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Original Research Article

Theoretical Investigation of Doping Effect of Fe for $SnWO_4$ in Electronic Structure and Optical Properties: DFT Based First Principle Study

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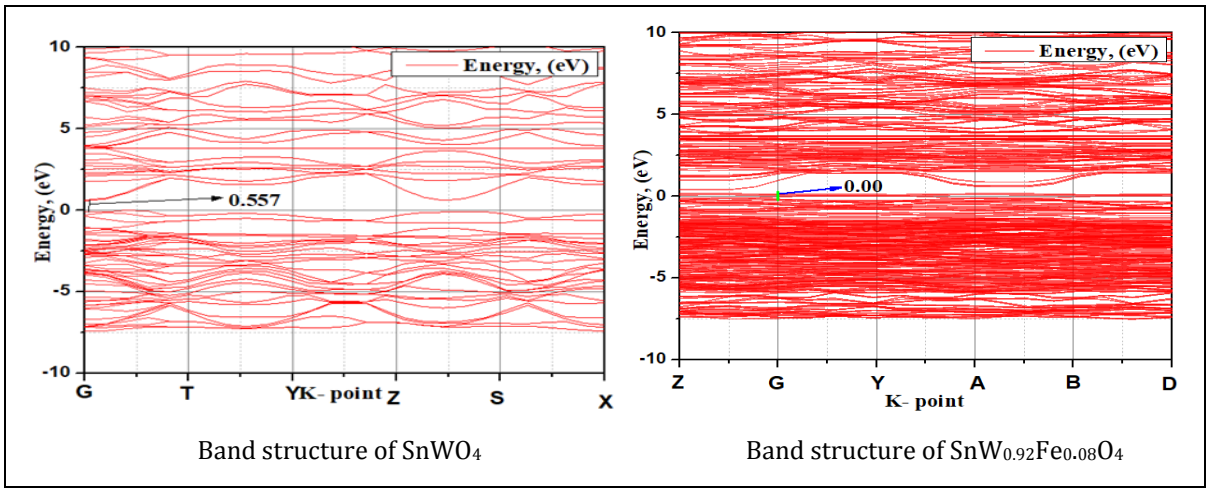
ABSTRACT

In this work, the electronic band structures, total density of state, partial density of state, and optical properties were investigated using the first principle method for $SnWO_4$ *via* generalized gradient approximation (GGA) based on the Perdew–Burke–Ernzerhof (PBE0). The estimated band gap was found to be 0.557 eV which is supported for good semiconductor. The density of states and partial density of the states were simulated for evaluating the nature of 5s, 4d 5p for Sn, 6s, 4f, 5d for W and 2s, 2p for O atom for $SnWO_4$. The optical properties for instance, conductivity, dielectric function, and the loss function were calculated. The main goal of this research study was to determine the Fe doping activity on the electronics structure and optical properties by 8%, and the band gap was recorded in 0.0 eV, showing as a superconductor. Regarding the optical properties, the loss function was decreased after doping.

GRAPHICAL ABSTRACT



Band structure of $SnWO_4$ Band structure of $SnW_{0.92}Fe_{0.08}O_4$

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Introduction

A familiar semiconductor is a compound or a solid materials which face some barrier to the flow of electricity *i.e.* their properties are almost like conductive or conducting materials [1,2]. Due to the semiconductor technology, over the last 60 years, continuous progress of semiconductor compound, the element of groups IV, II, VI, and III, V has been taken as of semiconducting compounds or crystals [3,4]. Moreover, semiconductors have been used in modern electronics technology such as mobiles, computers, laptops, and solar cells. Germanium silicon, carbon, selenium, and acid mixed water are the most commonly used semiconductors [5,6]. Besides germanium, silicon, bismuth, iron, and strontium are also widely used as semiconductor materials in present time in different advanced electronic device due to their great conductivity [7]. Moreover, the crystal of germanium, silicon, bismuth, iron, stronsium and antimony oxides has been established as semiconductor due to their thermal capacity. The main limitation of these crystal is the high forbidden energy gap despite of its outer cell having the same balance electrons [8]. To deteriorate this problem, doping technique has been employed at our present study.

