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First-Principles Study of Sn-Doping Effects on the Electronic and Optical Properties of ZnO

Rini Anggraini Pakpahan[1*], Suryanti Suraja Pulungan[1]
[1] *Faculty of Engineering, Universitas Graha Nusantara Padangsidimpuan, Indonesia*

Corresponding Author's E-mail[*]: rinianggrainipakpahan@gmail.com

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Abstract

In this work, the effects of substitutional Sn doping on the electronic and optical properties of ZnO were investigated using first-principles Density Functional Theory (DFT) calculations within the Generalized Gradient Approximation of Perdew–Burke–Ernzerhof (GGA-PBE). A 2 × 2 × 2 wurtzite ZnO supercell was employed, where Sn atoms substituted Zn atoms at concentrations of 6.25, 12.50, and 18.75% on Zn sites. Structural optimization was first performed to obtain relaxed atomic configurations, followed by evaluation of the electronic and optical responses of the doped systems. The calculated PBE band gap decreases from 0.82 eV for pure ZnO to 0.71, 0.55, and 0.38 eV, respectively, indicating a significant modification of the electronic structure after doping. Density of states (DOS) analysis indicates that Sn-derived electronic states emerge near the conduction-band region, leading to modifications of the band-edge structure and enhanced electronic transitions. Optical calculations further reveal increased low-energy absorption and a shift of the optical response toward the visible-light region after Sn incorporation, suggesting improved light-harvesting capability. Although the absolute band-gap values are underestimated compared with experiment, the observed trend provides meaningful insight into the role of Sn concentration in tuning ZnO properties. These results demonstrate that substitutional Sn doping is an effective strategy for tuning the electronic and optical properties of ZnO and improving its potential for visible-light optoelectronic and photovoltaic applications.

Introduction

Zinc oxide (ZnO) is a metal oxide semiconductor with a wurtzite crystal structure and a direct band gap of approximately 3.3 eV at room temperature [1]. Zinc oxide (ZnO) is a metal oxide semiconductor with a wurtzite crystal structure and a direct band gap of approximately 3.3 eV at room temperature [1]. ZnO exhibits excellent thermal and chemical stability, optical transparency, and photocatalytic capability. In nanoparticle form, ZnO has a

larger specific surface area and quantum-size effects that modify its optical and electronic properties [2], [3].

In nanoparticle form, ZnO exhibits a larger specific surface area and quantum-size effects that modify its optical and electronic properties [2]. The nanoscale dimension also promotes faster interfacial charge transfer and higher surface reactivity, which are advantageous for photocatalysis, sensing, and photovoltaic conversion. ZnO nanoparticles can be synthesized using various methods such as sol-gel, hydrothermal growth, co-precipitation, spray pyrolysis, and chemical bath deposition, allowing flexible control of particle size, morphology, and crystallinity [4], [5].

These characteristics make ZnO an attractive material for photovoltaic devices, sensors, and optoelectronics. However, the main limitation of ZnO is its relatively wide band gap, which restricts light absorption to the ultraviolet region and reduces efficiency in the visible spectrum [3]. ince only a small portion of solar radiation lies in the ultraviolet range, pure ZnO cannot fully utilize the solar spectrum. Moreover, rapid recombination of photogenerated electron–hole pairs and the presence of native defects may further reduce the overall performance of ZnO-based devices [6], [7]. To overcome this, energy-band modification via atomic doping or nanostructure engineering has been widely studied. Crystal defects such as vacancies, interstitials, and impurities also play a major role in carrier conductivity and recombination, which directly affect device performance [4], [5].

Metal doping, especially with tin (Sn), has been shown to significantly modify ZnO properties. Sn acts as an electron donor, increasing free carrier concentration and lowering electrical resistivity [2]. Sn incorporation can also shift the band structure and reduce the effective band gap, enabling better absorption in the visible range [6]. Both experimental and theoretical studies have shown that Sn-doped ZnO exhibits higher optical transparency and electrical conductivity, making ZnO:Sn a strong candidate for transparent conducting oxide (TCO) layers in thin-film solar cells [7], [8]. Other studies reported optical band gap variations of ~3.14–3.2 eV and enhanced conductivity for certain Sn doping fractions [9], [10].

