Diffusion of atomic impurities in liquid lead-bismuth eutectic using a machine-learning potential

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Reliable data on the diffusion of atomic impurities in liquid lead–bismuth eutectic (LBE) are critically important for predicting corrosion, mass transfer, and chemistry control in lead-cooled nuclear systems. However, direct experimental measurements of impurity diffusion coefficients in LBE — for steel components (Fe, Cr, Ni), oxygen, and hydrogen — remain extremely challenging. Reported experimental values exhibit wide scatter and strong dependence on indirect modeling assumptions [1].

Ab initio molecular dynamics (AIMD) provides an accurate description of liquid LBE and impurity–melt interactions [2], but its application to diffusion studies is restricted by the limited time and length scales accessible in first-principles simulations. Machine-learning interatomic potentials trained on ab initio data overcome these limitations by reproducing near–first-principles accuracy while enabling long-time, large-scale simulations required for statistically converged diffusion coefficients. The development of such potentials can be further automated using active learning techniques, allowing systematic and reliable modeling of impurity transport in liquid LBE.

In this work, we develop a machine-learning interatomic potential for the lead–bismuth eutectic system using an active learning approach. The resulting potentials are applied to calculate diffusion coefficients of atomic impurities — Fe, Cr, Ni, O, H, C, and Ti — in liquid LBE.

[1] Fazio *et al.* 2015 *Handbook on lead-bismuth eutectic alloy and lead properties, materials compatibility, thermal-hydraulics and technologies*
[2] Gil J and Oda T 2018 *Physical Chemistry Chemical Physics* **20** 30480–30491