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Influence of different exchange correlation potentials on band structure and optical constant calculations of $ZrGa_2$ and $ZrGe_2$ single crystals

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ABSTRACT

The all-electron full potential linearized augmented plane wave method was used to solve the Kohn Sham DFT equations. We have employed different approximations for the exchange correlation potentials, namely: LDA, GGA and EVGGA, and insignificant effect on the band structure and the density of states were found. Calculations show that there is a significant difference in the band dispersion with replacement of Ga by Ge that is attributed to the fact that in the $ZrGe_2$ compound Zr atom is situated at 4c site and two Ge atoms are situated at 4c site. Whereas for $ZrGa_2$ compound Zr is located at 4g site and the three Ga atoms are situated at 4h, 2c and 2a sites, respectively. There exists strong hybridization between the states. Moving from $ZrGa_2$ to $ZrGe_2$ has significant influence on the magnitudes and the peak positions of states. The optical properties of the two compounds were studied and analyzed.

1. Introduction

It is well known systematization of structural types with respect to the coordination of the atoms of the smallest sizes [1], which gives to classify structural types by classes, groups and to establish an affinity between structural types within the same class as well as between structural types, belong to different classes. Usually these approaches are different. In this work we try to look on the behavior of the corresponding energy band gaps. To study such relations the better way is to perform the calculations for the isostructural compounds.

Among the binary compounds particular interest present halides, germanides, antimonides, arsenides, etc. Partially covalence bonds prevailingly form more electronegative atoms and atoms with less electronegativity usually occupy empty structural positions or occupy voids in cluster layers or polyhedra formed by anions. Very often these atoms are characterized by shorter chemical bonds to anions. This phenomenon may be explained similarly to polyhedra Frank–Casper [2], i.e. like atomic agglomerates, where cationic electrons are shifted towards connections with anions.

As a consequence the compound possessing the lowest electronegativity for compounds of different classes at fixed structural type should be changed. As a consequence, in the Ref. [3] an attempt has been made to perform a classification of structural types with respect to the atoms with maximal sizes. Following the reasons presented above in the present work we explore the band structure performed within a framework of DFT method with different exchange correlation potentials: LDA, GGA and EVGGA. For this reason we have chosen compounds $ZrGa_2$ and $ZrGe_2$ [4] possessing the same structural fragments (Fig. 1). At the same time their electronic configuration is different from each other. The choice of the different exchange correlations approach should add to help the influence of this screening on the band structure behaviors. The quantum chemical simulations should show how sensitive they will be to such different potential screenings.

To the best of our knowledge no comprehensive work neither experimental data on the optical properties or first principles calculations on the structural, electronic, and optical properties of $ZrGa_2$ and $ZrGe_2$ compounds have appeared in the literature. Therefore as a natural extension to previous work on $ZrGa_2$ and $ZrGa_3$ compounds [5,6] a detailed depiction of the structural, electronic, and optical properties of $ZrGa_2$ and $ZrGe_2$ using full

