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The Interplay Of Lattice Distortion and Bands Near The Fermi Level in ATiO3(A=Ca,Sr, Ba)

In this paper, the structural and electronic properties of ATiO3 (A=Ca, Sr, Ba) have been investigated under the strain-free situation and realistic constraints using first-principles calculations. We endeavored to find out the relationship between the interplay between lattice distortions and bandgap in three ATiO3 family members that has remained skeptical to date. The simulations were done by employing the numerical atomic orbital method as implemented in the SIESTA code. Exchange and correlation functions were treated by the generalized gradient approximation. Since only intrinsic properties of the titanates were considered in these calculations no Hubbard term to deal with the on-site Coulomb repulsion on the Ti d-states was considered. In all the calculations herein, we replaced the core electrons by ab-initio norm-conserving pseudopotentials that followed the Troullier-Martins scheme in the Kleinman-Bylander fully non-local separable representation. We found out that the electronic structure was particularly sensitive to perturbations (compressive or tensile) as expected in most materials science studies in solid state chemistry and physics. Our results indicate that under mild strains; the bandgap (Egap), increased under compression and decreased under tension. In all the three materials, the bandgap and the lattice parameter (a) were found to relate as with 2.19< x< 3.1 for mild distortions. All these changes are attributed to the interplay of electrostatics and covalency in the crystals under study. This work acts as a yardstick on bandgap engineering to achieve desired properties in these octahedral titanates for feasible future applications in the electronics industry.

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