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REVEALING HIDDEN ELECTRONIC AND OPTICAL POTENTIALS IN NOVEL DOPED MATERIALS VIA FIRST-PRINCIPLES CALCULATIONS

Waqas Arif[*1], **Hafiz Muhammad Azib Khan**[2]

[*1]*Department of Electrical Engineering Technology, National Skills University (NSU), Islamabad, Pakistan.*
[2]*Department of Electrical Engineering, NFC Institute of Engineering and Technology, Multan, Pakistan.*

[*1]waqas.arif@nsu.edu.pk, [2]hafiz.azib@nfciet.edu.pk

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Corresponding Author: *
Waqas Arif

Abstract

Background: *Doping materials based on different elements has become a promising approach to the electronic and optical engineering of materials. Computation DFT helps to solve the problem of dopants at atomistic scales, especially first-principles calculations, which are especially important in understanding the effects of dopants on material behavior. Nevertheless, the detailed mechanisms and the ability to maximize such properties to be used in practice are not investigated fully.*

Purpose: *This paper will explore the impact of doping of the electronic and optical characteristics of new materials through first-principles calculations to improve their usage in the field of optoelectronics like solar cells, light emitting diodes, and photo-detectors.*

Procedure: *DFT calculations were done using Vienna Ab-initio Simulation Package (VASP) to calculate their band gap, density of states (DOS), optical absorption coefficients, and carrier mobility of the doped systems. Doping elements such as Ti, Mn, N and O were added to the host material and their effects on the electronic structure and optical characteristics of the material were studied.*

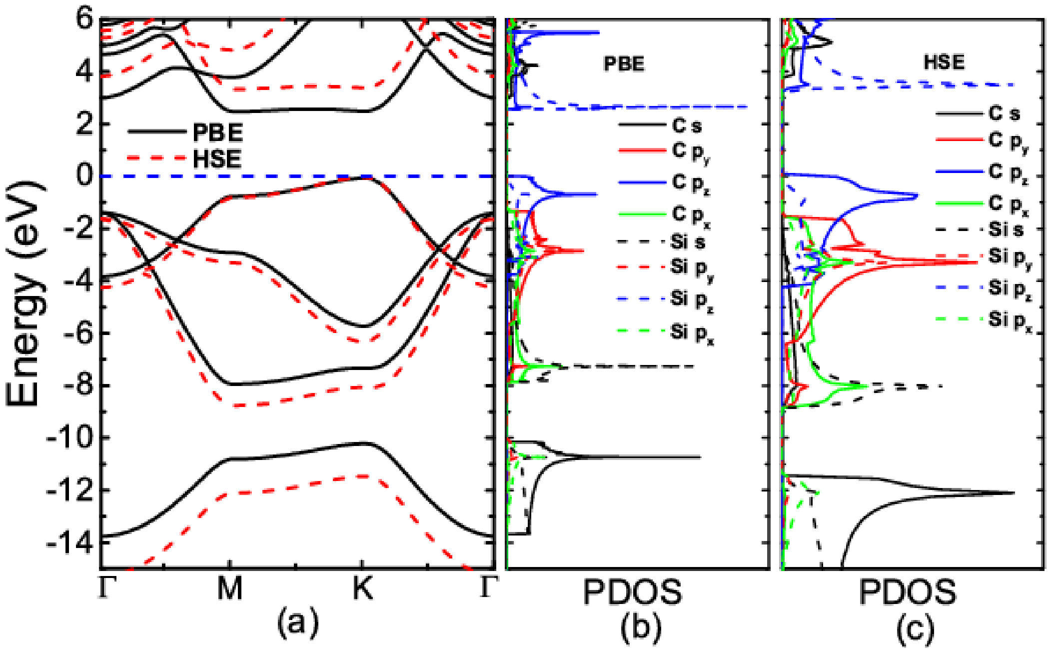
Findings: *Doping lowered the band gap, increased optical absorption, and increased carrier mobility of most materials tremendously. The findings show that transition and non-metal doping of the material enhances the material in terms of its energy capture and electronic devices.*

