22nd International Conference on
Diffusion in Solids and Liquids
22 TO 26 JUNE 2026 | RHODES, GREECE

ABSTRACT:

High-Fidelity Atomistic Simulations of Alloy Solidification

R. Freitas[1]
[1]Massachusetts Institute of Technology, Cambridge, MA, USA, 02139.

Atomistic simulations now achieve electronic-structure fidelity at the mesoscale, reshaping how these methods can be used to understand fundamental aspects of solidification. In this talk I will present recent work from my research group that uses high-fidelity atomistic simulations to study solidification in metallic alloys. I will discuss how machine learning potentials enable atomistic studies of increasingly complex chemistries with high fidelity, and I will highlight how these methods provide direct insight into the thermodynamic and kinetic processes governing solid-liquid interfaces, including chemical partitioning, solute trapping, and interfacial transport. Together, these developments establish atomistic simulation as a predictive framework for uncovering the fundamental physics of solidification and point to a broader role for these methods in informing materials processing.