M. Danet, reported that the tungstate oxide ($SnWO_4$) composites act as outstanding electrochemical properties and a promising anode material for lithium ion battery application [9]. Moreover, it has been used as gas sensors, catalysts or electro-chromic systems. The computational approaches were applied to determine the theoretical electronic structure, optical properties and Fe doping effect on $SnWO_4$.

On the other hand, the Sn and W metal based crystal has been estimated as good semiconductor and photocatalyst in the case of large range of absorption and doping can also enhance their activity [10,11]. To estimate this effect, Fe atom has been selected for their easily spread out and overlapping the valance band to conduction band as doping material [12-15].

Computational methods

The method of GGA with PBE0 was optimized of CASTEP code from the material studio 8.0 [16] was used to calculate the band structure, total density of state, and partial density of state. In this condition, the electronic band structure and density of state were calculated using the cut off at 489 eV, and k point at 4×4×2 with non-conserving pseudopotentials. Then the optical properties were simulated for calculation of conductivity, dielectric function and loss function in similar way. In addition, the geometric optimization was achieved, and the convergence criterion for the force between atoms was 3×10^{-6} eV/°A, the maximum displacement was 1×10^{-3}°A, and the total energy and the maximal stress were 1×10^{-5} eV/atom and 5×10^{-2} GPa, respectively.

Results and discussions

Optimized structure

The lattice parameters value are a = 5.062 Å, b = 5.630 Å and c = 12.057 Å while angels among them as α = 90.000A°, β = 90.000A° and γ = 90.000A°. The monoclinic $SnWO_4$ crystal and the space group is Hermanna Mauguin Pnna, orthorhombic crystal system, point group mmm, hall -P 2a 2bc, density 7.09 g/cm^3 are demonstrated in Figure 1a, and the Fe doped optimized structure is accounted in Figure 1b.