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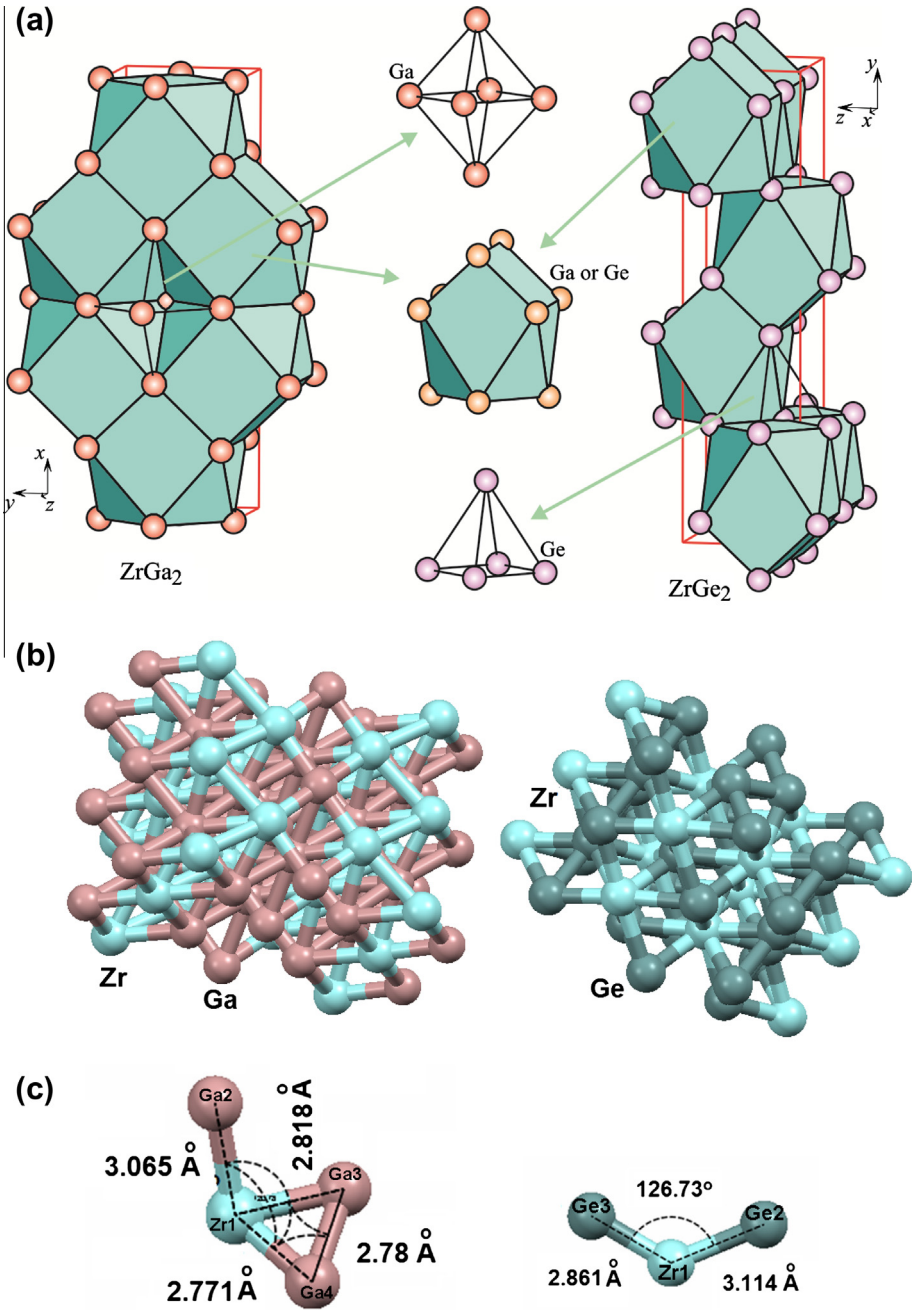

Fig. 1. (a) The crystallochemical transformation of the structure for crystals $ZrGa_2$ and $ZrGe_2$; (b) crystal structure of $ZrGa_2$ and $ZrGe_2$; and (c) asymmetry unit of $ZrGa_2$ and $ZrGe_2$.

potential method is timely and would bring us important insights in understanding the origin of the band structure and densities of states. Hence it is very important to use a full potential method. Present study is aimed towards such calculation by using the full potential linear augmented plane wave (FP-LAPW) method which has proven to be one of the most accurate methods [7,8] for the computation of the electronic structure of solids within a framework density functional theory (DFT). Our calculations will demonstrate the effect of using a full-potential on the structural, electronic and optical properties of the single crystals of $ZrGa_2$ and $ZrGe_2$.

In the Section 2 are given structural properties and principal computational details. The Section 3 present principal results concerning the band structure calculations and calculated optical dispersions of the principal optical functions. Comparison of the results obtained by LDA, GGA and EVGGA is presented.

2. Structural properties and computational details

For the calculations are chosen $ZrGa_2$ and $ZrGe_2$ single crystals. The crystal structures are listed in Tables 1 and 2 and illustrated at Fig. 1. Using the X-ray diffraction data (XRD) we have optimized the structure by minimization of the forces acting on the atoms. The structure is fully relaxed until the forces on the atoms reach values less than 1 mRy/a.u. Once the forces are minimized in this construction one can then find the self-consistent electron space density distribution at these positions by turning off the