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Theoretical investigation of structural, electronic and optical properties of Sc-doped SnO_2

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Abstract

In this study, the structural, and optoelectronic properties of $Sc_xSn_{1-x}O_2$ alloys with (x = 0, 0.0416, 0.0625 and 0.125) are investigated using the first principle method with a full-potential linearized augmented plane wave (FP-LAPW) as implemented in WIEN2k code, which is based on density functional theory (DFT). We used the generalized gradient approximation parameterized of Perdew-Burke and Ernzerhof (PBE-GGA) to calculate the structural properties, while the electronic and optical properties were determined using the Tran–Blahamodified Becke-Johnson (TB-mBJ) potential functional which gives improved band gaps compared to PBE-GGA.
The results reveal that by Sc-doping SnO_2 the band gaps broaden and remain direct at Γ. When substituting Sc-impurities, the Fermi level is displaced into the valence band due to the 3d-Sc orbital producing a p-type semiconductor. The optical response shows low absorption, reflectivity and the blue shifting of the optical transmittance in Sc-doped SnO_2 due to an increase in of the

band gap, according to the Burstein-Moss effect. Our results reveal that Sc-doped SnO_2 could be useful for transparent conducting applications.

Introduction

Transparent Conductor Oxide materials are a unique class that combine high electrical conductivity and optical transparency. TCOs have a potential applications in photovoltaic and optoelectronic devices [[1], [2], [3]], gas sensors [4], varistors [5], and catalytics [6]. The Tin Oxide SnO_2 crystallizes in a tetragonal rutile structure with space group no.136. $P4_2/mnm$ and it is expected experimentally to transform into a sequence of phases under pressure [7,8]. It is shown that the first transition appears at 11.8 GPa between the rutile structure and $CaCl_2$ (Pnnm) structure predicted by the theoretical study close to 11.6 GPa [9], the second transition at 12 GPa of the $CaCl_2$ (Pnnm) structure transforms to the α-$Pb0_2$ orthorhombic (pbca) structure. This second transition was calculated by Boujnah*et al.* [9] and has a value of 16.8 GPa SnO_2 undergoes a third transition to the Fluorite phase ($Fm\ 3^-\ m$) at approximately 21 GPa at ambient temperature, and the reported theoretical value of the cotunnite-type structure [9]is 68 GPa, which is larger than the observed value. SnO_2 has a direct wide band gap at room temperature experimentally and has a value of 3.6eV [10], and the good theoretical calculation using a hybrid functional(B3LYP), gave a band gap of approximately 3.5eV [11], which is higher than the limit visible light region with photon energy equal to 3.1eV, consequently the SnO_2 material has limited applications. We have many ways to modify the SnO_2 compound to become conductive, by intrinsic defects, or by applying strain pressure also by doping, in fact, adding dopant elements with a controller of carrier concentration in SnO_2 enhances the performance and shows some promise compared to the undoped SnO_2. Many works both experiments and theoretical studies have shown that the Transition-Metals (TM) dopant elements present different properties compared to pure SnO_2. It have been shown that pentavalent-ions (Ta, Nb, P, Sb and I) as doped, exhibit n-type conductivity, high charge carrier density and a widened optical bandgap [12]. The order of electrical conductivity increases with doping SnO_2 by Titanium (Ti) [13], by Antimony (Sb) and Fluorite (F) [14,15], while the conductivity deceases when doping SnO_2 by

