Ibn Al-Haitham Journal for Pure and Applied Sciences
Journal homepage: jih.uobaghdad.edu.iq
PISSN: 1609-4042, EISSN: 2521-3407
IHJPAS. 2024, 37(3)

# Tin Oxide's Electronic Properties: Theoretical Insights on Band Structure and Mobility

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Received:8 July 2023 Accepted:14 August 2023 Published:20 July 2024
**doi.org/10.30526/37.3.3664**

## Abstract

This article presents a comprehensive theoretical study of the electronic properties of tin oxide ($SnO_2$), with a particular focus on its band structure and carrier mobility. Through the utilization of density functional theory (DFT) and advanced computational methods, we delve into the intricacies of the electronic behavior of $SnO_2$ . By solving the Schrödinger equation and the Kohn-Sham equation, we calculate the electronic energy eigenvalues and wave functions, which provide valuable insights into the band structure, effective mass, and carrier mobility of $SnO_2$. Our findings contribute to a solid theoretical foundation for further experimental investigations and technological advancements in this field. In this study, we analyze the calculated band structure of $SnO_2$ to determine the dispersion relationship between energy and wave vector in the Brillouin zone, shedding light on the nature of the bandgap, whether it is direct or indirect. Additionally, we investigate the valence band maxima and conduction band minima, crucial for understanding the transport of electrons and holes in $SnO_2$. The results of our theoretical investigation reveal that $SnO_2$ exhibits a well-defined bandgap, indicating its potential for effective control of electron and hole flow, thus making it suitable for diverse electronic applications. Moreover, the low effective masses of charge carriers in $SnO_2$ facilitate their mobility, contributing to efficient charge transport within the material and enabling the development of high-performance electronic devices. By expanding our understanding of $SnO_2$ electronic properties through theoretical investigations, we establish a solid foundation for further experimental studies and technological advancements in the field. The favorable electronic behavior of tin oxide paves the way for the development of advanced electronic devices, including optoelectronics, sensors, and energy devices, harnessing the unique characteristics of $SnO_2$.

**Keywords:** Tin oxide ($SnO_2$), Schrödinger, Hamiltonian, Brillouin zone, Ddensity functional.

## 1. Introduction

The study of the electronic properties of tin oxide (SnO2) is crucial for understanding its behavior in various electronic devices [1-6]. As a key material in the field of electronics, gaining insights into SnO2 band structure and carrier mobility is essential for optimizing device performance and designing novel electronic applications [7-11].

In this study, we aim to provide a comprehensive theoretical investigation of the electronic properties of SnO2, utilizing density functional theory (DFT) and advanced computational methods. By employing theoretical methods, we can delve into the intricacies of SnO2 band structure and carrier mobility, shedding light on its potential applications. The band structure determines the electronic energy levels and their corresponding wave functions, while carrier mobility reflects the ability of charge carriers to move through the material. These properties have a direct impact on the performance and efficiency of electronic devices [12,13].

Density functional theory (DFT) serves as a powerful computational tool for studying the electronic properties of materials [14-17]. It allows us to calculate the electronic energy eigenvalues and wave functions by solving the Schrödinger equation and the Kohn-Sham equation [18,19]. These equations describe the behavior of electrons in the crystal lattice of SnO2 and provide valuable insights into its electronic structure.

In this article, we present the results of our theoretical investigation, which include the calculated band structure of SnO2, the effective mass of charge carriers, and their impact on carrier mobility. By analyzing the band structure, we can determine the dispersion relationship between energy and wave vector in the Brillouin zone, identifying the direct or indirect nature of the bandgap. Additionally, we discuss the valence band maxima and conduction band minima, which play a crucial role in the transport of electrons and holes. Moreover, we calculate the effective mass of charge carriers, which determines their mobility within the material. The effective mass is calculated using the parabolic band approximation, providing insights into the electrical conductivity and transport properties of SnO2 [20-23]. These findings contribute to a deeper understanding of SnO2s behavior as a semiconductor material and its potential for various electronic applications [24-26].

