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

ABSTRACT:

Ab Initio Machine-Learning Unveils Strong Anharmonicity in Non-Arrhenius Selfdiffusion of Tungsten

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The knowledge of diffusion mechanisms in materials is crucial for predicting their hightemperature performance and stability, yet accurately capturing the underlying physics like thermal effects remains challenging. In particular, the origin of the experimentally observed non-Arrhenius diffusion behavior has remained elusive, largely due to the lack of effective computational tools.

In this talk, I will introduce an efficient ab initio framework to compute the Gibbs energy of the transition state in vacancy-mediated diffusion including the relevant thermal excitations at the density-functional-theory level. With the aid of a bespoke machinelearning interatomic potential, the temperature-dependent vacancy formation and migration Gibbs energies of the prototype system body-centered cubic (BCC) tungsten are shown to be strongly affected by anharmonicity. This finding explains the physical origin of the experimentally observed non-Arrhenius behavior of tungsten self-diffusion.

A remarkable agreement between the calculated and experimental temperature-dependent self-diffusivity and, in particular, its curvature is revealed. The proposed computational framework is robust and broadly applicable, as evidenced by tests for a hexagonal closepacked (HCP) multicomponent high-entropy alloy. The successful applications underscore the attainability of an accurate ab initio diffusion database.

[1] X. Zhang, S.V. Divinski and B. Grabowski, Nat. Commun., 16, 394 (2025).