11th International Conference
on Advanced Materials

Rio de Janeiro Brazil
September 20 - 25

ICAM2009

Density-functional studies of $PbZr_{0.5}Ti_{0.5}O_3$: Monoclinic, Cubic and Tetragonal

N. H. Nicoleti[(1)*] and Júlio R. Sambrano[(1)]

(1) Grupo de Modelagem e Simulação Molecular, DM/FC, UNESP – Universidade Estadual Paulista, Bauru/SP, Brazil, nelionic@fc.unesp.br.

* Corresponding author.

Abstract – In this work, we examine the crystalline and electronic structure of the lead zirconate titanate - $PbZr_{0,5}Ti_{0,5}O_3$ (PZT), using the Density of Functional Theory (DFT) in set with hybrid functional B3LYP. The information that been collated with the experimental data, it indicates that in this concentration we have 3 possible structures for this material: monoclinic, cubical and tetragonal.

In the field of nanostructure materials special attention has been paid to ABO_3 perovskite oxides nanoparticles. In particular $PbZr_{0.5}Ti_{0.5}O_3$ (PZT) has received considerable attention due to its photoluminescence properties. The PZT is found at monoclinic, cubic and tetragonal phase [1]. Here, we use periodic methodology applied to density functional theory (DFT) to examine the structural and electronic properties of PZT [2]. Computational studies yield useful information regarding the electronic and structural properties of solids, which can provide a framework for the interpretation of experimental data in order to determine the influence of doping that often controls important aspects of solid-state chemistry [3]. Periodic DFT/B3LYP, were carried out by means of the CRYSTAL06 computer code. Pb, Zr, Ti and O centers have been described in the scheme: Pb_DURAND-31G*, Zr_ECP_HAYWSC_311d31G, Ti_86-411(d31)G and O_6-31d1 respectively. The models were built within the supercell 2x2x2 approach. The results are discussed in terms of density of states, band structures, charge distributions and compared with reported quantum mechanical calculations, as well as available experimental data. The main conclusion of this work can be summarized:

1) The calculated structural and electronic properties are in good agreement with other theoretical and experimental data, Table 1.

2) The calculated band gap of monoclinic, cubic and tetragonal is respectively: 3.97 eV and 3.79 eV to the cubic and tetragonal.

Keywords: DFT, electronic structure, perovskites.

This work is supported by: CNPq, FAPESP and Unesp.

Table 1: Experimental and theoretical data of the PZT.

Experimental			
$PbZr_{0.5}Ti_{0.5}O_3$	**Monoclinic**	**Cubic**	**Tetragonal**
Cell length (Å)	a = 5.73 b = 5.72 c = 4.12	a = b = c = 4.08	a = b = 4.03 c = 4.15
Cell angle (°)	$\alpha = \gamma = 90$ $\beta = 90.39$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$
Cell volume ($Å^3$)	135.02	68.17	67.33
Theoretical			
Cell length (Å)	a = 5.69 b = 5.66 c = 4.29	a = b = c = 4.07	a = b = 4.02 c = 4.21
Cell angle (°)	$\alpha = \gamma = 90$ $\beta = 90.60$	$\alpha = \beta = \gamma = 90$	$\alpha = \beta = \gamma = 90$
Cell volume ($Å^3$)	138.16	67.67	68.03

References

[1] D.E.Cox, B.Noheda, G.Shirane, Phys Rev Condensed Matter. 71, 13411 (2005).
[2] E. Orhan, F. M. Pontes, E. R. Leite, P. S. Pisan, J. A. Varela, E. Longo, ChemPhysChem. 6, 1 (2005).
[3] Z. Chen, Y. Chen, Y. Jiang, J. Phys. Chem. 106, 9986 (2002).