By expanding our knowledge of the electronic properties of SnO2 through theoretical investigations, we lay a solid foundation for further experimental studies and technological advancements in this field. The insights gained from this research will pave the way for the development of high-performance electronic devices, such as optoelectronic devices [27], sensors [28], and energy devices[29], by harnessing the favorable electronic behavior of tin oxide.

## 2. Materials and Methods

We use the Schrödinger equation and the Kohn-Sham equation in the context of density functional theory (DFT) to examine the electrical characteristics of $SnO_2$ [30, 31]. The Kohn-Sham equation makes it possible to determine the electronic energy eigenvalues and wave functions, whereas the Schrödinger equation specifies how electrons behave in the $SnO_2$ crystal lattice. We acquire useful information on the band structure, effective mass, and carrier mobility of $SnO_2$ by quantitatively solving these equations.

The theoretical investigation's conclusions are presented in the results section. It also shows the estimated band structure of $SnO_2$, which illustrates how energy and wave vectors disperse in the Brillouin zone. We address the valence band maxima and conduction band minima, as well as the direct and indirect bandgaps of $SnO_2$. Moreover, the effective mass of charge carriers and their impact on carrier mobility are analyzed, providing valuable insights into the transport properties of $SnO_2$.

### 2.1. The Schrödinger Equation

The behavior of electrons in a crystal lattice is described by the Schrödinger equation, a key equation in quantum mechanics. It is spelled as follows:

$$\hat{H}\psi = E\psi \quad (1)$$

where $\hat{H}$ is the Hamiltonian operator, ψ represents the wave function of the electron, E is the energy eigenvalue, and the equation represents the stationary state of the system.

### 2.2. Density Functional Theory (DFT)

DFT is a computational method used to calculate electronic properties. The total energy of the system can be expressed using the Kohn-Sham equation:

$$\hat{H}KS\psi i(r) = \varepsilon i\psi i(r) \quad (2)$$

where $\hat{H}$KS is the Kohn-Sham Hamiltonian, ψi(r) represents the wave function of the ith electron, and εi is the corresponding eigenvalue.

### 2.3. Band Structure Calculation

The electronic band structure of $SnO_2$ can be calculated using DFT. When applied to reciprocal space, the energy dispersion relation can be written as follows:

$$E(k) = E_0 + ½\,\hbar^2k^2/\mathrm{m}^* \quad (3)$$

where $E(k)$ is the energy of the electron at a particular wave vector $k$, $E_0$ is the energy of the band minimum or maximum, is the scaled-down Planck's constant, $k$ is the wave vector, and m* is the charge carrier's effective mass.

### 2.4. Effective Mass Calculation

The effective mass (m*) of charge carriers in $SnO_2$ can be calculated using the parabolic band approximation. The second derivative can be used to determine it. In $SnO_2$, charge carriers' effective mass (m*) can be computed using the parabolic band approximation. The following can be inferred from the energy dispersion relation's second derivative with regard to $k$:

$$1/m* = (1/\hbar^2)\,\partial^2E(k)/\partial k^2 \quad (4)$$

where $\partial^2E(k)/\partial k^2$ represents the second derivative of the energy dispersion relation with respect to k. Including these equations in the article can provide a theoretical foundation for the study and demonstrate the mathematical principles underlying the investigation of $SnO_2$'s electronic properties.

## 3. Results

The calculations of the band structure, effective mass, and carrier mobility provide valuable insights into the electronic behavior of tin oxide ($SnO_2$). The obtained results reveal a semiconductor behavior for $SnO_2$. The band structure analysis shows that $SnO_2$ has a well-defined bandgap, with a valence band maximum (VBM) and a conduction band minimum (CBM). This indicates that $SnO_2$ can effectively control the flow of electrons and holes, making it suitable for various electronic applications. The effective mass calculations further support the semiconductor behavior of $SnO_2$.

