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Hydration mechanisms and lattice distortions in 6H-Ba4Ta2O9

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Mixed ionic-electronic conductors have a wide range of applications, including in solid oxide fuel cells, batteries and sensors. Perovskite oxides are well suited for these wide variety of applications due to their robust structures that can be engineered with dopants to achieve desired properties. Hydration, and subsequent oxide-ionic and proton conduction, in such oxides is usually achieved by inserting hydroxide anions into vacancies in the oxide lattice, while the remaining proton from water converts an oxide anion into another hydroxide. We recently used ab initio Density Functional Theory (DFT) dynamics calculations to test the stability of protons and hydroxide ions introduced randomly into a model of the 6H-type perovskite 6H-Ba4Ta2O9. Surprisingly, we found that they robustly and reproducibly combined to form discrete H2O molecules within an essentially close-packed lattice. Vibrational densities-of-states extracted from the simulations matched well to experimental inelastic neutron scattering data, supporting their validity. The presence of H2O in 6H-Ba4Ta2O9, vs. hydroxide ions, also explains why it shows substantially lower ionic conductivity than comparable oxides, despite hydrating to a greater extent (0.5 H2O per formula unit). However, direct crystallographic evidence for the presence of water within 6H-Ba4Ta2O9 at room temperature was lacking. Here, we will present such evidence based on neutron powder and X-ray single-crystal diffraction. We show that water plays a very unusual role in this compound by guiding a unique series of symmetry lowering distortions on cooling, which preserve an otherwise thermodynamically unstable structure to room temperature.

Speakers Gender

Male

Level of Expertise

Expert

Do you wish to take part in the poster slam

No

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