LMS Seminar

From electrons to microstructure: predicting properties of multi-principal element alloys through statistical mechanics and machine learning

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Date, time, and venue

May 21, 2026 (2 – 3 pm), Amphithéâtre Pole Mecanique

Abstract

Multi-principal element alloys, sometimes also referred to as high-entropy alloys, exhibit a remarkable combination of mechanical and thermal properties that make them attractive for high-performance applications in aerospace, energy storage, and automotive engineering. However, the vast compositional space of these alloys makes structure-property-processing relationships difficult to establish, and the lack of accurate phenomenological models limits the development of improved alloy chemistries and processing routes. Addressing this challenge requires atomistic models that capture the structural and chemical disorder intrinsic to these alloys. Such models can be coupled with statistical mechanics techniques to derive thermodynamic, kinetic, and chemo-mechanical descriptions that feed into mesoscale and continuum theories of phase transformations and microstructure evolution. In this talk, I will present recent theoretical advances that enable the rigorous coarse-graining of electronic structure calculations through statistical mechanics and machine learning. I will show how these methods can be applied to design multi-principal element alloys and to reveal atomistic mechanisms underlying their sluggish diffusion and enhanced ductility.

About the speaker

Anirudh received a B.Tech. in Metallurgical and Materials Engineering from the Indian Institute of Technology, Madras, a M.S in Materials Science and Engineering from the University of Michigan, Ann Arbor and a Ph.D. in Materials from the University of California, Santa Barbara. He set up the laboratory of materials design and simulation (MADES) at EPFL in 2022. His research interests are in the computational design and discovery of advanced engineering materials.

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