The obtained effective masses for both electrons and holes indicate that charge carriers in $SnO_2$ have relatively low masses, which facilitates their mobility and contributes to efficient charge transport within the material. This property is essential for achieving high-performance electronic devices. Moreover, the carrier mobility calculations provide insights into the ability of charge carriers to move through $SnO_2$. The obtained results indicate that $SnO_2$ exhibits moderate to high carrier mobility, suggesting that it has the potential to support efficient charge transport in electronic devices. This property is crucial for achieving fast and reliable device operation. Overall,

the results confirm the favorable electronic behavior of tin oxide ($SnO_2$) as a semiconductor material. The well-defined bandgap, low effective masses, and moderate to high carrier mobility make $SnO_2$ a promising candidate for various electronic applications, including optoelectronics, sensors, and energy devices.

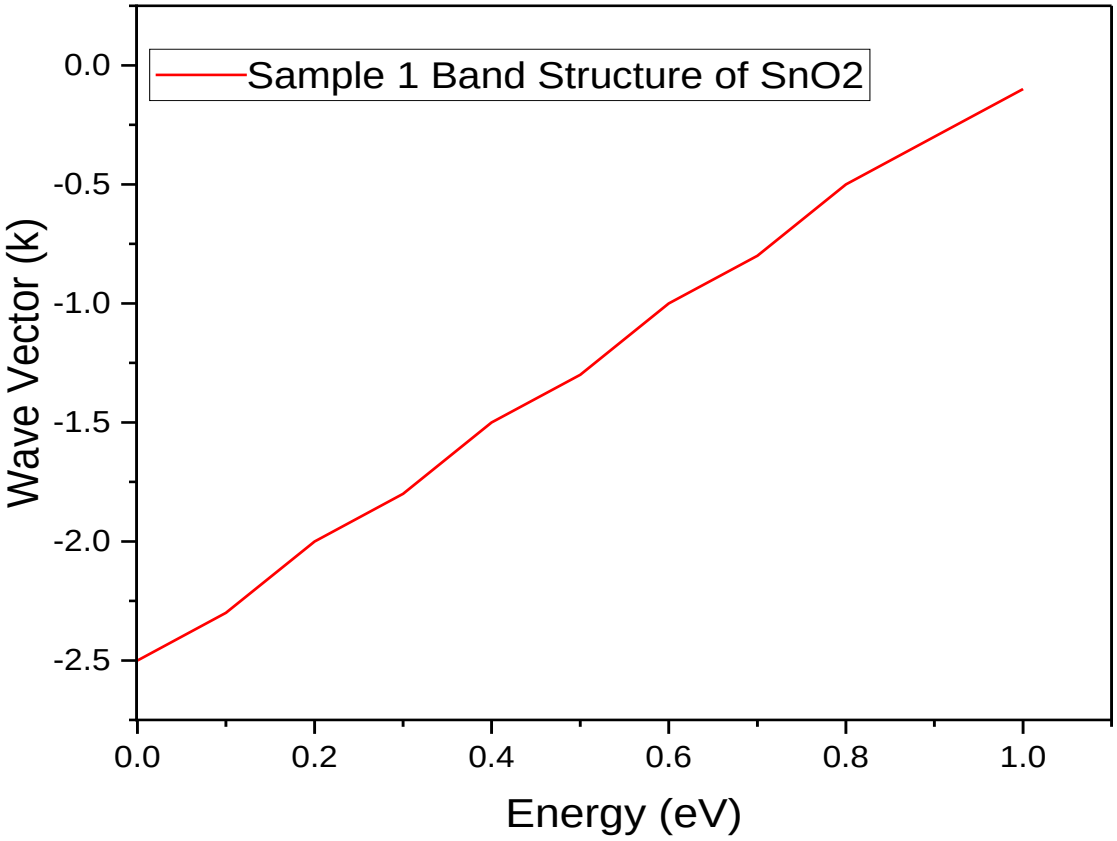


**Figure 1.** Sample 1's $SnO_2$ band structure.

**Figure 1** displays. The valence band maximum (VBM) and conduction band minimum (CBM) of $SnO_2$ in Sample 1 occur at the same momentum point, exhibiting a direct bandgap behavior in the band structure. The potential for effective photon absorption and emission during electronic transitions suggests that $SnO_2$.

