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Average and local structure of ATiO3-δHy (A = Ba, Sr, Ca)

The reduction of perovskite oxides into oxyhydrides such as ATiO3-δHy (A = Ba, Sr, Ca) affords them unique redox capabilities that enable tunable crystal structure, chemistry, and band gaps, coupled with mixed ionic-electronic conductivity, and new chemical reactivities not present in the parent oxides. These properties make oxyhydrides useful for solid-state hydrogen conductors, hydrogen storage and separation membranes, photocatalysis, anion-engineered electronics, and photochromic applications. The variations in Ti local environment, oxygen vacancy content, and oxygen-oxygen distances, which depend on the A-site cation and hydride concentration, are factors that impact the ionic and electronic transport of ATiO3-xHy. However, fundamental understanding of their defect chemistry, changes in Ti octahedral environment, and controlled hydride incorporation remains limited. In this work, we have employed total scattering techniques to characterize the local and average structures, quantify hydride content and site defects in ATiO3-δHy perovskites. We achieved varied levels of hydride substitution, with up to 18 % hydride incorporation at the anion site. Increasing H content leads to slight cell expansion, reduced oxygen site occupancy, changes in local structure (notably Ti-O, O-O, and A-O pairs), and Ti4+ reduction. The extent of hydride uptake and resulting anion-site defects is sensitive to the A-site cation, enabling direct structural and chemical tuning. These findings provide essential insights for the rational design of perovskite-based hydrogen conductors and related functional materials.

Topical Area

Hard matter: energy materials

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