

## First principles study of local and electronic structures of yttrium-doped $\text{Ba}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$

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Here we report the first principles study of yttrium-doped  $\text{Ba}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$  (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,  $\text{Ti}^{4+}$  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<sub>6</sub> 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.

**Primary author:** Mr THAMMADA, Wiriya (Department of Physics, Faculty of Science, Mahidol University)

**Co-author:** Dr SUEWATTANA, Malliga (Department of Physics, Faculty of Science, Mahidol University)

**Presenter:** Mr THAMMADA, Wiriya (Department of Physics, Faculty of Science, Mahidol University)

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