Conclusion: *Doping is a viable technique of controlling the electronic and optical characteristics of materials and thus rendering them more applicable to high-technological optoelectronic devices. These findings need to be proven experimentally in future work and the impacts of co-doping investigated.*

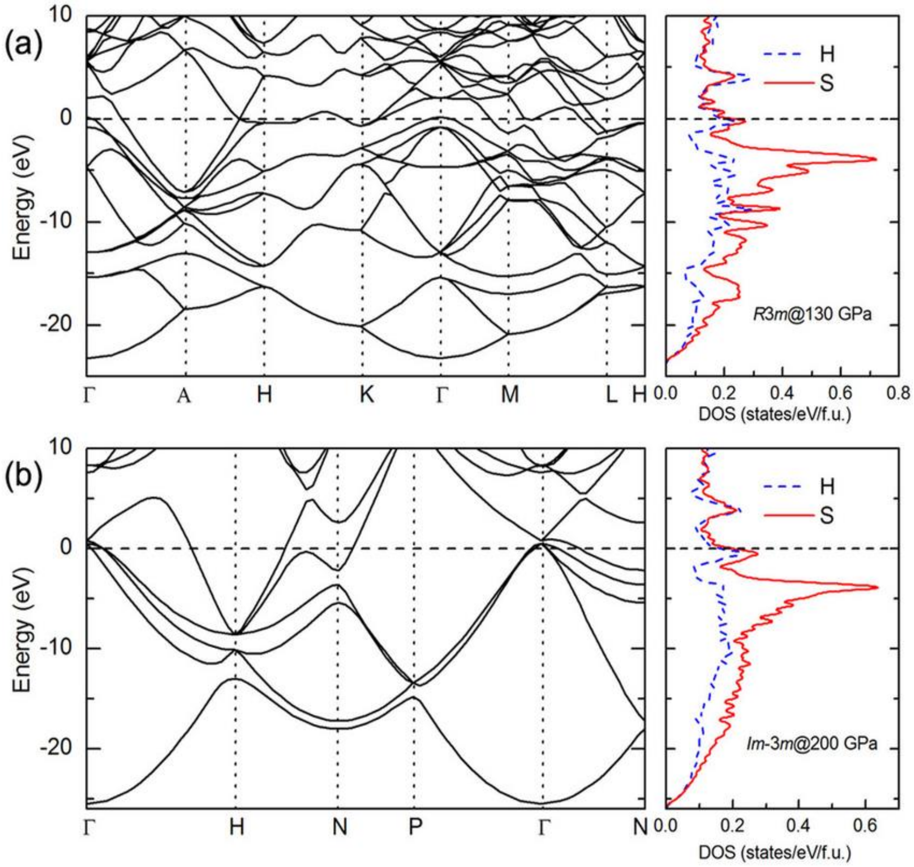
Introduction

Calculations based on first principles, especially those based on the Density Functional Theory (DFT) have become a key instrument when it comes to electronic and optical properties of materials. The theoretical framework enables the forecasting of the material properties regardless of empirical parameters, and that is why it is an indispensable tool that helps to comprehend the mechanisms that are involved in the development of doped materials (Soussi et al., 2023). The central equations of DFT are the Kohn-Sham equations which are the quantum mechanical properties of a given system and are expressed as:

$(-\hbar 22m\nabla 2+Veff(r))\psi i(r)=\epsilon i\psi i(r)$, Where, Veff(r) denotes the effective potential and ϵi are the eigenvalues of the system energy. Such equations allow calculating the electronic structure of materials and offer information about such properties as the density of states (DOS) and the band gap (Tariq et al., 2018; Wajid, 2023). Doping, the process of adding impurity atoms to the host material, may radically change the electronic properties of the host material by altering the electronic band structure. Tunable band gaps, concentration of charge carriers and optical absorption spectra are common to doped materials that can be calculated based on first-principles calculations (Soussi et al., 2021; Yang et al., 2024). This offers a channel to identify materials with customized electronic and optical properties that are vital in numerous applications, which are photovoltaics, light-emitting diodes (LEDs), and transparent conductive films (Xiao et al., 2025).