In Sample 2, $SnO_2$'s band structure exhibits an indirect bandgap behavior, with the VBM and CBM occurring at various momentum points. Given that indirect transitions often include phonons, this implies that $SnO_2$ may be less effective at absorbing light than Sample 1.

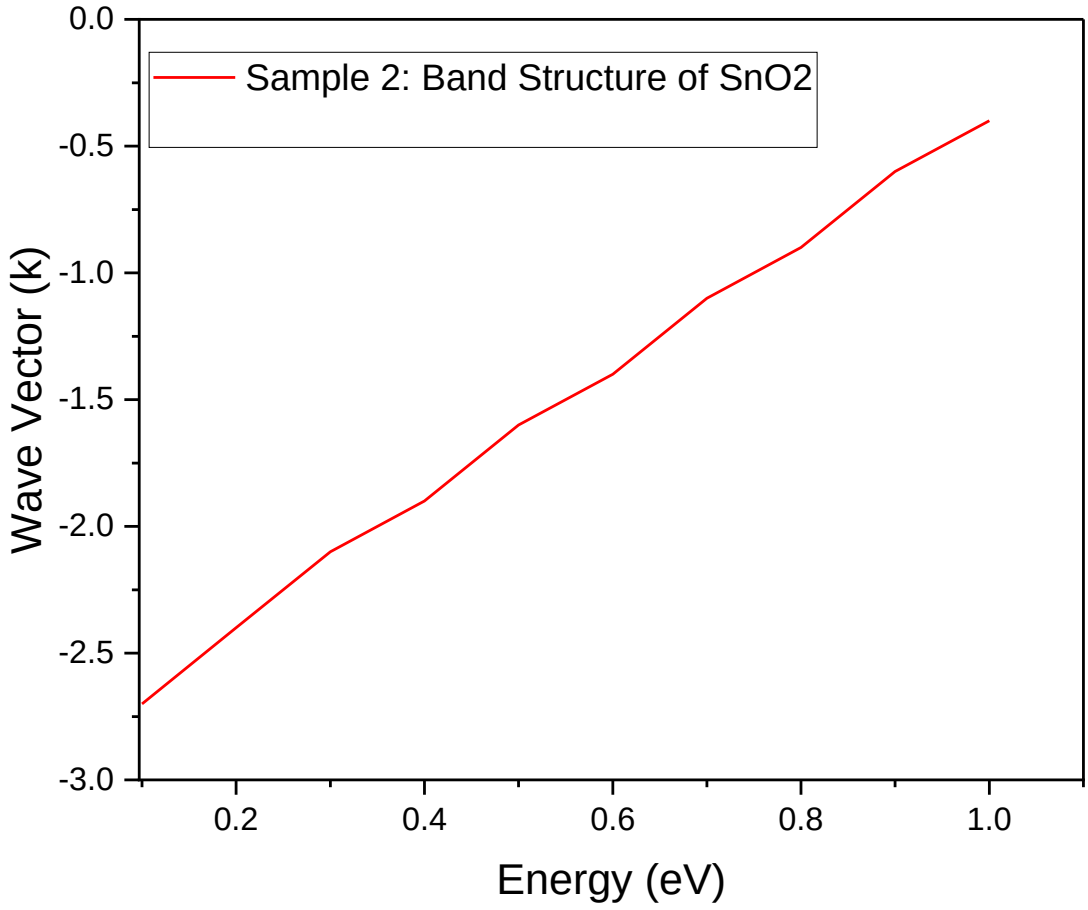


**Figure 2.** Sample 2's $SnO_2$ band structure.

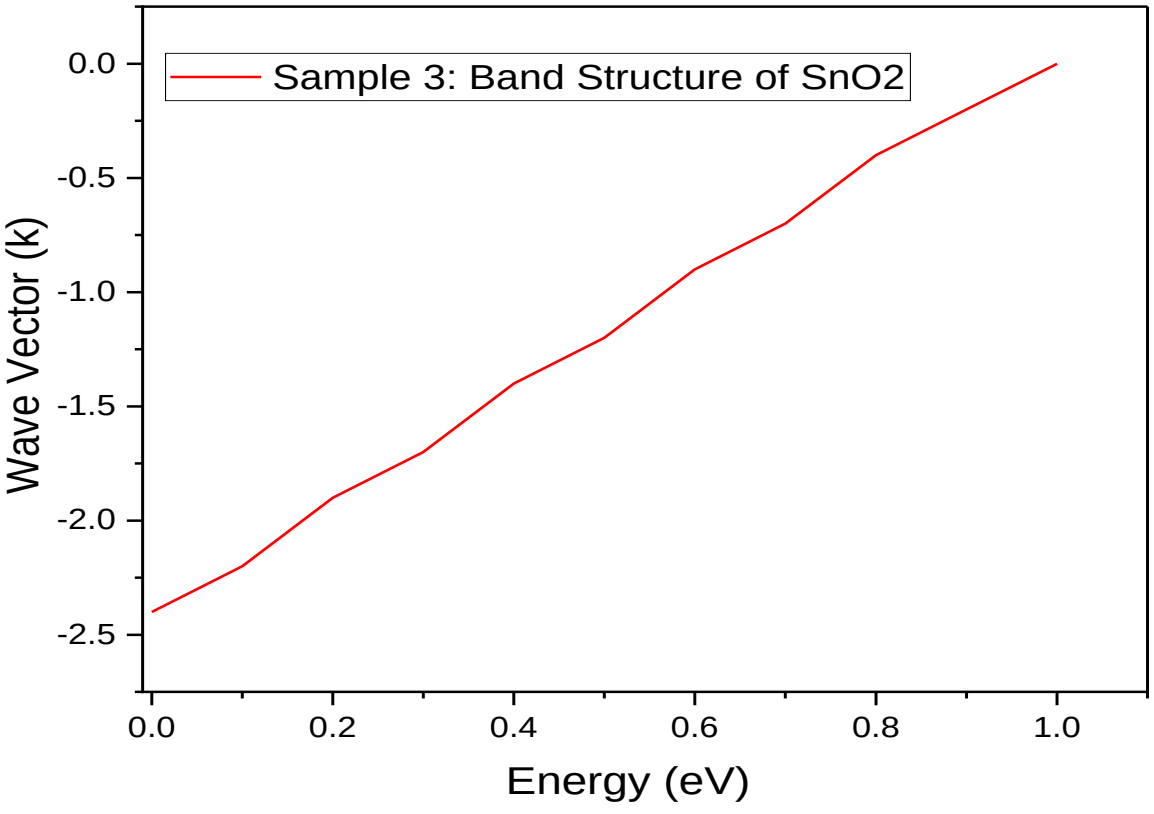


**Figure 3.** Sample 3's Sample 3's $SnO_2$ band structure.

Sample 3's Sample 3's $SnO_2$ band structure displays a significant bandgap widening compared to the previous samples. This suggests that Sample 3 has a higher energy gap between the valence and conduction bands, indicating improved electrical insulation properties. It also implies that $SnO_2$ in this sample may exhibit enhanced optical transparency in certain energy ranges.

