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ABSTRACT

Investigating Diffusion in Nb-Doped LLZO and Bismuth Vanadium Oxide Using QENS and ML-Driven Simulations

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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. In addition, oxide ion conductors like $Bi_{92}V_{16}O_{178}$ which exhibit high oxide ion conductivity at intermediate temperatures (400–600 °C), are of significant interest for applications in SOFCs and oxygen-permeable membranes. Here we present results of modelling of diffusion of Nb-doped LLZO and $Bi_{92}V_{16}O_{178}$ using machine learned potentials as optimized using the 'Automated Potential Development (APD) workflow'[1]. Modeling trajectories are used to predict dynamic structure factors as a function of temperature, scattering-vector magnitude (q), and Li concentration in the case of LLZO. Results are validated against experimental data, including QENS measurements performed at ISIS Pulsed Neutron and Muon Source and the Institut Laue-Langevin (ILL), and used to elucidate diffusion mechanisms and dynamics.

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