMS Corrosion and Environmental Effects Committee; TMS Chemistry and Physics of Materials Committee; TMS Nuclear Materials Committee; TMS Phase Transformations Committee; TMS Computational Materials Science and Engineering Committee

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