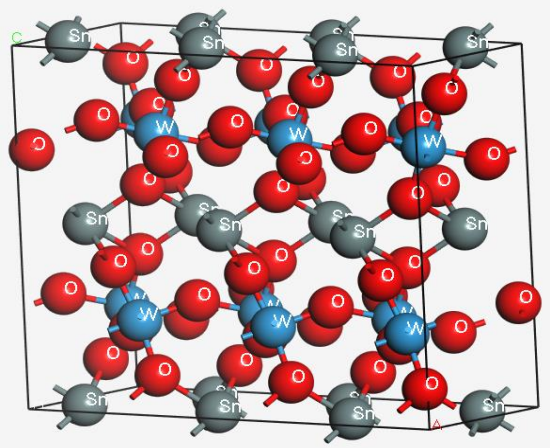


Figure 1a. Optimized structure of $SnWO_4$

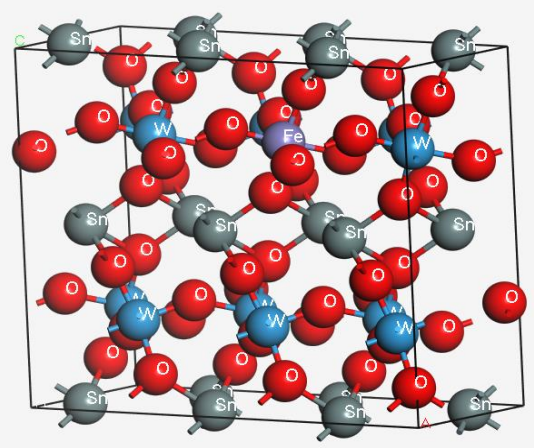


Figure 1b. Optimized structure of $SnW_{0.92}Fe_{0.08}O_4$

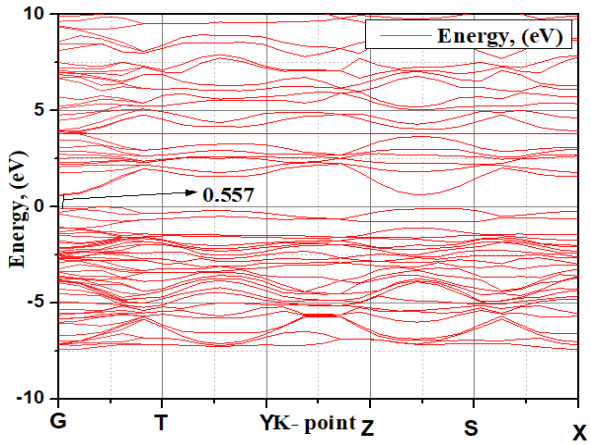


Figure 2a. Band structure of $SnWO_4$

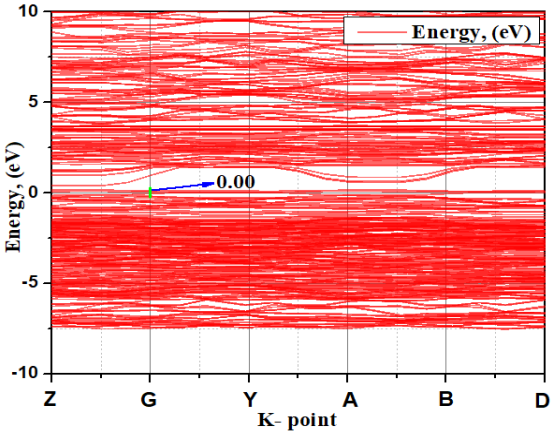


Figure 2b. Band structure of $SnW_{0.92}Fe_{0.08}O_4$

Electronic structure

To determine the electronic band structure of $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$, the Fermi energy level was set as zero. As seen in Figure 2a, and 2b, the minimum of conduction bands (MCB) was obtained in the G symmetry point, where as the maximum of valance bands (MVB) was also linked in G symmetry points. As both MCB and MVB are at point G symmetry, it is a called direct band gap, and it is calculated by 0.557 eV, and 0.00 eV for $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$, respectively. As can be seen in Figure 2a, both the upper and lower parts of the conduction band are well dispersive in the near Z, Y, S, and T symmetry points. Figure 2b reveals that, there are a lot of electronic band than Figure 2a which indicates the greater conductivity with deducing band gap.

Density of states and partial density of states

The density of the states indicates the nature of electronic band structures and the splitting of an orbital. PBEO calculated the density of total states (DOS) of Sn, W, Fe, and O elements for the $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$ crystals with GGA. Figure 3 shows that, the valence bands are mainly occupied by 5s, 4d 5p for Sn, 6s, 4f, 5d for W, 4s 3d and 4p for Fe and 2s 2p for O elements. Meanwhile, above the Fermi level, the conduction bands are composed of Sn in 5s,

4d 5p for Sn, 6s,4f, 5d for W, 4s 3d and 4p for Fe and 2s 2p for O elements orbital. As seen in Figure 3a, the total density of the state for the undoped $SnWO_4$ is lower than doped $SnW_{0.92}Fe_{0.08}O_4$. It is found that the DOS of s, p, d orbital and sum for $SnW_{0.92}Fe_{0.08}O_4$ is more delocalized than DOS of $SnWO_4$ showing in Figures 3a, 3b, 3c, 3d and 3e.

