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

ABSTRACT:

Physics-Informed AI for Thermodynamics and Kinetics

Baptiste Bienvenu, Li-Fang Zhu, Ali Tehranchi, Jan Janssen, Tilmann Hickel, Jörg Neugebauer
Max Planck Institute for Sustainable Materials, Düsseldorf, Germany.

Recent advances in materials science have introduced compositionally and structurally complex compounds, opening a vast configuration space for discovery. Traditional trial-and-error strategies cannot cope with the high-dimensional landscape, especially when novel diffusion processes or mechanisms are encountered. In this presentation, I will discuss how physics-informed artificial intelligence (PIAI) and data-driven workflows can increase the efficiency of ab initio-guided simulations, allowing us to describe complex materials in realistic environments rather than merely replacing them. By combining electronic structure theory, thermodynamic modeling, statistical mechanics, and machine learning, AI accelerates each tier of the simulation process—enhancing density-functional calculations, guiding kinetic sampling, and informing materials discovery approaches—while preserving physical fidelity. Automated digital workflows seamlessly link various simulation and machine learning techniques with AI-driven hypothesis generation, enabling rapid navigation of huge material configuration spaces. Real-world case studies related to fundamental processes in green steel synthesis, utilizing the vast composition space of high-entropy alloys for materials discovery or the fully ab initio description of thermodynamic bulk and defect phase diagrams, will illustrate this synergistic approach.