Diffusion and thermodynamics of defects in alkali feldspar simulated through machine learning force fields

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Exsolution microstructures of alkali feldspar $(Na,K)AlSi_3O_8$ which form during slow cooling of high-temperature rocks encode the rocks thermal history, but we do not yet fully know how to interpret them quantitatively. In this talk I will present computer simulations driven by machine learning force fields that shed light on the microscopic mechanism of diffusion that ultimately controls the evolution of the exsolution microstructures.

In Na-feldspar we find a new kind of Na^+-Na^+ dumbbell interstitial point defect and predict that this is the most stable interstitial defect over all temperatures. Our simulations of the dynamics of this defect combined with the calculated defect concentration quantitatively agree with experimental sodium self-diffusion data, which allows us to rectify past investigations on the mechanism and reconcile prior works on the anisotropy of cation diffusion.

I will also give a short overview of our recent work in which we use a combination of molecular dynamics and Monte Carlo simulations to calculate the mixing thermodynamics of Na-feldspar and K-feldspar above the alkali feldspar solvus. Our model correctly aligns with the literature data in that increasing Al-Si disorder corresponds to a more ideal mixture and we predict that the degree of Al-Si disorder is less relevant as long as disorder persists.