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High efficiency of transmittance and electrical conductivity of V doped ZnO used in solar cells applications

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ABSTRACT

The full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT) and Boltzmann's Transport theory, are employed to investigate theoretically the electronic structure, optical and electrical properties of vanadium -doped wurtzite ZnO with different concentrations (3.125%, 6.25%, 12.5%, 25%). The FP-LAPW based on the new potential approximation known as the Tran-Blaha modified Becke–Johnson exchange potential approximation (mBJ) was also applied with the primary goal of improving the electronic structure description specially the band gap energy. The calculated band structure and density of states (DOS) exhibit a band gap of pure ZnO (3.3 eV) closer to the experimental one. As well, our results indicate that the average transmittance in the 400–1000 nm wavelength region was 93%. We found that $Zn_{96.875}V_{3.125}O$ is the optimized composition of the V doped ZnO, which has the highest conductivity (3.2×10^3 $(\Omega cm)^{-1}$) and transmittance. The high transmittance and electrical conductivity indicate that hexagonal V:ZnO system is a potential as material for solar energy applications.

1. Introduction

Materials combining high electrical conductivity and optical transparency are vital for photovoltaic and optoelectronic devices, such as solar cells, light emitting diodes and touch screens [1–5]. Generally, the recent technology used Indium-doped Tin Oxide (ITO) materials like electrode in these applications. However, these ITO suffers from the scarcity and high cost of indium (In) [2,5]. This situation led to the search of an alternating in expensive non-toxic and abundant transparent conduction oxides (TCO) material with optical and electrical properties comparable or better to those of the current ITO materials.

Zinc oxide (ZnO) is a wide and direct band gap of 3.4 eV semiconductor with a large exciton binding energy around 60 meV [6]. ZnO is an interesting and multifunctional semiconductor that plays a leading role in II–VI semiconductor family. Additionally, ZnO intrinsically transparent nature over the whole visible range, abundant availability, low cost, high chemical and thermal stability make ZnO particularly attractive for photovoltaic (PV) and for optoelectronic applications, such as light emitting devices [7] and solar cells [8].

Recently, impurity-doped zinc oxide has been also suggested to be an alternative and attractive material for TCs applications. In fact, it exhibits promising electrical and optical properties [5,9–11]. The improving of the electrical and optical properties of n-type ZnO material (up to 10^{21} cm^{-3}) can be achieved by the doping of donor element, in this way ZnO has been commonly doped with Al, In, Ga, Sn and Si [12–17]. Recently some transition metals as V and Nb are used as dopants of ZnO to obtain transparent conductive oxide thin films and this encourages the preparation and study of doped ZnO thin films [18–21]. Furthermore, it is worth noting also that, the good TCOs should have some features like low absorption and reflectivity coefficient with a large transmittance in the large wavelength region, normally from Infrared (IR) up to UltraViolet (UV), and a high electrical conductivity as well.

More recently, the density functional theory (DFT) and Boltzmann equations transport calculations have been successfully applied to investigate the transparent electrode semiconductors such as Ga:ZnO, In:ZnO, La:ZnO and Si:ZnO [22–25]. Theoretically, several methods have been investigated in order to overcome the underestimation of band-gap values that calculated by the standard DFT method. Among them, the DFT based on the Tran–Blaha modified Becke–Johnson exchange potential approximation (mBJ) [26] can produce an accurate band gap value with a low cost of calculation.

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Therefore, through this work, we use this approach for studying the effect of vanadium doping on the electronic and optical properties of ZnO because of his most stable oxidation state V^{+5} in natural environment. In addition, V is a multi-electron donor, which is able to improve the electrical conductivity of ZnO-based semiconductors, V may be considered as a potential candidate for replacing the single electron donor of Al. Furthermore, to give a complete picture, the electrical properties will be calculated by using the Boltzmann transport theory that will be mentioned later on.

2. Computational details

Through This study, we have used ab initio calculations based on FP-LAPW method which has been performed to solve the Kohn–-Sham equations within the DFT, it is implemented in WIEN2k package [27]. The parameterization of the exchange-correlation energy has been done within the Gradient Generalization Approximation by Perdew, Burke and Ernzerhof (GGA-PBE version) [28] to optimize the volume and the internal position parameters of pure ZnO. To perform our main calculations, we use the modified Becke-Johnson (TB-mBJ) developed by Tran and Blaha [26,29] applied the Becke-Johnson (BJ) potential to a series of insulating systems. Using such potential it was found that the resultant band gaps are noticeably improved compared to the standard LDA/GGA [30,31]. The TB-mBJ potential can be written as::

$$\upsilon_{\chi,\sigma}^{mBJ}(r) = c\upsilon_{\chi,\sigma}^{BR}(r) + (3c-2)\frac{1}{\pi}\sqrt{\frac{5}{12}}\sqrt{\frac{2t_\sigma(r)}{n_\sigma(r)}} \quad (1)$$

where n_σ is the spin-dependent electron density and t_σ is the spin-dependent kinetic-energy density. $\upsilon_{\chi,\sigma}^{BR}$ is the Becke–Roussel potential [32]. The parameter c was proposed to be determined self-consistently from the density by:

$$c = \alpha + \beta\left(\frac{1}{V_{cell}}\int_{cell}\frac{|\nabla n(r')|}{n(r')}d^3r'\right)^{1/2} \quad (2)$$

where V_{cell} means the unit cell volume, α=−0.0012 *and* β=1.023 $bohr^{1/2}$ are parameters fitted according to experimental values [26].

