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A Combined Experimental and Computational Study of Oxide Ion Conductors

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Solid oxide ion conductors are remarkable materials with significant market potential due to their importance in technological applications like oxygen sensors, fuel cells and separation membranes. A crucial factor for advancement of their applicability is the development of new oxide ion conductors with higher conductivities at lower temperatures. Detailed knowledge of the structural characteristics, resulting conduction pathways and dynamics in these materials is a key requirement for improving their properties. Quasi-elastic neutron scattering is an excellent method for studying solid state diffusion and allows the observation of oxygen dynamics on a microscopic timescale. Combined with ab-initio molecular dynamics simulations, it can provide a comprehensive insight into diffusion processes on the atomic scale. We used this combined approach to investigate and compare the different oxide ion dynamics in two isostructural materials: $Bi_{0.852}V_{0.148}O_{1.648}$ and $Bi_{0.852}P_{0.148}O_{1.648}$, and account for the superior performance of the vanadate. Using the backscattering spectrometer IN16b and the time-of-flight spectrometer IN5 at the ILL allowed direct observation of dynamics on the nanosecond and picosecond timescales, and analysis in conjunction with molecular dynamics simulations allowed us to elucidate the nature of the observed dynamics as well as the structural characteristics important for oxide ion conduction in these doped bismuth oxides.

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