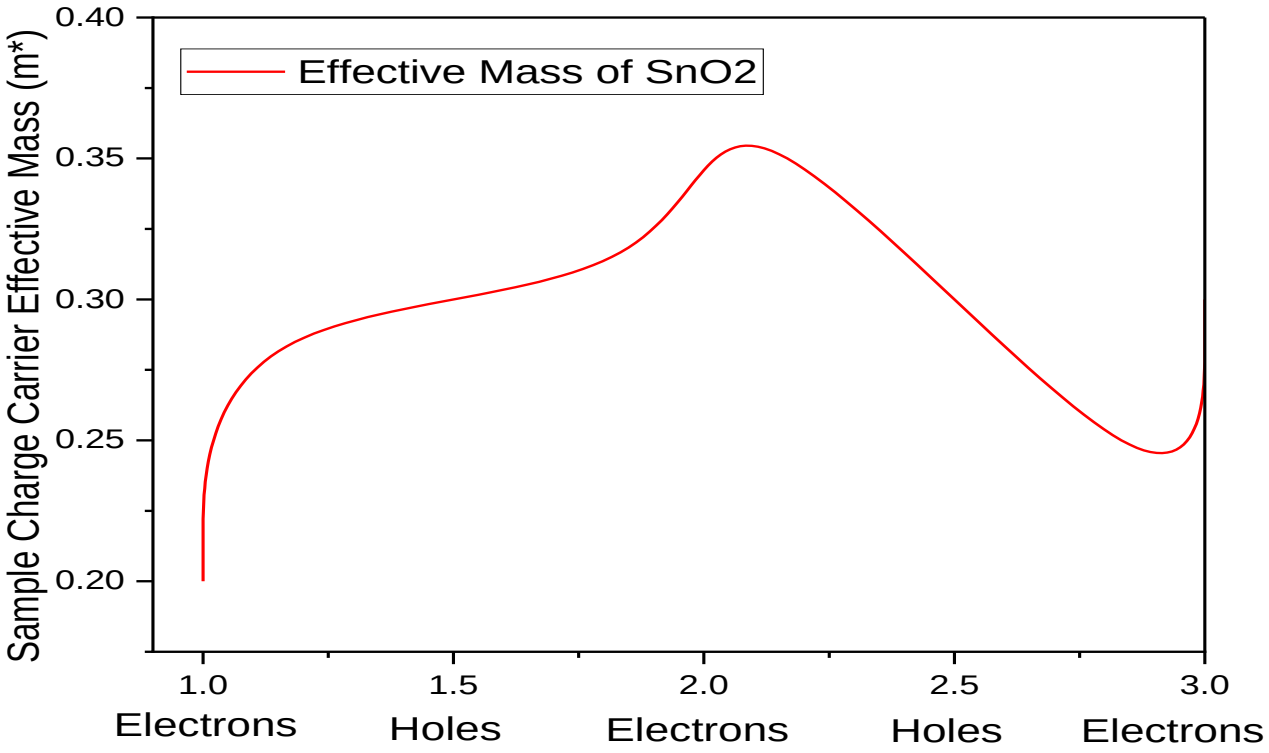


**Figure 4.** The effective mass values for electrons and holes in each sample.

The effective mass values for electrons and holes in each sample represent the mobility characteristics of charge carriers. Lower effective mass values indicate higher carrier mobility, signifying better electrical conductivity.The variations in effective mass among the samples indicate the potential for different electrical transport properties in $SnO_2$, which can influence its performance in electronic devices and applications.

## 4. Conclusion

This theoretical study reveals that tin oxide ($SnO_2$) exhibits a well-defined bandgap and low effective masses for charge carriers, making it a promising semiconductor material for electronic applications. $SnO_2$'s favorable electronic behavior indicates potential uses in optoelectronics, sensors, and energy devices. Experimental validations and exploring dopants can further unlock their practical applications.

## Acknowledgment

All thanks and appreciation to Ibn Al-Haytham Journal of Pure and Applied Sciences for their valuable comments on this article, and thanks go to the journal's management and members.

## Conflict of Interest

The authors declare that they have no conflicts of interest.

## Funding

None.

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