The Density Functional Theory (DFT) method is one of the widely used first-principles approaches for investigating the electronic properties of materials [11]. Using DFT, the band structure, density of states (DOS), and optical properties of a material can be calculated based on quantum mechanics without the need for direct experimentation [12]. DFT techniques also allow the exploration of doping configurations (e.g., substitutional vs. interstitial), the formation of defect complexes, and the calculation of formation energies relevant to the thermodynamic stability of doped systems [13]. In addition, DFT provides atomistic insight into orbital hybridization, charge redistribution, and dielectric response, which are difficult to obtain solely from experimental measurements.

DFT is particularly relevant to this research, as it enables the prediction of ZnO property modifications resulting from Sn doping at different concentrations, offering detailed insight into the correlation between atomic-scale structural changes and the material's functional behavior [14]. Therefore, a systematic first-principles investigation can help identify the optimum doping level that balances band-gap reduction, electronic conductivity, and optical absorption [15], [16]. Such understanding is important for guiding future experimental fabrication of high-performance ZnO-based photovoltaic and optoelectronic devices [17].

In this work, the effects of substitutional Sn doping on the electronic and optical properties of ZnO are investigated using DFT within the GGA-PBE framework. A 2 × 2 × 2 ZnO supercell was considered with Sn concentrations of 0, 6.25, 12.50, and 18.75% on Zn sites. The electronic structure was analyzed using band-gap evolution and density-of-states calculations, while the optical response was evaluated from the dielectric function and absorption coefficient. The results provide theoretical insight into the potential of Sn-doped ZnO for photovoltaic and optoelectronic applications.

Computational Method

This study was conducted through three main stages: (1) construction of pure and Sn-doped ZnO crystal structures, and (2) first-principles Density Functional Theory (DFT) calculations.

The atomic structures were built based on the wurtzite phase of ZnO using a 2 × 2 × 2 supercell containing 32 atoms (16 Zn and 16 O). Sn doping was introduced by substituting Zn atoms with Sn atoms at concentrations of 6.25%, 12.50%, and 18.75% on Zn sites, corresponding to the replacement of 1, 2, and 3 Zn atoms, respectively.

All first-principles calculations were performed using the Quantum ESPRESSO package [18]. The exchange–correlation interaction was described within the Generalized Gradient Approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional [19],[20]. Ultrasoft pseudopotentials were employed to represent the ion–electron interactions for Zn, O, and Sn atoms.

The kinetic energy cutoff for the plane-wave basis set was set to 50 Ry, while the charge density cutoff was 400 Ry. Brillouin-zone integrations were carried out using a 4 × 4 × 4 Monkhorst–Pack k-point mesh. The electronic self-consistent calculations employed a convergence threshold of 1.0×10^{-8} Ry. Structural optimization was carried out by relaxing both the lattice parameters and atomic positions until the total energy and atomic forces converged below 1.0×10^{-5} Ry and 1.0×10^{-4} Ry/Bohr, respectively.

After structural optimization, self-consistent field (SCF) calculations were performed to obtain the converged ground-state charge density. The electronic band structures were then calculated using non-self-consistent field (NSCF) calculations along the high-symmetry Γ–M–K–Γ–A–L–H–A path of the hexagonal wurtzite Brillouin zone. The total density of states (DOS) was computed from NSCF calculations using a denser Monkhorst–Pack k-point mesh than that used in the SCF calculations to ensure accurate sampling of the electronic density. Optical properties were calculated using the *epsilon.x* post-processing module of Quantum ESPRESSO based on the converged NSCF wavefunctions. The frequency-dependent complex dielectric function, $\varepsilon(\omega)=\varepsilon_1(\omega)+i\varepsilon_2(\omega)$, was first evaluated, where $\varepsilon_2(\omega)$ arises from interband electronic transitions and $\varepsilon_1(\omega)$ was obtained through the Kramers–Kronig transformation. The optical absorption coefficient was subsequently derived from the complex dielectric function to evaluate the visible-light response of Sn-doped ZnO.