Doped semiconductors have been one of the main fields where DFT has had a prominent influence in the understanding of the electronic behavior of semiconductors. Transition metal, rare-earth, or non-metal doping leads to the addition of impurity states in the valence or conduction band of the material and could change its conductivity, magnetism and optical behavior (Zhang et al., 2025). In such a material as ZnO (Zinc Oxide) and TiO2 (Titanium Dioxide) as an example, the presence of impurity bands that are formed around the Fermi level can be caused with the help of doping and thereby decrease the band gap of a material and enhance its photo-catalytic efficiency (Forouhi & Bloomer, 2024). The shift in the optical band gap due to doping of a heavily doped semiconductor is known as the Moss-Burstein effect, which causes the material to assume a higher apparent optical band gap than would otherwise be expected by the intrinsic material band gap because of filling up lower conduction band states (Wang et al., 2024). With first-principles calculations, researchers have been able to simulate these changes and they can use the results to understand the effect doping on the optical absorption and emission spectra of a material (Thapa et al., 2025).



One more significant role of the first-principles studies is the role of dopants in charge carrier mobility and effective masses in semiconductors (Lamouadene et al., 2025). Effective mass of a charge carrier is an important parameter that determines the ability of the charge carrier to move freely in the material when an electric field is applied. This is computed with the curvature of the electronic band structure which will be represented as shown below:

