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Electronic properties of ABO_3: Periodic Density Functional Study

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Abstract – The electronic properties of cubic ABO_3, where A = Ba or Sr and B = Zr or Ti, were investigated by means of periodic methodology based on DFT theory. The bands structures shows that the fundamental energy gap are indirect between *R* and *Γ*, for all models. The contributions of the different bands was analyzed from the density of states. The results are in good agreement with the experimental data.

The ABO_3 (A = Ba or Sr and B = Zr or Ti) perovskites oxides have attracted considerable attention in the last years, and are suitable for various technological applications. This materials are used in thermal barrier coating material for supersonic jets by aerospace, related industries, computer memory, solar cells, and catalysts, among others. Due to this, investigation of these compounds are very important. Many research groups have devoted considerable attention on the development of high density ceramics with tecnological applications.

Correlations between theoretical and experimental techniques can bring clarification about the structure of this material; in this work we used DFT therory, with hybrid functional B3PW, using the program CRYSTAL06.

We focus our study on the cubic structure (space group *Pm3m*) of the perovskites. In this structure, the A atom is coordinated by twelve oxygen atoms and the B with six oxygen atoms, in an octahedral configuration. As a first step, a optimization procedure of the lattice parameter ***a*** was carried out, yielding a value as Table 1 for B3PW.

The simulations yields a bulk band gap, as Table 1, in good agreement with the experimentally observed gap. For all perovskites, the band gap is indiret between *R* and *Γ* points of the Brillouin zone.

The principal atomic orbital (AO) component indicates that upper valence bands and bottom conduction bands are mainly derived from orbital 2p of O and d_{xz}, d_{yz} and d_{xy} of Zr or Ti, respectively, with a litte contribution of AO of atoms Ba and Sr.

Theoretical calculations can provide important informations regarding the electronic and structural properties of solids and interpretation of experimental data. Band structure, total and projected density of states and density maps will be discussed.

Table 1. Experimental and Theoretical lattice constant ***a*** (in Å) and band gap (in eV)

Material	$a_{experimental}$	$a_{theoretical}$*	Band gap $_{experimental}$	Band gap $_{theoretical}$*
$BaZrO_3$	4.192[1]	4.207	5.33[2]	5.80
$SrZrO_3$	4.109[3]	4.106	5.21[4]	4.90
$BaTiO_3$	3.977[5]	3.980	3.20[6]	3.50
$SrTiO_3$	3.944[7]	3.888	3.40[8]	3.67

* this work

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