Indium (In), Aluminium (Al) and Copper (Cu) [[16], [17], [18]]. The ferromagnetism properties of SnO_2 are approved by doping with Transition Metals (TM) elements: Cobalt (Co) [[19], [20], [21]], Vanadium (V) [22], Chrome (Cr) [23,24], Manganese (Mn) [25], Iron (Fe) [26,27] and Nickel (Ni) [[28], [29], [30]].
Yttrium (Y) and Scandium (Sc) have paid more attention especially for their exceptional properties. M. Boujnah et al. [31] reported that 3d transition metals (Sc, Ti and V) doped rutile SnO_2 display a new transparent conducting oxide with p-type semiconducting valuable for solar cells. Yttrium (Y) doped TiO_2 was found to be successful in improving photocatalytic activity and extending the absorption edge towards visible light [[32], [33], [34]]. In addition, 4d transition metals (Y, Ag, Cd, Nb, Mo) doped TiO_2 reduced the energy gap of rutile TiO_2, leading to the same redshift in the optical absorption edge [35] with photocalytic activity being evidently enhanced [34]. In previous studies, Y doped ZnO can enhanced the UV emission and decreased the deep level emission (DLE) band in the green range of ZnO [[36], [37], [38]], and doping with Y ions reduced the nonradioactive recombination centres and increased the possibility of the near band edge transition of ZnO. In the present work, Scandium ion is chosen because is suitable for incorporated into SnO_2, which leads to similar crystalline size of Sc^{3+}cation to Sn^{4+}, good dispersion and enhanced separation of electron-hole pairs [32].
The main purpose of this work is to study Scandium (Sc) doped SnO_2. The calculations are performed using Wien2k code based on the DFT formalism. The paper is organized as follows: After the present introduction, the computational method and details used in our work are given in section II. Section III shows our results and a discussion of the structural, electronic and optical properties of Sc doped SnO_2 have been given and discussed. We will conclude with a summary in section IV.

Section snippets

Computational details

First principle methods such as Density Functional Theory (DFT) [39,40] and Full-Potential Linearized Augmented Plane Wave) « FP-LAPW » [41] plus the generalized gradient (GGA) of the exchange potential of Perdew, Burke, and Ernzerhof (PBE) [42] and Tran–Blaha modified Becke–Johnson exchange potential approximations (TB-mBJ) [43] implemented in the WIEN2k code were used to calculate the structural, electronic and optical properties of $Sc_xSn_{1-x}O_2$ compounds at concentrations x = 0.0416, 0.0625

Structural properties

Tin oxide is crystallized with a tetragonal structure of rutile type with the space group $P4_2/mnm$ and lattice parameters a = b = 4.738 Å and c = 3.187 Å [46]. The conventional structure of SnO_2 has two types of Sn and O atoms, which are located in positions 2a: (1/2; 1/2; 1/2). (0; 0; 0) and 4f: (u; u; 0), (1-u; 1-u; 0), (1/2+u; 1/2-u; 1/2), (1/2-u; 1/2+u; 1/2), respectively, with *u* = 0.306 [47]. To study the effect of the Sc doping concentration (4.16%, 6.25% and 12.5%) of SnO_2, We have

Band structure

The study of the electronic properties of semiconductors provides valuable information about their potential applications in the fabrication of electronic and optoelectronic devices. The band structures of pure and Sc-doped SnO_2 at 4.16%, 6.25% and 12.5% r along the Γ-X-M-Γ-Z-R-A-Z path in Tetragonal Brillouin zone in the energy range of −10 eV–10 eV are shown in Fig. 4. Our calculations have been performed using the lattice parameter calculated in the previous section and based on the (GGA -

Optical properties

Optical properties are directly related to the crystal structure and topology of the band structure. The calculations of the optical properties of Sc doped SnO_2 with different concentrations at zero pressure and zero temperature are performed according to the FP-LAPW method using the TB-mBJ approximation. The linear response of materials can be described by the complex dielectric function $\varepsilon(\omega)$ of the system by Ref. [67]:$\varepsilon(\omega) = \varepsilon_1(\omega) + i\,\varepsilon_2(\omega)$
The evolution of the dielectric function $\varepsilon(\omega)$ is

Conclusion

In summary, the structural, and optoelectronic properties of $Sc_xSn_{1-x}O_2$ compounds with (x = 0%, 4.16%, 6.25% and 12.5%) have been investigated using FP-LAPW. The results reveal that Sc-doping of the SnO_2 lattice increased the lattice parameter. Additionally, the formation energy calculations reveal that the doped systems remain thermodynamically stable after doping. The band structure and density of states calculations show a Γ direct band gap for pure SnO_2. When substituting impurities, the

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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