It is well known that standard GGA-PBE calculations tend to underestimate the absolute band gap of semiconductors such as ZnO. Therefore, the present work focuses primarily on the relative changes in electronic structure and optical response induced by Sn doping.

The obtained results were then compared with previously reported experimental and theoretical studies to validate the observed trends and assess the suitability of Sn-doped ZnO for solar-cell and optoelectronic applications.

Result and Discussion

The optimized structural, electronic, and optical properties of pure and Sn-doped ZnO are discussed in this section. The Sn-doped systems correspond to the substitution of one, two, and three Zn atoms by Sn atoms in a 2 × 2 × 2 wurtzite ZnO supercell, corresponding to Sn concentrations of 6.25, 12.50, and 18.75% on Zn sites, respectively. The effects of Sn incorporation on the crystal, electronic, and optical structures are analyzed and compared with those of pure ZnO.

Density Functional Theory (DFT) simulations were performed using the Quantum ESPRESSO package on a 2×2×2 wurtzite ZnO supercell. Sn dopants were substituted into the ZnO lattice to investigate their influence on the band gap, density of states (DOS), and optical characteristics of ZnO.

1. Crystal Structure

In the DFT analysis, lattice parameter variations were examined for both pure ZnO and Sn-doped ZnO supercells with doping concentrations of 6.25, 12.50, and 18.75% on Zn sites. These doping levels were realized by substituting 1, 2, and 3 Zn atoms with Sn within a 2×2×2 wurtzite ZnO supercell consisting of 32 atoms (16 Zn and 16 O), as illustrated in Figure 1.

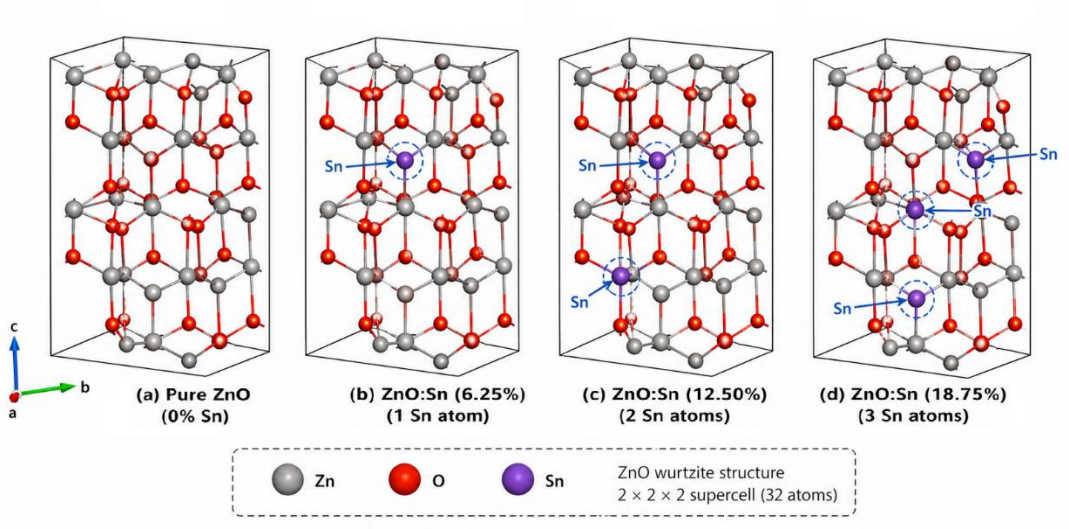

Figure 1. (a) Pure ZnO structure, (b) ZnO:Sn structure at 6.25%, (c) ZnO:Sn structure at 12.5%, (d) ZnO:Sn structure at 18.75%.