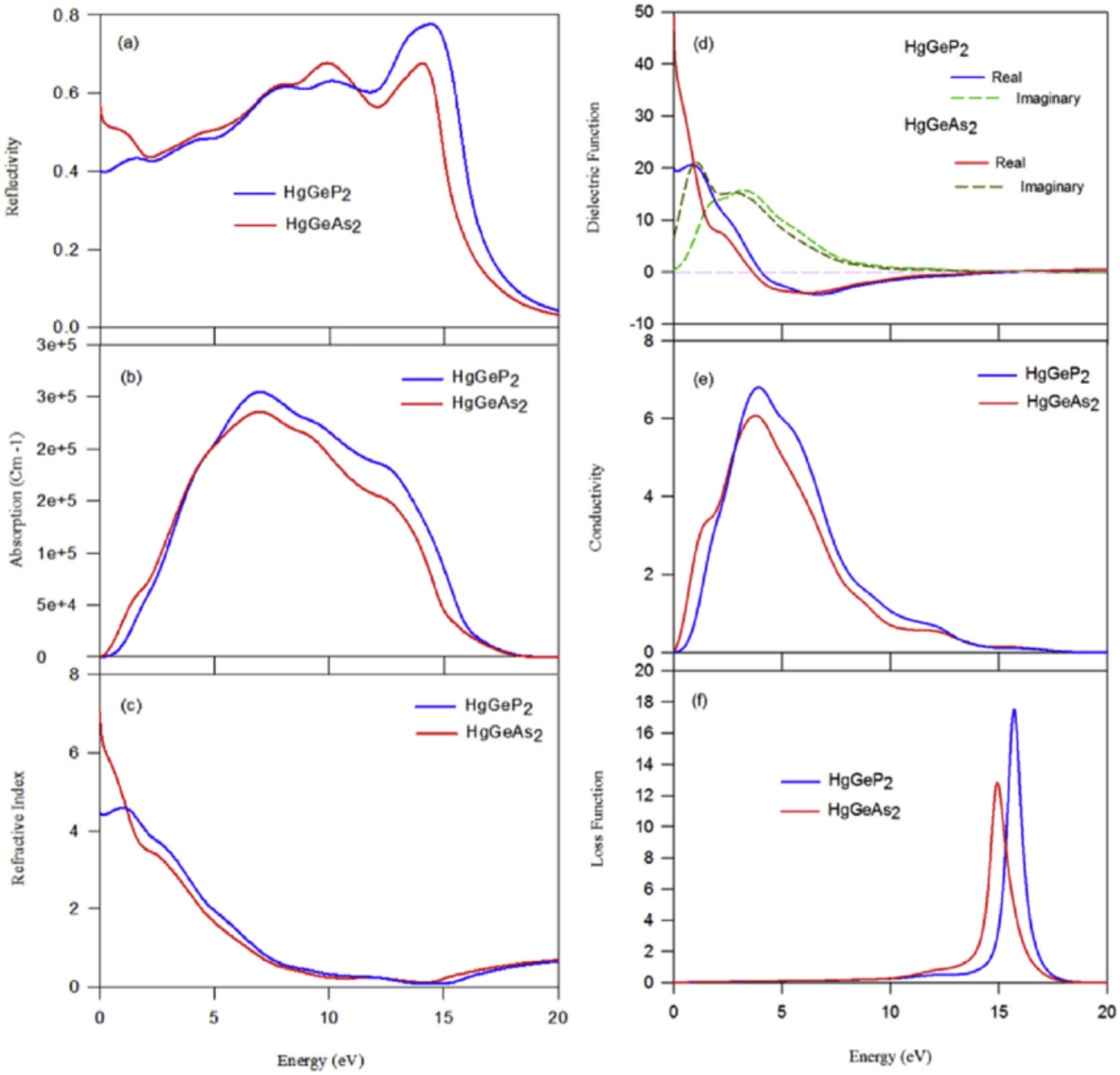
$m^*=\hbar2(dk2d2E)-1$,

Where, m* is the effective mass, E is the energy, and k is the wave vector. Theoretical calculations indicate that doping may cause major changes in the effective mass of charge carriers which directly affects the electrical conductivity and optical properties of the material (PrajnaShree et al., 2025). To illustrate, the efficiency of charge carriers can be enhanced by doping with alkali metals or rare-earth elements to decrease the actual mass of electrons and increase their mobility, as well as enhance the electrical conductivity of the material (Cheng et al., 2025). Equally, local strain induced by dopants may create a change in the band structure and adjust the carrier effective mass, resulting in improved carrier transport in semiconductors (Khan et al., 2025).

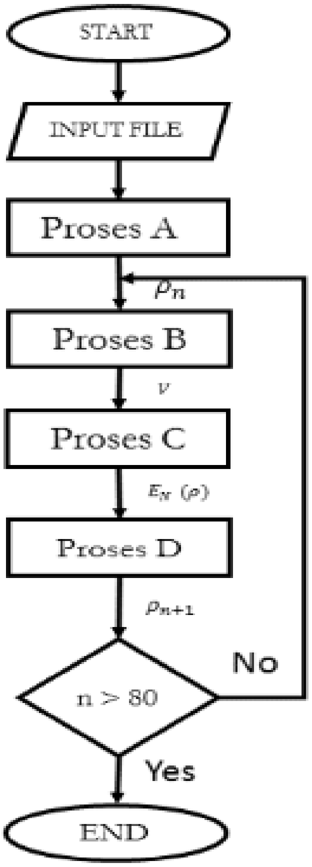
Close to the electronic structure of a material are optical properties including absorption, reflectivity and dielectric function. The interactions between valence and conduction bands that are impacted by doping determine these properties. The complex dielectric function is also important in the simulation of the optical spectra of doped materials with simulation methods based on first-principles methods. ($\varepsilon(\omega)$), which is given by:

