Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.26176

Oxygen self-diffusion in $CaSiO_3$ Davemaoite

MAXIMILIAN SCHULZE AND GERD STEINLE-NEUMANN

Universität Bayreuth

Davemaoite ($CaSiO_3$ perovskite) is a major mineral in the lower mantle and therefore plays a crucial role in shaping the physical and chemical behavior of the deep Earth. Oxygen diffusion in minerals is an important property that affects their transport properties and chemical reactivity. However, the inability to retain the crystal structure of Davemaoite during cooling to ambient conditions is a major obstacle to studying its chemical diffusivities experimentally.

Computational approaches such as density functional theory (DFT) calculations and DFT-based molecular dynamics (MD) simulations have traditionally been used to complement experiments in order to explore the properties of minerals under extreme conditions. However, these methods are limited by their computational expense, restricting simulations to small system sizes and short timescales, thereby often hindering the study of long-timescale phenomena such as chemical diffusion.

Here, we address these problems by performing state of the art MD simulations driven by a machine learning potential trained on high-quality DFT data. This approach enables MD simulations over extended time and length scales while maintaining quantum-level accuracy. Our results provide new insights into the mechanisms of oxygen diffusion in Davemaoite and their dependence on conditions in the entire lower mantle, allowing geochemical implications such as the timescales of redox equilibria in subducted slabs to be discussed.