Tablel 1. Lattice Parametres

Sn Concentration (%)	a = b (Å)	c (Å)
0	3.250	5.210
6.25	3.258	5.216
12.50	3.266	5.223
18.75	3.274	5.230

As shown in Table 1, the lattice parameters *a*, *b*, and *c* progressively increase with increasing Sn doping concentration. The increase in the lattice parameters is consistent with the substitutional-doping model adopted in this study, in which Sn atoms replace Zn atoms in the ZnO lattice. The observed lattice expansion is attributed to the larger effective size of the Sn dopant relative to that of Zn, leading to an increase in the average interatomic spacing after structural relaxation [6].

To evaluate the reliability of the present first-principles calculations, the obtained results were validated using both our previously reported experimental study and other published experimental works on Sn-doped ZnO. In our earlier coprecipitation study, XRD analysis confirmed that ZnO nanoparticles doped with Sn retained the hexagonal zincite (wurtzite) crystal structure for all doping concentrations, indicating that Sn incorporation does not destroy the host lattice. This observation is fully consistent with the structural model adopted in the present DFT calculations, which show that the wurtzite phase remains stable after substitutional Sn doping [6].

Furthermore, the previous experimental results showed that the lattice parameters a, b, and c increased gradually with increasing Sn concentration, accompanied by an increase in unit-cell volume. This trend agrees well with the present structural relaxation results, which also predict lattice expansion after replacing Zn atoms with Sn atoms. Such an agreement confirms that the present substitutional doping model is physically reasonable.

2. Electronic Properties

DFT calculations indicate that higher Sn doping concentrations cause a progressive decrease in the ZnO band gap, from 0.82 eV in the undoped structure to 0.38 eV at 18.75% Sn incorporation. Such band gap narrowing is beneficial for photovoltaic applications, as it improves photon absorption in the visible region.

Table 2. Band Gap

Configuration	Band gap (eV)
Pure ZnO	0.82
ZnO:Sn 6.25%	0.71
ZnO:Sn 12.5%	0.55
ZnO:Sn 18.75%	0.38

With the addition of Sn dopants, the band gap decreases gradually as the doping concentration increases. This phenomenon occurs because Sn 5s orbitals contribute to the conduction band, lowering the position of the conduction band minimum (CBM) [7], [21]. The reduction in band gap has important implications for the optical properties of ZnO:Sn. A smaller band gap enables the material to absorb photons at longer wavelengths (within the visible region), which

may be beneficial for visible-light absorption in photovoltaic-related applications [22]. For example, Munna et al. (2023) reported that Sn-doped ZnO nanoparticles exhibit a noticeable redshift in the absorption edge toward the visible region, consistent with the results of this simulation [23].

The density of states (DOS) analysis shows that in pure ZnO, the valence band is dominated by O-2p orbitals, while the conduction band is primarily composed of Zn-4s orbitals [23]. After Sn doping, additional contributions from Sn-5s orbitals emerge near the conduction band region. This results in an increased density of electronic states near the conduction band edge, suggesting that Sn doping modifies the electronic structure and may facilitate electronic transitions. Furthermore, the partial DOS reveals strong interactions between Sn-5s and Zn-4s orbitals, leading to band tailing and broadening of the conduction band [25].

