Proton Delocalization in Scandium and Yttrium Doped Barium Zirconate

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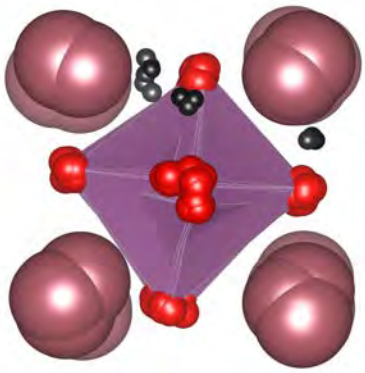
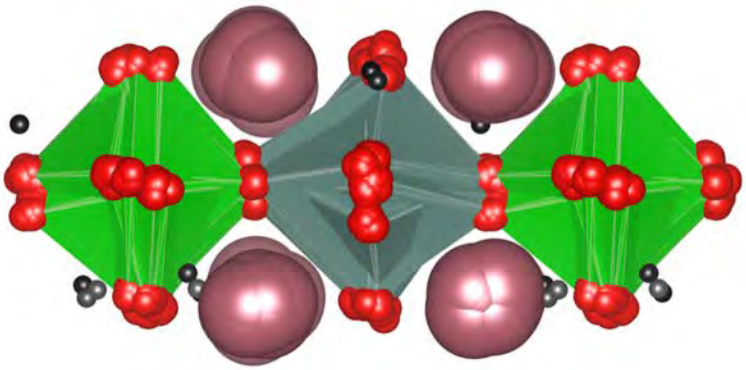
This study aims to understand how scandium and yttrium dopants affect the ground state wavefunction of the promising fuel cell barium zirconate, $BaZrO_3$, and how the wavefunction might affect the conductivity in the temperature range of 300-600 K. Diffusion Monte Carlo (DMC) is used to find the ground state wave function in the two doped $BaZrO_3$ systems. The Vienna Ab initio Simulation Package (VASP) is used to find Born-Oppenheimer potential energy surface on which the nuclei move. At the start of the DMC simulation, walkers are placed at every minimum in the potential energy surface and the trial energy is set to the average potential energy over all the walkers. The wavefunction or distribution of walker configurations as the simulation proceeds for each doped system is visualized. The weight of a walker is used to change the proton gray scale value. In the scandium doped system, our results show that the wavefunction or walker distribution is localized on both H_I^{Far} and H_I^{Close} locations after many time steps. In the yttrium system, the wavefunction of protons is localized on H_I^{Far} and H_{II}^{Far} sites. These are the lowest two energy sites for each system and the sites favored by the electron density.



Proton Density in Scandium System



Proton Density in Yttrium System