

First-principles study of proton diffusion in BaFeO_{3-δ}

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Ceramic fuel and electrolyzer cells based on proton-conducting electrolytes usually employ a mixed electronic-proton-conducting cathode. While this ensures increased performance, it creates complex interactions between electrons and protons in the cathode material itself. Here, we explore the impact of these interactions on proton diffusion in cathode materials, specifically, in the BaFeO_{3-δ} perovskite system.

Density functional theory (DFT) calculations and nudged elastic band (NEB) method for the calculation of minimum energy paths and migration barriers of proton transfer.

Analysis of the electronic structure of BaFeO₃ shows that electron holes have a dominant O2p character, so that a variation in hole concentration affects the properties of oxygen ions. This manifests in systematic variations of the oxygen vacancy formation energy and the material's propensity for water absorption as a function electron hole concentration.[1] Long-range diffusion of protons involves proton transfer between two neighboring oxygen ions that approach each other in a transient lattice vibration. The associated migration barrier is calculated as a function of oxygen vacancy (thus also electron hole) concentration. We observe systematic variations, which we describe by using various geometrical and electronic descriptors, and compare it to barriers in the BaZrO₃ electrolyte.

The proton migration barriers in BaFeO_{3-δ} show systematic variations with oxygen vacancy and thus electron hole concentration.

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References

[1] Hoedl, Gryaznov, Merkle, Kotomin, Maier, J. Phys. Chem. C 124, 11780 (2020).