DSL2026
22-26 JUNE
RHODES - GREECE

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

ABSTRACT:

Predicting Diffusion and Phase Formation Across the Periodic Table with Foundational Machine Learning Interatomic Potentials

The reach of atomistic thermodynamic and kinetic simulations has long been restricted by a fundamental bottleneck: the prohibitive computational cost of first-principles methods and the rigid approximations of lattice-based models, which confined high-fidelity studies to small systems and simple chemistries. The emergence of machine learning interatomic potentials (MLIPs) has been transformative in overcoming these limitations, offering near-quantum accuracy at a fraction of the computational cost.

This presentation introduces the Graph Atomic Cluster Expansion (GRACE), a framework that unifies various MLIP architectures and provides the mathematical foundation for simulating atomic interactions across the periodic table. I will demonstrate that the foundational parameterizations provided by GRACE allow for accurate simulations, with particular emphasis on diffusion in topologically close-packed structures, the computation of free energies, and phase formation and stability.

The presentation will conclude by addressing current frontiers in foundational MLIP development. I will discuss the systematic generation of comprehensive training datasets to ensure model transferability and the ongoing work to incorporate complex physical phenomena—such as magnetism, charge transfer, and long-range electrostatics—which are vital for a truly universal simulation of the periodic table.