Simulating Proton Conduction Pathways in $SrZrO_3$

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The recent energy crisis has stimulated research in fuel cell development as a source of alternate energy. Fuel cells constructed of perovskite oxide ceramics exhibit conductivity primarily upon the introduction of a cationic dopant to the system. Our primary goal is to compare the effect of dopant on the proton conduction pathways of the perovskite. Replacing Zr^{4+} with the Al^{3+} dopant results in widening of the highlighted oxygen-oxygen distance in Fig.1. In addition, the angle indicated approaches 90° in the Al^{3+} doped system. Both changes reduce the orthorhombic distortions. Conjugate gradient and Nudged Elastic Band methods are used with density functional theory to create an energy map of proton binding sites and transition states. With this map, low-energy, simple pathways can be found by color-coding graph theory ideas. Finally, the paths found for the doped and undoped $SrZrO_3$ systems are compared.

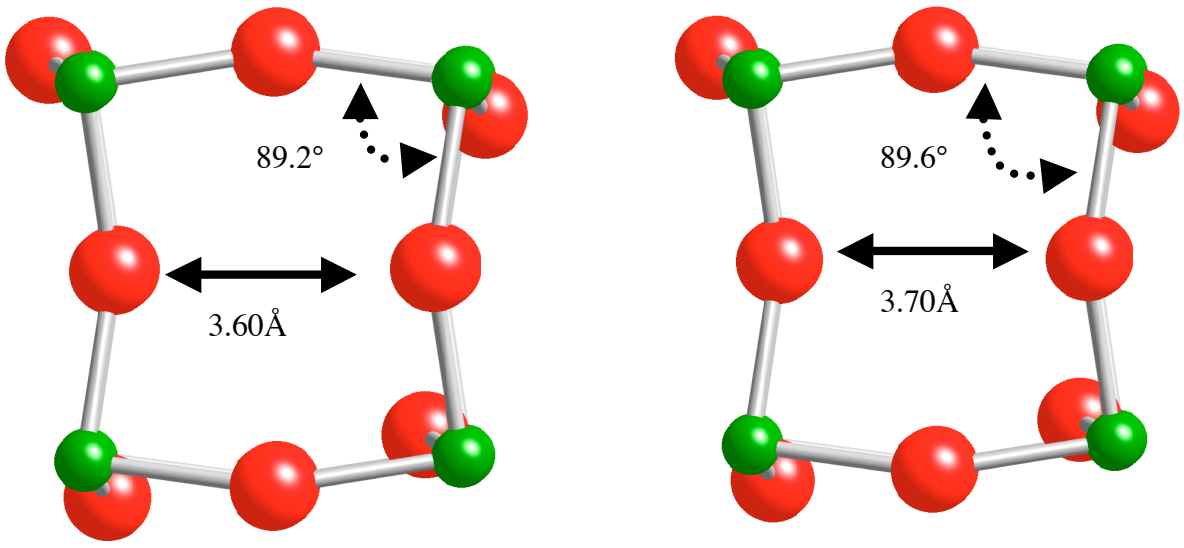

Figure 1: Oxygen atoms are in red, zirconium in green and aluminum in pink. The aluminum doped $SrZrO_3$ system is on the right. This system is clearly more cubic in structure, due to the right hand corner angle approach 90° and the subsequent increase in the width of the "bowtie" shape.