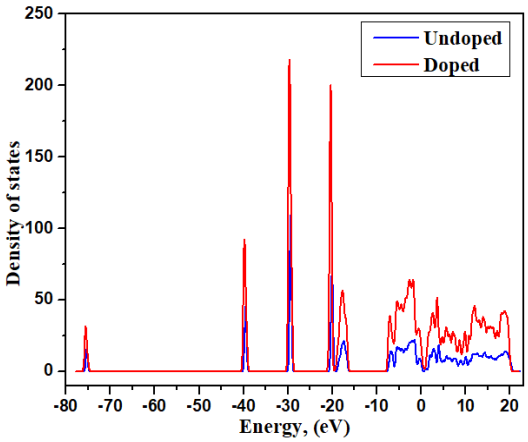


Figure 3a. Total density of States $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

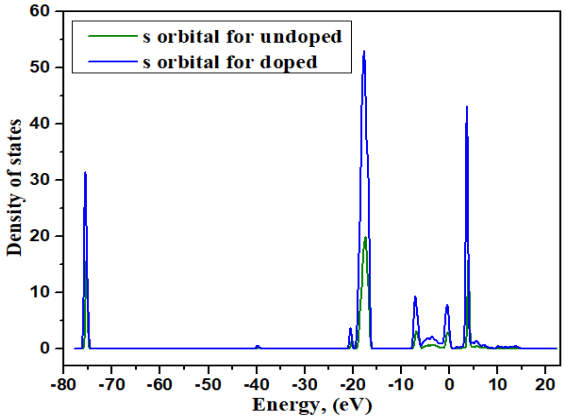


Figure 3b. Density of States of s orbital for $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

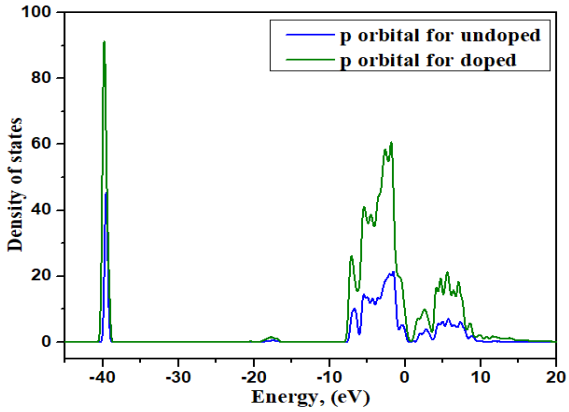


Figure 3c. Density of States of p orbital for $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

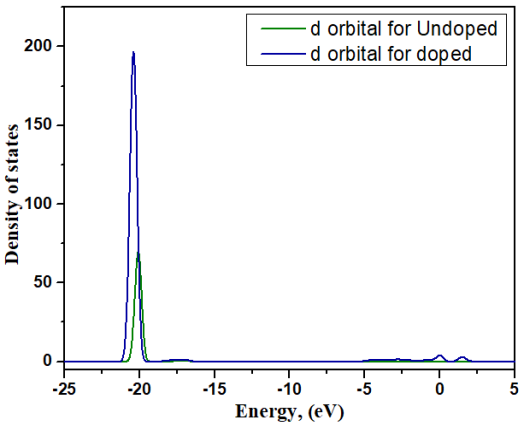
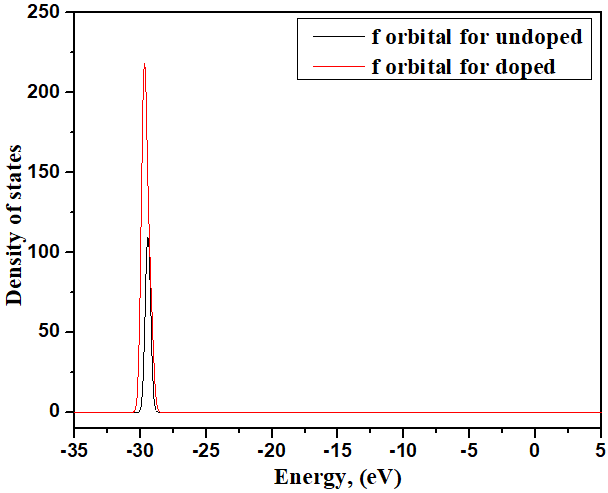


Figure 3d. Density of States of d orbital for $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

Figure 3e. Density of States of f orbital for $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$



Optical properties

Dielectric function

The dielectric function is an essential tool to investigate their optical properties, which is related to adsorption properties as the following equation for solid [17].