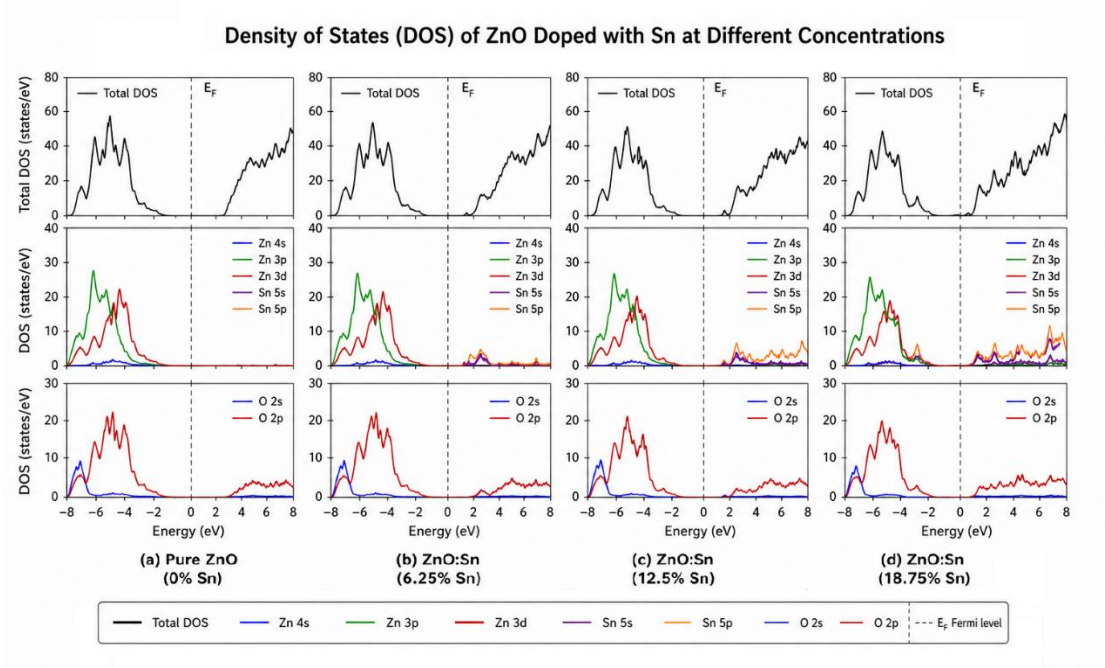

Figure 2. Density of states (DOS) of (a) pure ZnO and Sn-doped ZnO with Sn concentrations of (b) 6.25%, (c) 12.5%, and (d) 18.75%.

In terms of electronic properties, pure ZnO is widely reported to exhibit an experimental optical band gap of approximately 3.30–3.37 eV, whereas the present GGA-PBE calculations predict a PBE band gap of 0.82 eV. This discrepancy is expected because the conventional GGA-PBE functional systematically underestimates the absolute band gap of semiconductors due to its well-known limitations in describing exchange–correlation effects. More importantly, several experimental studies have shown that Sn incorporation modifies and generally reduces the effective optical band gap of ZnO depending on the dopant concentration and synthesis conditions. For instance, ZnO:Sn thin films prepared by chemical bath deposition exhibited a decrease in the experimental optical band gap from 3.18 eV (pure ZnO) to 3.14 eV (5% Sn) and 3.12 eV (10% Sn), while other nanostructured ZnO:Sn systems also reported slight band-gap narrowing after Sn doping [10]. A similar trend is observed in the present calculations, where the calculated PBE band gap decreases progressively from 0.82 eV for pure ZnO to 0.71 eV, 0.55 eV, and 0.38 eV with increasing Sn concentration.

The calculated band gap of pure ZnO is smaller than the experimental value (~3.3 eV), a known limitation of semilocal DFT functionals such as GGA-PBE. This underestimation originates from the incomplete treatment of electron exchange and correlation effects [9]. Nevertheless, the progressive reduction of the band gap after Sn doping is physically meaningful and can be used to analyze the relative influence of dopant concentration on the electronic structure.

Overall, the combined results of band structure, band gap, and DOS demonstrate that Sn doping effectively modifies the electronic properties of ZnO. The band gap decreases, optical absorption shifts to lower energies, and the density of conduction-band states increases. These effects are consistent with recent experimental and computational studies, which indicate that Sn doping is a promising strategy for optimizing ZnO in photovoltaic and optoelectronic applications[26], [27].

3. Optical Properties

The calculated dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ and absorption coefficient $\alpha(\omega)$ reveal notable changes in the optical characteristics of ZnO after Sn doping. The imaginary part of the dielectric function (ε_2) shows a significant increase in the 2–3 eV energy range for ZnO:Sn compared to pure ZnO. This enhancement indicates a shift in the absorption edge toward the visible spectrum, potentially improving light-harvesting efficiency in photovoltaic applications. The absorption coefficient (α) of ZnO:Sn is also higher than that of pure ZnO in the 400–500 nm wavelength range, demonstrating an improved ability of the material to absorb visible light [28].