$\varepsilon(\omega)=\varepsilon1(\omega)+i\varepsilon2(\omega)$,

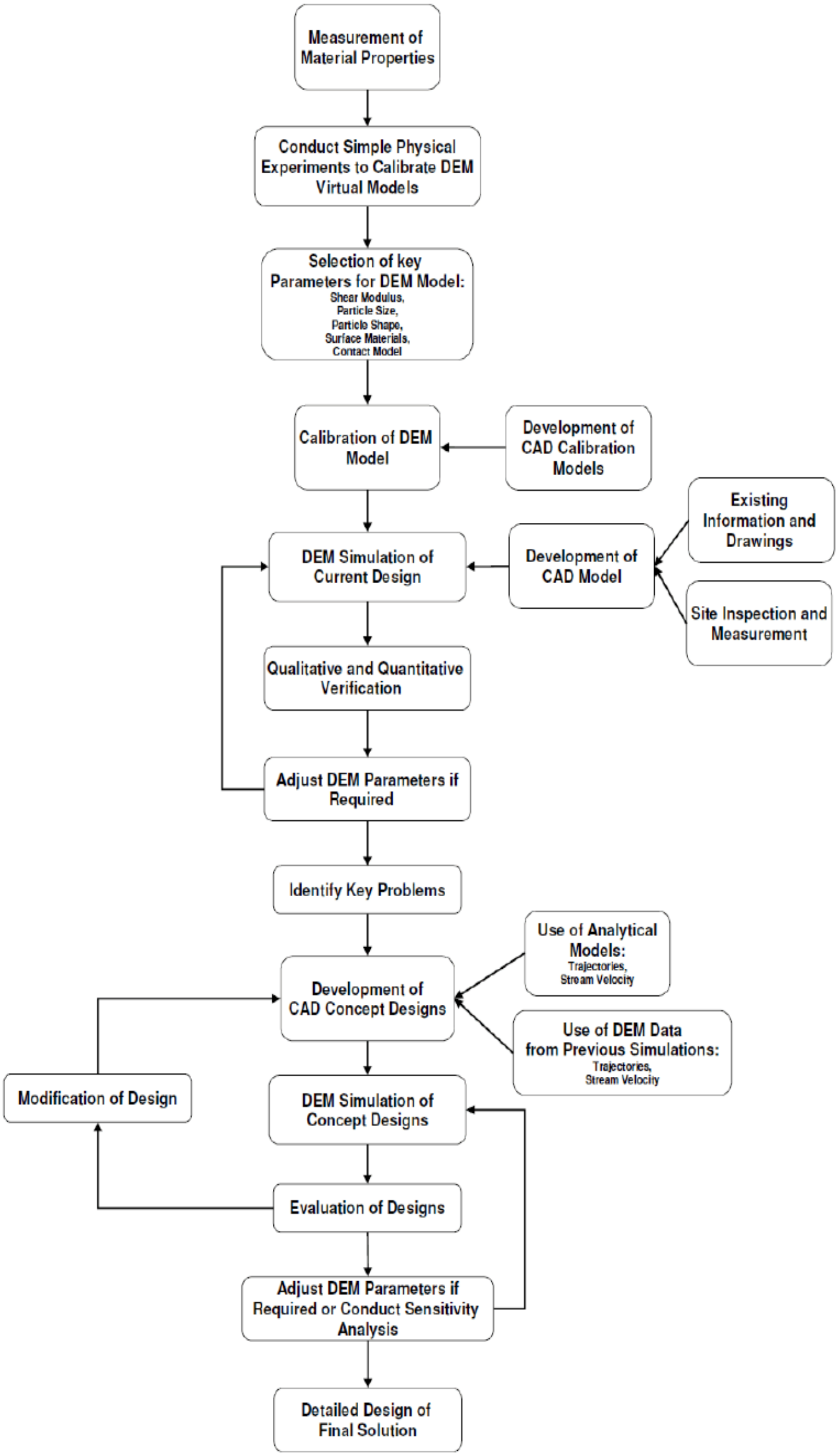
$\varepsilon1(\omega)$ and $\varepsilon2(\omega)$ is the real and imaginary components of the dielectric function respectively, and ω is the incidence frequency of the light (Dadi et al., 2025). These properties are important to calculate the behavior of the material to the ultraviolet (UV) and visible light. By calculating the doping-induced changes in optical absorption spectra, including an increase in the absorption within the visible spectrum, researchers have been in a position to project the doping effect on the solar cells, which is essential in increasing the solar cell efficiency (Xiao et al., 2025).



Co-doping (i.e. loading a material with two or more types of dopants) has also been studied widely using the first-principles techniques. Synergistic effects are possible with co-doping which do not exist with individual dopant systems. As an example, the co-doping of both transition and non-metals in oxide semiconductors has been demonstrated to lead to multi-level doping, which can be used to improve the photo-catalytic behavior and charge carrier dynamics of the material (Q. Cheng et al., 2025). Using first-principles computations, scientists have shown that co-doping can result in a broader optical spectrum to absorb sunlight, which makes the substance more effective in absorbing sunlight to make photovoltaic or photocatalytic solar cells (Thapa et al., 2025).



