Proton conduction pathways in $SrAl_xZr_{1-x}O_3$ and $BaY_x Zr_{1-x}O_3$ perovskite systems.

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Proton-conducting perovskites show good potential for use in fuel cell technologies. Perovskites are ceramic oxides with an ABO_3 structure. In this study we consider Al^{3+} doped $SrZrO_3$, and Y^{3+} doped $BaZrO_3$. The orthorhombic character of $SrZrO_3$ decreases with increasing concentration of Al^{3+} dopant while cubic $BaZrO_3$ shows slight distortions in the presence of Y^{3+} dopant. In the $SrZrO_3$ system, Zr^{4+} is replaced by Al^{3+}; in $BaZrO_3$ the dopant is Y^{3+}. When a small dopant such as Al^{3+} is used, the proton closest to the dopant tilts toward it, as its +3 charge is not as repulsive as the +4 charge of zirconium. Binding site energies are calculated with the VASP (Vienna *ab initio* Simulation Package) for both systems. Transition state energies are calculated using the Nudged Elastic Band method (NEB). The map of binding and transition state energies generated is used to analyze proton conduction pathways with an adjacency matrix algorithm, color coding and Kinetic Monte Carlo (KMC).