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# Oxide Ion Dynamics in $\text{Bi}_2\text{O}_3$ -based Solid Electrolytes: Combining Quasielastic Neutron Scattering with Ab Initio Molecular Dynamics

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Solid oxide ion conductors are important materials in applications like oxygen-permeable membranes and solid oxide fuel cells (SOFC). In the latter, they are used as solid electrolytes. Current SOFC electrolyte materials, however, require high temperatures to achieve a sufficiently high oxide ion conductivity for device applications. Developing materials with excellent ionic conductivity at intermediate temperatures (400–600 °C) is a crucial step in making SOFC more widely applied. Understanding the relationship between structural properties and high ionic conductivity is therefore an important part of current research on energy materials. Quasielastic 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:  $\text{Bi}_{0.852}\text{V}_{0.148}\text{O}_{1.648}$  and  $\text{Bi}_{0.852}\text{P}_{0.148}\text{O}_{1.648}$ , 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 structural characteristics important for oxide ion conduction in these doped bismuth oxides.

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