Effect of oxygen vacancy on proton binding site energies of 12.5% Y-doped $BaZrO_3$

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Proton conductivity of perovskites has made them promising material for fuel cells. A recent experimental study[1] suggested that oxygen vacancies caused by doping the perovskite can enhance the proton conduction. We considered 23 Glazer distortions[2] as well as three previously optimized structures[3] for a 2×2×2 system of 12.5% Y-doped $BaZrO_3$ to find the lowest energy structure. The lowest energy stureture of 12.5% doped system without vacancy shows a lattice size of 4.25, 4.25, 4.25 Å and angles of 90., 90., 90.° via calculations using conjugate gradient optimization in the Vienna *Ab initio* Simulations Package(VASP)[4]. Three types of possible oxygen vacancies are identified from the system and the energy of all 92 proton binding sites are considered for each type. Calculation indicates that the energy of proton binding sites is highly dependent on proximity of dopant, local hydrogen bonding, and oxygen vacancy location. Bader calculation[5] shows that some binding sites closed to the oxygen vacancy do not have enough electron density to bind a proton. In addition, some sample transition states calculated via nudge elastic band (NEB)[6,7] method in VASP are shown.

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