Effect of Substituted Mn on Electronic Characteristics of Indium Oxide and Zinc Oxide via Density Functional Theory Studying

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Abstract

Objective: One of the main raising issues in chemical industries is improving the materials electric properties. For this purpose, we investigate the effect of substituted Mn on Indium and Zinc oxides by density functional approach.

Methods: The impact of transition metal (Mn) on the electronic characteristics of Indium Oxide (In2O3) and Zinc Oxide (ZnO) have been investigated, utilizing first-principles computation approach according to the density functional approach (DF), by Generalized Gradient Approximation (GGA).

Results: Obtained results for band structure and density of states show that band gap values for indium oxide and zinc oxide are 1.4 eV, 0.75 eV respectively. Substitution of Manganese alters the energy gap and a spin splitting influence is seen. Doped Indium Oxide with Mn and doped Zinc Oxide with Mn have a spin polarized band structure with different band gap for spin up and down states.

Conclusion: We observed for doped ZnO in the spin-down state, a half-metallic behavior, whereas for the spin-up state it remains semiconductor.

Keywords: Building Integrated Photovoltaics, Li-Fi, V2V Communication, Visible Light Communication

1. Introduction

Metallic oxides are indicating one of the biggest bound of characteristics ferroelectric, superconducting, ferromagnetic, multiferroic, magneto-resistive, dielectric, and heat conductivity. Of applicable issue are called Amorphous Semiconducting Oxides (ASOs) and Transparent Conducting Oxides (TCOs).

TCOs like In2O3, SnO2, CdO and ZnO are n-kind wide bound semiconductors. Light layers of these elements have been provided with different techniques and extensively utilized in optoelectronic tools, as transparent electrodes in flat panel shows, in slight-layer transistors, in infrared reflectors, light-emitting diode, solar cells and imagers. They show great transmittance in the near-infrared and visible areas. The optical and electrical characteristics of these elements could be altered by stat- ing defilements. The characteristics of doped TCO layers are so sensible to the kind of defilements. It is further fascinating to examine the compounds of these elements to recognize how the formation and characteristics are changed when the configuration varies.

In2O3 and ZnO are oxides of group IIIB-IVB metals. These are two type of important of Transparent conducting oxides (TCO). In2O3 exists in three different space group symmetries I2 1, Ia 3, and Ic 3c. Between these configurations, In2O3-Ia 3c with a bound of about Eg = 3.7 eV has been generally examined both empirically and
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Theoretically, \( \text{In}_2\text{O}_3 \) crystallizes in a cubic bixbyite-type formation that has 80-atoms in its unit cell with the lattice constant \( a = 10.117 \, \text{Å} \). It has two kinds of Indium and one kind of Oxygen atoms at Wyckoff positions 8b, 24d and 48e.

The next most significant TCO, practically for photovoltaic usage, is ZnO. Zinc oxide is a direct wide-band semiconductor (3.3 eV at 300K) that is extensively utilized for green production, blue-ultraviolet, and white light-emitting tools. The crystal formation of ZnO is wurtzite, zinc blende, and rock salt, while the thermodynamically stable stage is wurtzite. The zinc blende ZnO formation is metastable and could be organized just via hetero epitaxial development on cubic substrates, like ZnS GaAs/ZnS. The lattice constant was \( a = 4.655 \, \text{Å} \).

In this article, we have compared effect of spin polarization Mn dopant on electronic properties of In2O3. In the cubic bixbyite structure and ZnO in phase cubic zinc blend. Transition metal pollutions are important from 2 points of view. First related to acceptor-like doping in the electronic characteristics context. The other related to the magnetic characteristics while the transition component focusing is comparatively great though still in the dilute border so as not to change the central fundamental of the ZnO matrix.

2. Method of Calculation

The evaluations are conducted via a self-consistent theme by resolving the Kohn-Sham equations utilizing the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) approach in the frame of Density Functional Theory along via the GGA utilizing WIEN2k.

The computations conducted via 400 k-points and \( R_{\text{k max}} = 7 \) for the convergence factor in that the evaluations organized and converge in indexes of the intended bound. The amount of \( G_{\text{max}} = 12 \), and the muffin-tin radii for In, Zn, O and Mn were \( R_{\text{MT}}(\text{In}) = 2.0 \, \text{au} \), \( R_{\text{MT}}(\text{Zn}) = 1.9 \, \text{au} \), \( R_{\text{MT}}(\text{O}) = 1.6 \, \text{au} \) and \( R_{\text{MT}}(\text{Mn}) = 1.8 \, \text{au} \). The iterations were stopped while the entire charge differences were less than 0.0001e among stages. The cut-off energy that states the divisions of the valence and core stages was selected to be -6Ry.

