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First principles study of local and electronic structures of yttrium-doped $Ba(Zr_xTi_{1-x})O_3$

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Here we report the first principles study of yttrium-doped $Ba(Zr_xTi_{1-x})O_3$ (Y-doped BZT) for $x = 0.125$, 0.250, and 0.375 supercells as a promising rare earth doped lead-free ferroelectric material. The local and electronic structures of Y-doped BZT and pure BZT relaxed supercells are systematically investigated in term of atomic pair distribution functions (PDFs), A and B site cation off-centering, and electronic density of states (DOS) respectively. The PDF spectrums show the increasing of structural disorder as a function of Zr concentration, while the short-range disorder is strongly influenced by the size of cation and their corresponding vacancies. Moreover, the drastic diffusion in PDF spectrums of Y-doped BZT reflects the compositional fluctuation on the local environment of the supercells. For cation off-centering, Ti^{4+} play a major role as the active ferroelectric distortion in BZT. However, the substitution of yttrium ions into BZT matrix enhanced the lattice distortion as observed from the increasing of off-centering magnitude for both A and B site cations. The calculated total and projected DOSs on d states of cations and O-$2p$ states confirm the strong hybridization between Ti $3d$ and O $2p$ states, thus implying the covalent bonding in Ti-O_6 octahedral. On the other hand, the little effects of yttrium ions on the electronic structures, especially the highest and lowest valence and conduction bands, were observed.

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