

Toward Long Range Proton Conduction Across (310) Tilt Grain Boundaries in BaZrO₃
Jiayi Chen, Wanshu Zhu, Luong Nguyen and Maria A. Gomez

Department of Chemistry

Mount Holyoke College

50 College Street, South Hadley MA 01075

Fuel cells show great potential as alternative energy sources. Y doped BaZrO₃, among other conductive perovskites, has shown excellent proton conductivity and stability(1). Since transmission of protons is rate-determining step in fuel cell generation of electricity, it is crucial to study the proton conduction mechanism. Earlier studies in our group have revealed the proton conduction mechanisms in single perfect crystals of Y doped BaZrO₃ and other perovskites. However, crystals are usually not perfectly formed and often contain grain boundaries. Our study will consider proton conduction in systems including grain boundaries based on the (310) surface.

(1)M. A. Gomez, M. Chunduru, L. Chigwesh, L Foster, S. J. Fensin, K. M. Fletcher, and L. E. Fernandez, *The effect of yttrium dopant on the proton conduction pathways of BaZrO₃, a cubic perovskite*, J. Chem. Phys. **132** (2010) 214709; M. A. Gomez, M. Chunduru, L. Chigwesh, K. M. Fletcher, *The effect of dopant at the Zr site on the proton conduction pathways of SrZrO₃: An orthorhombic perovskite*, J. Chem. Phys. **133** (2010) 064701.