Proton Conduction Pathways in $BaZrO_3$

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Perovskite oxides have shown promise as potential fuel cells, gas sensors, and membranes. Their ability to conduct protons relies on the system being doped to create a charge imbalance. Generally, this is done by replacing a tetravalent atom with a trivalent dopant. The charge imbalance created is crucial to the process of proton conduction. The resulting oxygen vacancy can be filled with water, which contains protons that are subsequently conducted through the perovskite.

This study focuses on $BaZrO_3$. This particular perovskite is cubic when undoped, but can be doped to create a more orthorhombic structure. This allows for inter-octahedral proton transfers, as well as creating a much larger number of specific binding sites for the proton. In this study Y^{3+} is used as a dopant. The transitions between the binding sites will be analyzed using both NEB and a dimer method to find the barriers for different pathways through the system. Then, using a Kinetic Monte Carlo algorithm, the most energetically favorable path will be found.

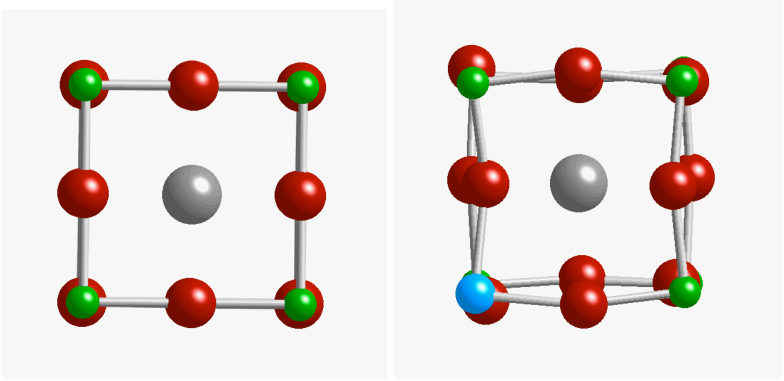

Figure: The cubic undoped $BaZrO_3$ system is shown on the left, and the Y-doped system is shown on the right. Doping the system results in two oxygens moving farther away, and two moving closer together, which allows for inter-octahedral transfers of the proton.