The radii of the muffin-tin spheres R*mt* (Zn) = 1.99, R*mt* (O) = 1.66 and R*mt* (V) = 2.03 Bohr. We make harmonic expansion up to l_{max} = 10, and set $R_{mt} \times K_{max}$ = 7.0, where K_{max} is the cut-off wave vector in the first Brillouin zone (BZ), while a fine k-mesh with 1000 k-points in the irreducible wedge of the first Brillouin zone is used for the undoped ZnO. We decrease the k-points by decreasing the concentration of the doped element. The self-consistent calculations are considered to be converged only when the integration of absolute charge-density difference per formula unit between the successive loops is less than 0.00001|*e*|, where *e* is the electron charge.

Using the results from band structure calculations with both GGA and mBJ approximations, the transport calculations were performed employing the BoltzTraP code [33] that is based on semi-classic Boltzmann theory and the rigid band approach. The electrical conductivity as a function of temperature and the chemical potential can be written as:

$$\sigma_{\alpha\beta}(T,\mu) = \frac{1}{\Omega}\int \sigma_{\alpha\beta}(\varepsilon)\left[-\frac{\partial f_0(T,\varepsilon,\mu)}{\partial\varepsilon}\right]d\varepsilon \quad (3)$$

Where the term Ω is the volume of the unit cell and f_0 is the Fermi-Dirac distribution function. The term $\sigma_{\alpha\beta}(\varepsilon)$ represents energy projected transport distribution tensor which contains the system dependent information, and can be writing as:

$$\sigma_{\alpha\beta}(\varepsilon) = \frac{e^2}{N}\sum_{i,\vec{k}}\tau_{i,\vec{k}}\upsilon_\alpha\left(i,\vec{k}\right)\upsilon_\beta\left(i,\vec{k}\right)\frac{\delta\left(\varepsilon-\varepsilon_{i,\vec{k}}\right)}{d\varepsilon} \quad (4)$$

Where N is number of k-points, *i* is the band index, *k* is the wave vector and $\upsilon\alpha(i,\vec{k})$ is the group velocity, which can be obtained from the band structure calculations as:

$$\upsilon_\alpha\left(i,\vec{k}\right) = \frac{2\pi}{h}\frac{\partial\varepsilon_{i,\vec{k}}}{\partial k_\alpha} \quad (5)$$

Where the term $2\pi/h$ is the reduced Planck constant. The other transport parameters are derived from the electrical conductivity. Thereafter, we will calculate the transport coefficients at the Fermi level where the transport information is concentrated.

3. Results and discussion

1. Electronic properties:

The structure optimization was first performed for ZnO Wurtzite bulk. The optimized lattice parameters are a=3.26 Å, c=5.21 Å which are in good agreement with experimental data a=3.25 Å, c=5.21 Å [34]. Fig. 1 reveals the band structure of ZnO along the high-symmetry lines across the first irreducible Brillouin zone calculated with GGA and mBJ approximations. From here on we've used the mBJ potential for the calculation of electronic and optical properties because it provided results more conform to experimental ones. The energy is given relative to the top of the valence band. We also plot the total DOS of ZnO to compare the valence band and band gap with those of band structure. From the band structure, the valence band maximum (VBM) and the conduction band minimum (CBM) are located at the same Γ point, indicating the pure ZnO is a direct band gap semiconductor. The total density of states (DOS) of pure ZnO as well as projected DOS related to partial of Zn and O. The valence band (VB) ranges from −6 to 0 eV composed mainly of and hybridization O 2p and Zn 3p states, and the conduction band is composed of Zn 4s states. The Fermi level was set as the maximum of the valence band.

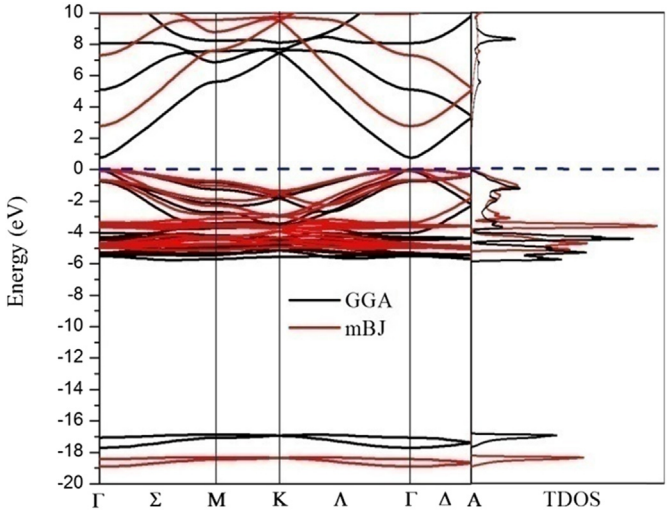

Fig. 1. Band structures along high-symmetry lines of the BZ compared with Total Density of states of pure ZnO with GGA and mBJ approximations.