The effect of yttrium concentration on the proton conduction pathways in barium zirconate

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Doped perovskites show good promise as fuel cell proton conducting membranes. Proton conduction in 6.25 % yttrium doped barium zirconate is explored. The dopant increases octahedral distortions as it did in the 12.5% yttrium doped system. However, the distortion is barely perceptible in the region between the dopants. The proton binding site energy roughly increases with distance away from the dopant. Rotational and intra-octahedral transfer barriers have been found between proton binding sites using the Nudged Elastic Band (NEB) method. Inter octahedral transfer barriers are found for some sites but when the octahedral distortion is barely perceptible, the proton prefers to make two intra-octahedral transfers rather than a single inter-octahedral transfer. Graph theory and kinetic Monte Carlo are used to find multi-step proton conduction pathways in this lower concentration dopant system. The pathways are compared and contrasted with higher dopant concentration system from our earlier studies..