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Hydration mechanisms and proton conduction in the mixed ionic-electronic conductors Ba4Nb2O9 and Ba4Ta2O9

Mixed conductors – materials that exhibit significant mobility of more than one type of charge carrier such as oxide ions, protons and electrons – have a range of important applications including solid oxide fuel cell membranes, electrodes, batteries and sensors. We recently studied the behaviour of hydrogen in the mixed ionic-electronic conductors γ-$Ba_4Nb_2O_9$ and 6H-$Ba_4Ta_2O_9$, using a combination of experimental (neutron diffraction and inelastic neutron scattering) and computational (*ab initio* molecular dynamics) methods. While these compounds have isostructural low-temperature polymorphs, they adopt distinct forms in the high-temperature conducting regime. We found that they also have distinct mechanisms for hydration and ionic conduction. Hydration of γ-$Ba_4Nb_2O_9$ is localised to 2-D layers in the structure that contain a 1:1 ratio of isolated but adjacent NbO_4 and NbO_5 polyhedra. OH- and H+ ions combine with two polyhedra respectively to form complete layers of NbO_4OH polyhedra, giving rise to a stoichiometric hydrated form γ-III-$Ba_4Nb_2O_9$.1/3H_2O. Protons then diffuse through these 2-D layers by "hopping" between oxygen atoms on adjacent polyhedra. In the case of 6H-$Ba_4Ta_2O_9$, hydration occurs by intercalating intact water molecules into the structure up to a maximum of ~0.375 H_2O per formula unit. This explains the unusual local and long-range structural distortions in the hydrated form observed by neutron diffraction. Diffusion then occurs by water molecules moving between neighboring symmetry equivalent positions. These fundamentally different hydration and proton conduction mechanisms explain why 6H-$Ba_4Ta_2O_9$ has the less well-defined and higher maximum water content, while γ-$Ba_4Nb_2O_9$ has the higher proton conductivity.

Topic

Advanced Materials

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