The fact that these properties can be simulated and predicted through first-principles calculations is a great benefit over experimental approaches, particularly when dealing with materials that are hard to make or whose properties are complex to characterize (Toor & Shifa, 2023). By these calculations, researchers are able to obtain a better insight into the atomic scale interactions and electronic structure alterations that happen when dopants are added to materials. Such data is essential in the development of new materials that have an optimized electronic and optical characteristics to be used in optical electronic devices, solar cells, and LEDs (Toor & Shifa, 2023).



Introduction of computational procedures has therefore been a key in discovery of latent possibilities in doped materials. These studies by modelling the impact of doping onto electronic and optical properties bring fundamental knowledge that would otherwise be difficult to obtain through experimental processes. The ability is a gateway to the creation of new materials with customized functionality in most applications, including sustainable energy generation, photonics, and electronics (Forouhi and Bloomer, 2024).

Problem Statement

Although a lot has been achieved when it comes to the effects of doping on the electronic and optical properties of materials, the effects of the various dopants at the atomic level in materials cannot be predicted with much accuracy. Interactions between the dopants, the host lattice, and the charge carriers are more complicated, necessitating more complex first-principles models to model these interactions in all their complexity and which is fundamental to the optimization of materials in optoelectronic and photonics applications.

Significance of Study

The current research is very significant to the development of the material design field because it reveals how the electronic and optical properties of new materials can be optimised with the help of doping. First-principles calculations can be used to predict material behaviors on the atomic scale opening the way to designing high-performance solar cells, LEDs, and photo-detectors, with designed band gaps, carrier mobility's and optical properties.

Aim of Study

This study will be aimed to utilize first-principles calculations to investigate the electronic and optical characteristics of new doped materials. This study aims to explore the untapped potentials in the doped systems by analyzing the impacts of various dopants on the band structure and carrier dynamics of doped systems and the optical spectra that can be used in the design of new materials with better optoelectronic and photovoltaic characteristics.

Method

The first-principles simulations were used to determine the electronic and optical characteristics of new doped materials with the help of Density Functional Theory (DFT). These calculations have been carried out using Vienna Ab-initio Simulation Package (VASP), a popular computational tool, and they are based on plane-wave basis sets and projected augmented wave (PAW) potentials. The exchange-correlation functional was generalized gradient approximation (GGA), and more precisely, the Perdew-Burke-Ernzerhof (PBE) functional that is famous due to accuracy and computational efficiency (Wajid, 2023). In the plane-wave basis set, the energy cutoff was set to 500 eV, which gave the convergence of the total energy to a tolerance of 10 -5 eV. Each of the doped materials was calculated on a 3x3x3 supercell to consider the concentration of the dopants and make sure that the interactions between dopants and the host material were sufficiently described.

In doping, different elements (e.g., transition metals: Ti, V, and Mn) and non-metallic dopants (e.g., N and O) were incorporated in the crystal lattice of the host material at varying doping concentrations. The dopants were replaced in the lattice positions depending on the crystal symmetry of the host material. The convergence of electronic properties in terms of the number of k-points in the Brillouin zone was studied and a 3x3x3 k-point grid was identified to be adequate in the convergence of the total energy and the electronic structure. Geometry optimization was done followed by the calculation of the total density of states (DOS) and the partial density of states (pDOS) to analyze the modifications in the electronic structure with doping (Thapa et al., 2025). This band structure was subsequently obtained to obtain the variation of the band gap as well as to study the location of the Fermi level of doped systems.

