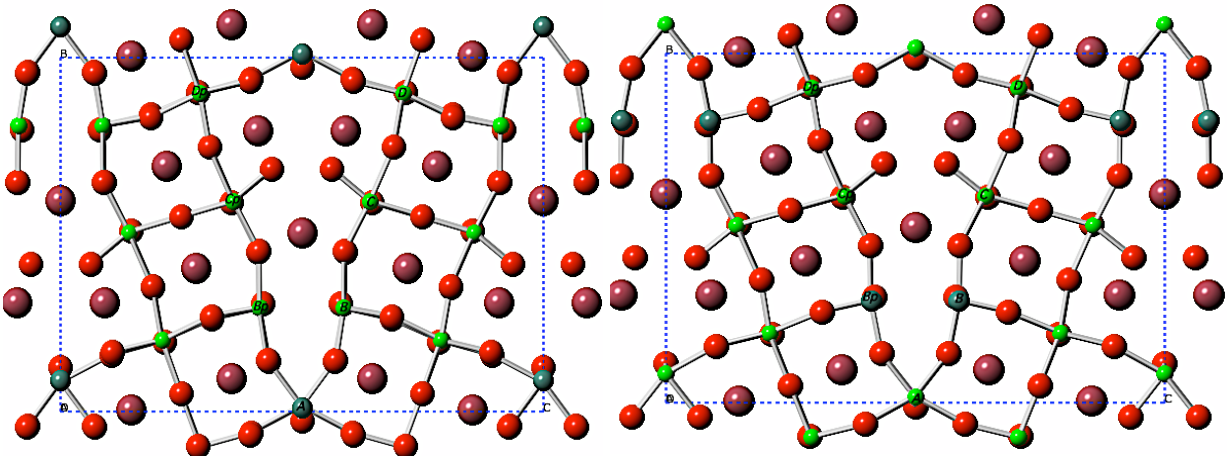
How grain boundary energies are affected by varying combinations of dopant sites and its concentration

Leixin Zhu, Dana L Fry, Fan-Jean Liu, Rachel Krueger, Monica Chelliah and Maria A. Gomez
Department of Chemistry, Mount Holyoke College

Solid oxide fuel cell (SOFC) is an electrochemical conversion device that has a solid oxide or ceramic electrolyte. Yttrium doped $BaZrO_3$, a type of SOFC electrolyte, has displayed high efficiency and stability in proton conduction; however, grain boundary impedance causes critical limitations to proton conduction. Since yttrium tends to aggregate closer to the grain boundaries of $BaZrO_3$, the increase of concentration of Y dopant impacts different proton transfer pathways and results in different activation barriers. Density functional theory calculations with LDA, PW91 and PBE functional performed on symmetric Σ5 (310) grain boundaries in 3.57% $Y/BaZrO_3$ showed consistent ordering on the energies of each potential doping site. PBE functional was chosen for single point energy calculations for a spectrum of combination of dopant sites in 14% and 7% $Y/BaZrO_3$.



(a) (b)

Figure 1. (a) the lowest energy doping site (site A) for both 3.57% doped system and 7% doped system; (b) the lowest energy doping sites for 14% doped system (site BBp).