Abstract Book

International Conference on Smart Materials
Smart/Intelligent Materials and Nanotechnology
and
2nd International Workshop on
Functional Materials and Nanomaterials

Smartmat-'08
& IWOFM-2

22-25 April 2008
Chiang Mai, Thailand

Supported by

The Effects of Excess Titanium and Crystal Symmetry on Electronic Properties of Pb $(Zr_{1-x}Ti_x)O_3$

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In this paper the structural and electronic properties including band structure, energy gap, and the density of states have been studied for different phases of $Pb(Zr_{1-x}Ti_x)O_3$ compounds in the ranges from x=0 to x=1. The calculations were performed in the framework of density functional theory (DFT), using the full potential-linearized augmented plane wave (FP-LAPW) method with the generalized gradient approximation (GGA).As PZT compounds are ferroelectric and strongly correlated materials, it seems one needs to use an orbital dependent potential for the exchange-correlation terms. However, in order to see the effect of orbital-dependent potential, we calculated the electronic properties of $PbTiO_3$, using GGA, LDA+*U* and GGA+*U* approaches. Applying the orbital dependent potentials results in the shift of the binding energies of certain orbital levels to the experimentally determined positions. In general, our results show that for all cases (x=0, 0.33, 0.5, 0.66 and 1) by increasing the amount of Ti atoms the band gap decreases, because of the strong hybridization between Ti-3d and O-2p orbital. But the decrease of the crystal symmetry results in band gap widening. For the monoclinic phase (x =0.5) the effect of excess Ti on the band gap is less than the effect of crystal symmetry, so there is an increase in the band gap.