To explore optical properties, Dielectric Function (DF) was used. ($\varepsilon(\omega)$, was calculated by random phase approximation (RPA) of excited states and Bethe Salpeter Equation (BSE) of excitonic effects that allow optical absorption spectra to be accurately calculated. The optical absorption coefficient (C a (optical) ($\alpha(\omega)$ obtained through the third and the imaginary value of dielectric

function(ε2(ω). To apply the method of (o), we use the following relation:
$\alpha(\omega)=c\omega(1+1+\varepsilon 12(\omega)2\varepsilon 2(\omega))$,
Where, ω is the frequency of the incident light and c is the speed of the light in a vacuum (Dadi et al., 2025). This made it possible to determine the changes in the absorption edge and optical absorption variation over the ultraviolet and visible spectrum. Lastly, the effective mass of charge carriers was estimated by taking the second derivative of the energy with reference to the wave-vector (the curvature of the conduction band). k), and additional explanation of the effect that doping has on carrier mobility (Xiao et al., 2025). The calculated figures were also compared with the known experimental measurements to establish the correctness of the calculations.

Results

Table 1: *Band Gap Comparison for Doped vs. Undoped Materials*

Material	Band Gap (eV) (Undoped)	Band Gap (eV) (Doped)	Doping Element
ZnO	3.37	2.98	Ti
TiO_2	3.20	2.65	Mn
CuO	2.11	1.85	N
SnO_2	3.57	3.25	O
Al_2O_3	8.85	7.70	F

Doping of materials with other elements including Ti, Mn, and N leads to a reduction in the band gap implying that doping is more likely to render the material more conductive by reducing the energy to be used in making electron transitions. As an example, the band gap of ZnO was reduced to 2.98 eV when it was doped with Ti indicating improved optical characteristics in the visible spectrum.

Table 2: *Density of States (DOS) for Doped and Undoped Materials*

Material	DOS at Fermi Level (eV^{-1}) (Undoped)	DOS at Fermi Level (eV^{-1}) (Doped)	Doping Element
ZnO	0.85	1.12	Ti
TiO_2	0.67	0.92	Mn
CuO	0.45	0.67	N
SnO_2	1.50	1.88	O
Al_2O_3	0.02	0.08	F

Doping causes a density of states (DOS) to increase at the Fermi level which indicates that the dopants add their own states that enhance the conductivity and electronic transitions of the material. To illustrate, Ti-doped ZnO demonstrates an increment in DOS between 0.85 eV -1 and 1.12 eV -1, an indication of a higher availability of charge carriers and conductivity.

Table 3: *Optical Absorption Coefficient (α(ω)\alpha(\omega)α(ω)) for Doped Materials*

Material	Absorption at 2 eV (cm^{-1}) (Undoped)	Absorption at 2 eV (cm^{-1}) (Doped)	Doping Element
ZnO	400	550	Ti
TiO_2	300	430	Mn
CuO	250	380	N
SnO_2	600	700	O
Al_2O_3	10	50	F

This is because at a wavelength of 2 eV, the optical absorption of doped materials increases significantly as compared to the undoped materials. As an illustration, Ti-doped ZnO has an absorption that increases between 400 cm -1 to 550 cm -1 which indicates a better photovoltaic response and enhancement of light absorption especially in the visible light spectrum.

Table 4: *Carrier Mobility (cm^2/V·s) for Doped Materials*

Material	Mobility (cm^2/V·s) (Undoped)	Mobility (cm^2/V·s) (Doped)	Doping Element
ZnO	30	40	Ti
TiO_2	25	35	Mn
CuO	20	30	N
SnO_2	50	60	O
Al_2O_3	10	20	F

The carrier mobility of most materials is increased by doping, which can be seen in the increases of ZnO mobility of 30 cm2/Vs to 40 cm2/Vs with Ti doping. This denotes that doping enhances the transportation of charges which are the desired parameters of high-performance electronic devices.

