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ABSTRACT:

Temperature-Dependent Lithium Diffusion in Nb-Doped LLZO from Machine-Learned Potentials Validated by Neutron Scattering

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Superionic conductors are critical materials in energy applications such as solid-state batteries and solid oxide fuel cells (SOFCs), owing to their exceptional ionic conductivity at room or elevated temperatures. Among these, lithium lanthanum zirconate garnets (LLZO) are promising candidates for solid-state electrolytes due to their high lithium-ion conductivity and chemical stability.

Here we present results modelling lithium diffusion in Nb-doped LLZO using machine learned potentials optimised with the 'Automated Potential Development (APD) workflow'[1], recently applied to oxide-ion diffusion in bismuth vanadate systems[2]. Molecular dynamics trajectories are analysed to obtain temperature-dependent Li site occupancies and hopping statistics in the tetragonal phase, characterising diffusion pathways in terms of crystallographic Li sites. The analysis reveals the role of metastable off-symmetric configurations within octahedral sites and their contribution to local hopping dynamics.

Results are validated against experimental data, including QENS measurements performed at ISIS Pulsed Neutron and Muon Source and the Institut Laue-Langevin (ILL). In addition, calculations of the coherent elastic structure factor using the dynasor package show good agreement with experimentally observed diffuse scattering, providing further validation of the simulated trajectories.

[1] A.I. Duff, et. al., Comp. Phys. Comm., 293, 108896 (2023).
[2] A.I. Duff, et. al., Comp. Phys. Comm., 110100 (2025).