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Optoelectronic properties of the new quaternary chalcogenides $Zn_2CuInTe_4$ and $Cd_2CuInTe_4$: Ab-initio study

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ABSTRACT

In order to exploit the fundamental properties of the new tellurides quaternary diamond-like structure $Zn_2CuInTe_4$ and $Cd_2CuInTe_4$, first principles investigation in the framework of the Full-Potential LAPW scheme have been carried out for that purpose. We used the Wu and Cohen generalized gradient approximation (GGA-WC) to calculate the optimized structure that corresponds to the global minima of the energy. Enthalpy of formation shows that the most stable structures are the relaxed ones. The EV-GGA and the TB-mBJ approximations were also used for electronic and optical properties. The equilibrium electronic parameters found are in good agreement with the previous results. The real and thecient, the opt imaginary parts of the dielectric function, the refractive index, the extinction coeffiical conductivity, the absorption coefficient, the loss function and the reflectivity are reviewed in the large spectral range of photon energy. The present study demonstrates a variety of novel electronic and optical properties, which make these compounds highly promising for optoelectronic materials.

1. Introduction

Bring by the desire to find other materials with new or improved properties, computational physics for materials quickly emerged as a very promising tool used in this materials science. All indications are that this trend will continue to accelerate and that progress in many areas will increasingly depend on the development of new concepts and new calculation techniques. Over the past few years, the improvement of computational techniques has made us possible to discover a variety of compounds with different lattices parameters, varied band gap energy and interesting optical properties for the development of new devices for a multitude of optoelectronic applications.

Materials science is a field that is changing at a very fast pace and currently gives very promising results looking at the scale manometric. It is driven by the desire to find other materials with new or improved properties. The contribution of

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calculations from first principles to materials science is more important than ever. The main reasons are the steady progression of computer power and continuous progress in the methodology, both the efficiency and accuracy of the calculation methods and its approximations.

Knowing the structure, it is possible to calculate a large number of properties of a material, even before it is synthesized, hence the crucial importance of the structural prediction for the design of semiconductor materials. The electronic structure is undoubtedly the most important information on a material, since it directly or indirectly determines almost all the properties of the material.

Tellurides quaternary diamond-like structure represented by the general formulae A_2-I-III-VI_4 (A = Zn and Cd) are materials containing one or more chalcogenide elements (group VI in the periodic table, e.g. sulfur, selenium or tellurium) as a substantial constituent. Taking into account the chemical composition $A_2CuInTe_4$ (A = Zn and Cd), these quaternary materials have tetrahedrally coordinated crystal structures, and their properties are much more diverse given the increased number of elements [1], so they may have wide applications in optoelectronic, photovoltaic, thermoelectrics [2], spintronics [3], magnetic and magneto-optical applications [4]. As the name suggests, tetrahedral structures are characterized by tetrahedral bonding, every atom in the structure has four nearest neighbors [5].

$Zn_2CuInTe_4$ and $Cd_2CuInTe_4$ are a member of quaternary I-II_2–III–VI_4 compounds with cubic lattice. The structure of these compounds can be derived from the II–VI cubic zinc blende structure. According to *Nolas et al.* [6] the polycrystalline $Zn_2CuInTe_4$ and $Cd_2CuInTe_4$ were synthesized from highly pure elements (99.999% of purity) sealed in a quartz ampoule under vacuum with a nominal stoichiometry of I-II_2-III-VI_4 and heated at 973 K over 4 days [6]. The structure of the samples was examined by Powder X-ray diffraction (XRD), and the refinement results indicate that the two specimens have a not ordered cubic zinc-blende structure. For the type structure, the unit cell contains four Zinc or Cadmium, two Copper, two Indium and eight Tellurium atoms.

In this present paper we studied the structural, electronic, optical and properties of our selected compounds by first principles calculations with F-cubic crystalline structure. For our acknowledgments no optical properties have been investigated at the present time for these systems. The calculations were performed within the WIEN2 K code. For such a purpose, we employing the experimental data as the input parameters in order to obtain our optimized results. We then compared our results to previously reported X-ray diffraction (XRD) data.

This article is organized as follows. In Section 2, the computational technique is described. Results and discussions will be presented in Section 3, and a summary of this work is given in Section 4.

2. Method of calculation

The most successful approach to finding solutions to the Schrödinger equation that describes the quantum behavior of atoms is used in this study. In our calculations, the lattice parameters and positions of the constituent atoms have been chosen as determined in the experimental works cited above [6]. The F-cubic phase was adopted for $Zn_2CuInTe4$ and $Cd_2CuInTe_4$ Tellurides quaternaries. The minimum energy has been calculated employing the first principles self-consistent FP-LAPW method with the WIEN2k computational code [7]. The structures were fully optimized (cell parameters, volume cells, and atomic positions) with a residual force threshold of 0.1 mRy. In order to get a good description of structural optimization we used the GGA method constructed by *Wu* and *Cohen* in WC-GGA [8]. The generalized gradient approximation of Engel-Vosko (EV-GGA) [9] and the modified Becke-Johnson scheme (TB-mBJ), proposed recently by Tran and Blaha [10], were also used for electronic and optical properties. These approximations are primordially identified through theoretical models that seek to better represent the terms of exchange and correlation of Kohn and Sham. The unit cell is divided into non-overlapping muffin-tin (MT) spheres around the atomic sites, and an interstitial region. Here we used the following muffin-tin radii R_{MT}; Zn = 2.4, Cu = 2.4, Cd = 2.5, In = 2.5 and Te = 2.5 for $Zn_2CuInTe4$ and $Cd_2CuInTe_4$. The $R_{MT}K_{max}$ parameter was taken equal to 9.0 for structural optimization. To ensure the correctness of our calculations, we have taken l_{max} = 10 and G_{max} = 14.

3. Results and discussion

3.1. Structural properties

The crystalline structures of our compounds were simulated by using a supercell containing 16 non-equivalent atoms ($2 \times 2 \times 2$) in order to mimic the zinc blende structure with four different atoms. In Fig. 1 we presented the F-cubic structure of $Zn_2CuInTe_4$.

Each Tellurium (Te) atom is closely surrounded by four atoms, two Zinc (Zn) one Copper (Cu) and one Indium (In), located at the corners of a nearly regular tetrahedron. Each Zn/Cu/In atom is similarly surrounded by four Tellurium atoms. The distances between atoms for both materials with un-relaxed and relaxed structures are shown in Table 1.

With the framework of WIEN2 K, we will address the study of structural, electronic and optical properties of the materials considered here. It us therefore seems essential to study the structural properties firstly before we passing to the study of optoelectronic properties.

The minimization process is performed to find the relaxed positions of atoms and they are shown in Tables 2 and 3 for $Zn_2CuInTe_4$ and $Cd_2CuInTe_4$ respectively, along with common standard positions.