Modeling Proton Conduction Through (311) O-Terminated $BaZr_{0.875}Y_{0.125}O_3$

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Perovskite oxides have attracted much interest due to their possible use in proton conducting fuel cells. Our objective is to understand grain boundary structure and how it affects preferred proton conduction pathways in the Y doped perovskite oxide $BaZrO_3$. Prior studies have shown the O terminated (311) $BaZrO_3$ surface to be the most energetically favored surface.[1] Twist and tilt boundaries based on this surface are considered. The grain boundaries are optimized using density functional theory with the PBE functional. These grain boundaries will be used to find proton conduction pathways.

[1] S. Islam, talk at the 2010 Solid State Protonic Conductors 15; H. J. Zhou, Y. B. Mao, and S. S. Wong, "Shape control and spectroscopy of crystalline $BaZrO_3$ perovskite particles," J. Mat. Chem. **17** (2007) 1707-1713.