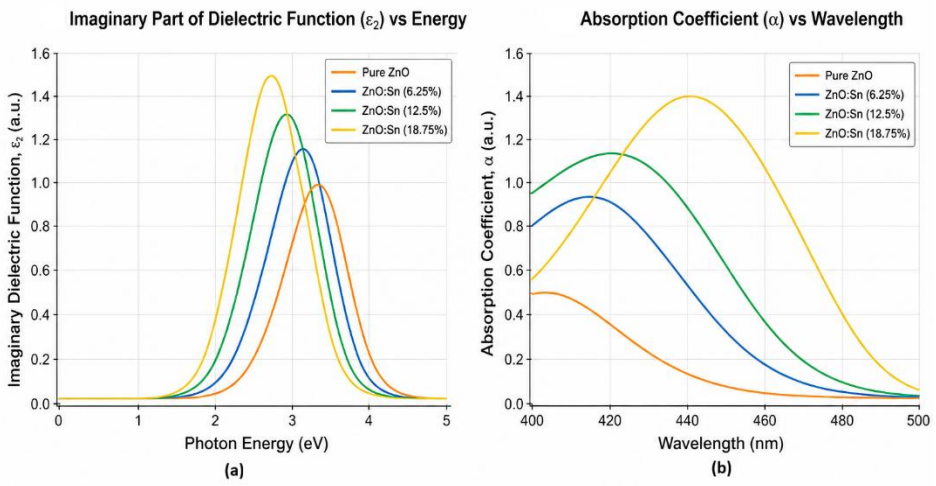

Figure 3. (a) Dielectric function $\varepsilon_2(\omega)$, and (b) absorption coefficient $\alpha(\omega)$.

The introduction of Sn atoms into the ZnO structure results in significant modifications to the optical properties of the material. Using a 2×2×2 supercell, Sn doping at concentrations of 1 atom (6.25%), 2 atoms (12.5%), and 3 atoms (18.75%) produces observable changes in both ε_2 and α. As the Sn concentration increases, the absorption edge shifts to lower energies and the absorption coefficient increases, indicating that Sn doping effectively broadens the visible-light absorption spectrum.

The calculated optical response is also supported by previous experimental studies. Several UV–Vis investigations reported that Sn doping shifts the absorption edge of ZnO toward the visible-light region and increases optical absorption intensity. Such behavior has been attributed to defect-assisted transitions, donor levels introduced by Sn ions, and band-gap narrowing effects. These observations are in good agreement with the present dielectric function and absorption coefficient results, where Sn-doped ZnO exhibits stronger absorption in the visible range compared with pure ZnO. Therefore, the simulated optical enhancement is consistent with experimentally observed photoresponse improvements in Sn-doped ZnO materials [29], [30].

These improvements are highly beneficial for photovoltaic applications, as a broader visible-light absorption range allows the material to harvest a larger portion of the solar spectrum. Consequently, Sn-doped ZnO has the potential to enhance photoexcitation rates, increase carrier generation, and improve overall solar energy conversion efficiency.

Conclusion

This study systematically investigated the effects of substitutional Sn doping on the electronic and optical properties of ZnO using first-principles Density Functional Theory (DFT) within the GGA-PBE framework. The results show that increasing the Sn concentration significantly modifies the electronic structure of ZnO and progressively reduces the band gap from 0.82 eV (pure ZnO) to 0.71, 0.55, and 0.38 eV for 6.25, 12.50, and 18.75% on Zn sites, respectively. Although the absolute values are underestimated compared with experiment, the observed trend confirms that Sn incorporation effectively narrows the band gap and enhances the material's visible-light response. Density-of-states analysis further indicates that Sn-related states are located near the conduction band, leading to changes in electronic transitions.

Optical calculations reveal improved low-energy absorption and a shift of optical activity toward the visible region after Sn doping, indicating better light-harvesting capability. Overall, the findings demonstrate that substitutional Sn doping is a promising strategy for tuning ZnO properties and improving its potential for photovoltaic, transparent-electrode, and other optoelectronic applications.

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