The computations are conducted via using the empirical information for the lattice constants. Next via optimizing the whole energy of the crystal to the volume, the analytical lattice constants are received. The last computation conducted by the analytical lattice constant and relaxed form for compounds. The optimization plots are presented in Figure 1. Deduced findings are in continent with the others outcomes.

3. Results and Discussion

3.1 Electronical Results

3.1.1 Band Structure

In this paper, the value of the bound of In2O3, In1.5Mn0.5O3, ZnO and Zn0.875Mn0.125O evaluated from
the band form as explained in Figures 2-5 utilizing GGA technique. The scale of energy in graphs 3 and 4, is in eV and the Fermi level is set to zero on the energy scale. The valence bands were divided by 1.4 eV and 0.75 eV for undoped In$_2$O$_3$ and ZnO energy gap directly from the conductivity band stages at Γ point. Empirical amount of In$_2$O$_3$ direct bound is almost 3.6 eV at Γ point and experimental results of ZnO show a direct band gap about 3.3 eV$^{18}$. These amounts of bounds are smaller than the empirical findings since that the well- known gap issue, whereby the DFT underestimates the bounds. Obtained outcomes of band gap for In$_2$O$_3$ and ZnO are in good agreement with the theatrical recent investigations, like the two stated in$^{3-6}$.

The calculated band structure of In$_{1.5}$Mn$_{0.5}$O$_3$ in up and down spins stages is shown in Figure 3. In these three cases, energy gap is indirect (at Γ point) and is equal to 0.7 eV, 2 eV for up and down spins stages, respectively. Doped Indium Oxide via Mn has as pin polarized band structure with different band gap for spin up and down states. Therefore this subject (spin polarization effect) indicates different electronical properties of this compound.

The obtained results of band structure for Zn$_{0.875}$Mn$_{0.125}$O is shown in Figure 5, with due regard to spin effect can be seen a half-metallic behavior for Zn$_{0.875}$Mn$_{0.125}$O in spin down state, because the Fermi level intersects a band for only one spin direction, but spin-up being semiconducting (Figure 5).
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Figure 5. Band structure of Zn_{0.875}Mn_{0.125}O. (a) With spin up. (b) With spin down.

3.1.2 States Density

The electron dispensation in an energy spectrum is defined via the DOS and could be evaluated in photoemission work. The whole DOS for O, In and In_{2}O_{3} were illustrated in Figure 6. It is demonstrated that the valance bands are formed significantly since the O-2p orbits and conductivity bands regarding In-5s and In-5p orbits. The most of 4d orbits for indium in the valence band were among –10 to –15 eV, there is also small contribution for 4d-orbits of indium in the valence band top. The great dispersion and s-kind specification in conduction band bottom show the high conductivity and mobility for this compound. There are relation among O-2p and In-4d orbitals near to the valance bandtop.

Figure 7 shows the total DOS spectrum for In_{1.5}Mn_{0.5}O_{3} and Mn in spin up and down states. In Figure 7(a), it could be observed that Mn-3d stages are revealed significantly at the valance band top and have a good overlap between Mn-3d and O-2p orbitals, while in Figure 7(b) the 3d states of Mn are located mostly at the conduction band bottom and tiny hybridization has among O-2p and Mn-3d.

Figure 6. Total density of states of O, In and In_{2}O_{3}.
In Figure 8, the total DOS spectrum are shown for O, Zn, ZnO as a function of energy between -20 – 15 eV. There were a huge amount of localized stages at the valance band top the originating significantly from the O-2p and Zn-3d orbitals. The valance band that is among -6 eV to 0 eV (Fermi energy), is made of the O-2p orbital hybridized via the Zn-3d orbital. The lower portion of valance band is made via O-2s orbital. The main contribution to the conduction band bottom is essentially made of Zn-4s.

The evaluated whole density of stages of $\text{Zn}_{0.875}\text{Mn}_{0.125}\text{O}$ and Mn in spin up and down states are shown in Figure 9, it can be seen that the Mn-3d orbital in spin up state is located in the valance band and powerful hybridization has with O-2p, while for spin down state of this compound, the 3d states of Mn are located at the of the conductivity band bottom.

4. Conclusion

Here, we were investigated the electronic characteristics of $\text{In}_2\text{O}_3$ and ZnO in undoped and doped with Mn states
Effect of Substituted Mn on Electronic Characteristics of Indium Oxide and Zinc Oxide via Density Functional Theory Studying utilizing the FP-LAPW approach via the GGA. The findings of obtained indicate that the energy gap for In$_2$O$_3$ and ZnO is changed by substitution of Mn element on In, Zn in In$_2$O$_3$ and ZnO, respectively. It can be seen that energy gap is different in the two up and down spins stages for doped In$_2$O$_3$ and doped ZnO. Therefore spin splitting effect explain different electrical properties for these compounds.

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6. References

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