$$\varepsilon = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

Where ε_1 (ω) and ε_2 (ω) are denoted the dielectric constant (real part) and the dielectric loss factor (imaginary part) respectively. The dielectric function has a relationship with the space of materials that are physically equivalent to the permittivity or absolute permittivity. The real part of the dielectric function represents the energy storage capability in the electric field, and the imaginary part represents the energy dissipation capability of the dielectric materials. As seen in Figure 4, the imaginary part is less than the real part from 0 eV to 5 eV frequencies, but from 17 eV to 30 eV, the imaginary part and real part is overlapping, for the doped and undoped.

Loss function

There are two regions for electronic energy loss function such as high energy region and low energy region for the optical properties. The first region is the high loss energy region with change of frequency or spectra after the ionization edge which can say the oxidation state of d orbital splitting for metals of center atom in complex compounds, having range the more 20 eV. The other one is the low energy loss function, including the energy less than 1, which can provide information about the composition and electronic structure. The energy loss function for optical properties is linked to dielectric constant of the materials within the range of validity of the dielectric theory. As can be seen in Figure 5, the loss function for $SnW_{0.92}Fe_{0.08}O_4$ is about lower compared with that of the undoped.

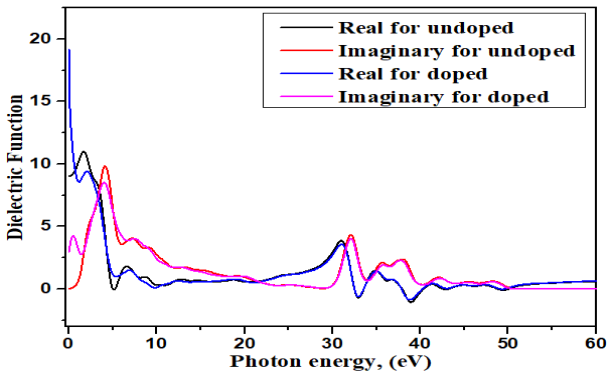


Figure 4. Calculated dielectric function of $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

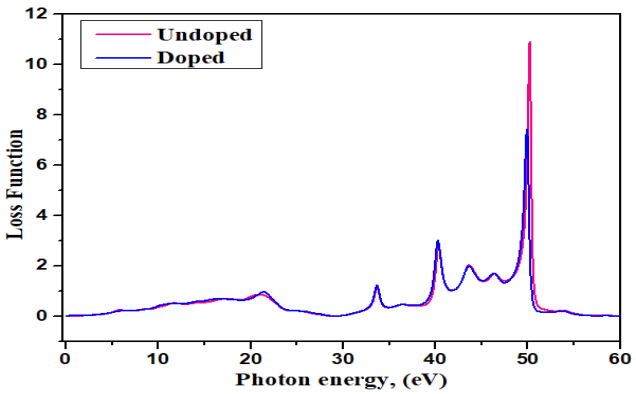


Figure 5. Calculated Loss function of $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$

Conclusion

This research study presents a theoretical investigation on the effect of Fe doped on electronic structure, by evaluating the optical properties of the $SnWO_4$ using first-principle computational tools regarding use as conductor. In pristine, and 8% doping in $SnWO_4$ crystals were simulated and made a comparative study on their structural and optical properties. From the band gap study, $SnWO_4$ and $SnW_{0.92}Fe_{0.08}O_4$ can be said as a good semiconductor and superconductor respectively, having band gap 0.557 eV, and 0.00 eV. The main finding of this study, Fe doping on $SnWO_4$ was recorded as reducing the band gap at 0.00 eV. It was observed that the imaginary part of the dielectric constant was less than the real part up to 5 eV frequencies; however, both the real and imaginary part overlapping from 17 eV to 30 eV for doped as well as undoped. In addition, the loss function was almost constant except at 50 eV energy where loss function decreased for the doped one.

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Disclosure statement

No potential conflict of interest was reported by the author.

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