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First-Principles Investigations of Pb Anti-Site Defects in $PbZrO_3$ and $Pb(Zr, Ti)O_3$ Perovskites[1] RICARDO KAGIMURA, DAVID J. SINGH, Oak Ridge National Laboratory — Lead zirconate (PZ) and lead zirconate titanate (PZT) have the perovskite type structure, ABO_3. Bivalent lead (Pb^{+2}) ions occupy the A site, while tetravalent titanium and zirconium (Zr^{+4}, Ti^{+4}) ions occupy the B site at random of the PZT solid solution. Also, lead can be tetravalent (Pb^{+4}), such as in PbO_2 structure. Recent experimental work has reported that tetravalent Pb ions can locate at the B site of the PZT perovskite forming a lead zirconate-titanate-plumbate solid solution. The experimental results suggest that, based on a $PbZrO_3$-$PbTiO_3$-$PbPbO_3$ ternary solution phase diagram [G. Suchaneck *et al.*, Ferroelectrics **318**, 3 (2005)], the substitutional Pb atom prefers to occupy the Zr site instead of the Ti one. In this work, we report density functional supercell calculations for pure $PbZrO_3$ perovskite and for ordered $Pb(Zr_{1/2}Ti_{1/2})O_3$ solid solution with different configurations for the Zr and Ti atoms. We investigate the anti-site defect energies and the effects on the electronic structure.

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Ricardo Kagimura
Oak Ridge National Laboratory

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