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## Proton dynamics in proton-conducting brownmillerite-based barium indate oxides

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Proton-conducting oxides are an important class of materials for next-generation, intermediate-temperature solid-state electrolytes in e.g., proton conducting fuel cells. While most development efforts have been directed toward materials exhibiting the cubic perovskite structure, in recent years several promising alternative structures have emerged. One of these is the pseudo-cubic structure obtained upon hydration of brownmillerite-type barium indate phases. Unlike in cubic perovskites, pseudo-cubic barium indate phases exhibit several proton sites with distinct local environments. In this context, we report on a comprehensive study of the proton local environments and dynamics in the model system  $\text{BaInO}_3\text{H}$ , using inelastic and quasielastic neutron scattering techniques and ab initio molecular dynamics simulations. We show that, while the signature of up to four proton sites can be detected in the vibrational spectra, the diffusive proton dynamics can be described through the two main proton sites: the H(1) “perovskite-like” proton site and the H(2) proton site characteristic of the pseudo-cubic structure. We show that preferential motions, already observed at room-temperature, are hydroxyl reorientations for H(1) and proton transfers for H(2). We also show that the activation of the more energetic counterpart motions of H(1) and H(2) is necessary to observe interexchange between sites and long-range diffusion in the nanosecond timescale.

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