Exploring proton pair motion in yttrium doped barium zirconate

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Abstract

Proton conductivity is essential to hydrogen fuel cells. Yttrium doped barium zirconate is one of the fastest solid-state proton conductors. While previous studies[1, 2] suggest that proton tuples move as pairs in yttrium doped barium zirconate, a systematic catalog of all possible close proton-tuples moves is missing. Such a catalog is essential to simulating dual proton conduction effects. Density functional theory and PBE functional are utilized to obtain the total electronic energy for each proton tuple. Conjugate gradient and Nudged Elastic Band (NEB) methods are used to find the minima and transition states for proton tuple motion. In the lowest-energy configuration, protons are in close proximity to each other and the dopant significantly affecting the backbone structure. The image below shows the lowest energy proton tuple as well as the pathways to move away from this lowest energy structure with energy barriers in eV for each type of move. Protons need less energy to overcome forward barrier in intra octahedral transition than rotation in most of the cases. We also found weaker barrier when proton moves to sites on the same plane with dopant.

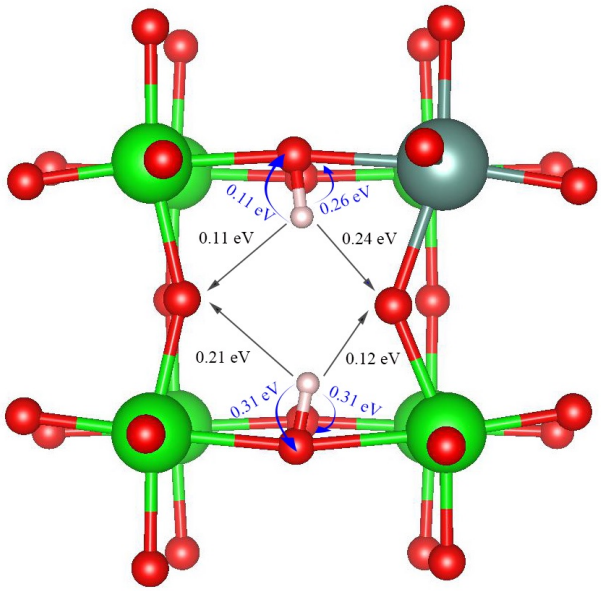

FIG. 1. The lowest energy proton tuple in the Y-doped BaZrO3 system. The arrow indicates all the possible single-step motion to escape the lowest energy structure.