PERIODIC QUANTUM MECHANICAL ANALYSIS OF BARIUM TITANATE WITH PHOTOLUMINESCENT PROPERTIES

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ABSTRACT

The material researched in this study is barium titanate (BT). This material displays a perovskite-type structure, which is usually found as a crystalline phase (BT-c), where titanium is hexacoordinate with oxygens and barium at its corners. When it is found as an amorphous phase (BT-a), the titanium is hexa- and pentacoordinate. The method used to obtain BT has been the polymer precursor method (PPM).The advantage of this method is its low cost and easy reproducibility. This material displays ferroelectric and optical properties. One of its most important properties is the photoluminescence of the amorphous structure at ambient temperature.

The objective of the present work has been the performance of a quantum mechanical study to research the optical, structural and electronic properties, for a more detailed interpretation of the experimental results obtained.

KEY WORDS: photoluminescence, barium titanate, ab initio

1. COMPUTATIONAL DETAILS

The calculations were made using the Crystal 98 computational packages for periodic systems for BT-c and BT-a. The ab initio calculations made under Hartree-Fock level using the density functional theory proposed by Lee, Yang and Parr, combined with the change functional, B3LYP, which was demonstrated by Muscat et al. The lattice parameters were optimized for simulation of the crystalline phase, using the X-ray diffraction crystallographic data as a starting point.

2. RESULTS AND CONCLUSIONS

With the analyses of the theoretical calculations, the band structures (Figure 1) and state densities (DOS) (Figure 2) were verified of the compound, enabling comparable theoretical gap values to be found with the experimental values (3.55 eV and 2.67 eV) for crystalline and amorphous BT respectively. These results agree with the experimental data, where the photoluminescent emission for amorphous BT at ambient temperature was verified.

In the results of the theoretical calculations of the DOS analysis, the appearance of new electronic levels for BT with the application of a deformation in the Ti-O bond can be observed, indicating formation of the pentacoordinate species.

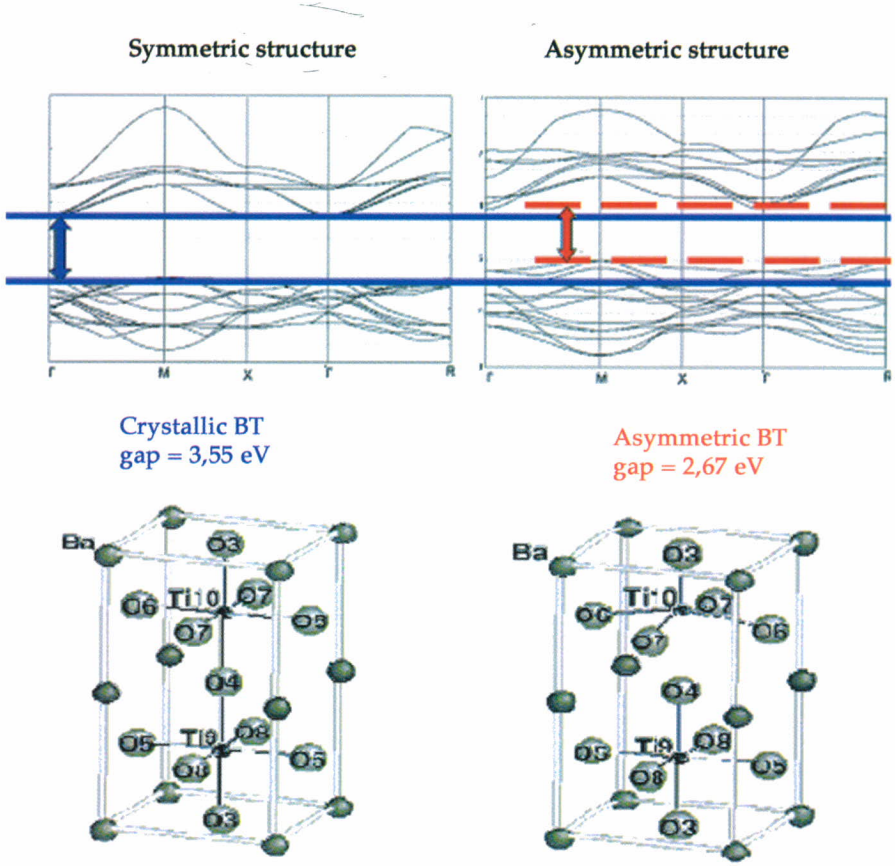

Figure 1. Band structures of BT. (a) crystalline. (b) asymmetric

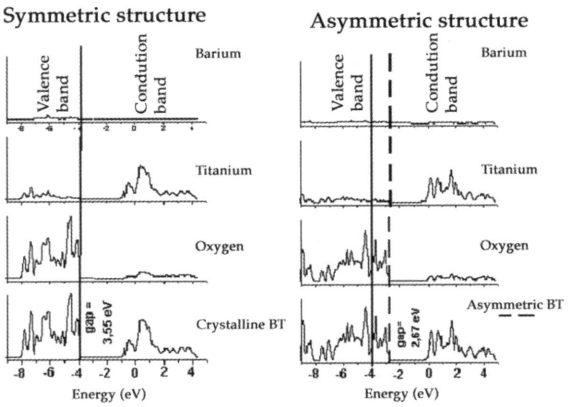

Figure 2. DOS of BT.

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