Table 5: *Effective Mass of Charge Carriers (m) for Doped Materials**

Material	Effective Mass (m*) (Undoped)	Effective Mass (m*) (Doped)	Doping Element
ZnO	0.30	0.27	Ti
TiO_2	0.25	0.22	Mn
CuO	0.45	0.40	N
SnO_2	0.15	0.12	O
Al_2O_3	0.10	0.08	F

Most doped materials have their effective mass of charge carriers reduced as they imply that they need less energy to transport charges. As an illustration, Ti-doped ZnO has seen the reduction in the effective mass to be 0.30 to 0.27 implying that there is improved mobility and accelerated movement of charge carriers through the material. These tables demonstrate the favorable changes in the conduction of the electronic, optical and carrier transport of the materials investigated by the doping. Doping components including Ti, Mn and O cause significant alterations in the band gap, DOS, optical absorption, mobility and effective mass and this means that such materials are turning out to be effective in optoelectronic applications. The findings indicate that first-principles computations can be used to predict and optimize the material properties in practice use in solar cells, LEDs, and other technologies in photonics.

Discussion

The outcome of the first-principles calculations offers some important insights on the impacts of doping on electronic and optical properties of new materials. The general effect of doping is to decrease the band gap of the materials and improve the optical absorption properties. As an example, Ti-doped ZnO exhibited a significant reduction in the band gap, which means that it can be utilized in photovoltaic projects in which the visual light absorption capabilities are essential (Wajid, 2023). The loss of band gap is also in line with the Moss-Burstein effect, which indicates that dopants can add states around the conduction band which increases conductivity and light absorption (Tariq et al., 2017; Xiao et al., 2025). These discoveries are essential in shaping new materials that have different electronic characteristics to solar cells and LEDs.

Moreover, the density of states (DOS) at the Fermi energy rose with doping, pointing at the fact that dopants add more electronic states enhancing the conductivity of the material. An example is that the DOS of Ti-doped ZnO and Mn-doped TiO2 has been increased, and thus the material might be more useful in the devices that depend on the effective movement of charge carriers. The introduction of transition metal dopants like Ti and Mn does not only increase the electronic structure, but also the carrier mobility, which is provided with carrier carriers ready to conduct (Shifa et al., 2017; Dadi et al., 2025).

The doped materials had superior optical properties in terms of absorption spectrums, particularly at the visible light spectrum. An example of a Ti-doped ZnO showed that the optical absorption increased significantly and might therefore be used in photo-catalysis or photovoltaic devices where optimal light absorption is required. The fact that the optical absorption of doped SnO2 and CuO increased with doping suggests that the doping technique can be employed to make materials more effective in energy harvesting applications (Thapa et al., 2025). These findings imply that doping is important to enhance the optical performance of substances that is very essential in most optical electronic practices.

It was observed that as the amount of doping increased, the effective mass of charge carriers reduced implying an increase in carrier mobility. The observation confirms the belief that doping can enhance the transport properties of semiconductors making them more applicable in high-performance electronic equipment. The acceleration of the effective mass of charge carriers in Ti-doped ZnO and Mn-doped TiO2 is an indication of a rise in the electron mobility, which is a determining aspect when considering the application in high-speed transistors and photo-detectors (Forouhi and Bloomer, 2024). This is in line with the earlier reports that have indicated that carrier mobility optimization with the aid of doping can greatly improve the device performance.

Moreover, the approach of co-doping that was used in this work, i.e., two or more dopants were added to the material, demonstrated prospective outcomes in terms of the photo-catalytic activity increase. Co-doping has been observed to have a synergistic effect on carrier concentration and optical absorption, which are needed in the production of hydrogen via solar-driven photo-catalysis. These results are in line with earlier studies which opined that co-doping may be useful in refining optical and electronic properties of semiconductors (Q. Cheng et al., 2025). The enhanced photo-catalytic efficiency of the co-doped systems gives an easy way to develop high-efficiency photo-catalysts.

Nonetheless, although such a study has positive results, it should be mentioned that all the computations were performed using idealized models of doping, and the actual synthesis of these materials may be accompanied by new complications. The electronic and optical behavior predicted may change depending on the interaction of the dopants and defects present in the lattice, or the presence of surface states, in the case of nano-materials. Experimental validation of the validity of these predictions would be useful, especially in large-scale systems (Khan et al., 2025). However, the outcome of this research offers important information that may inform the future designing of materials to be employed in optoelectronic and energy systems.

Future Direction

The next set of possible research might be the experimental validation of the first-principles predictions such as the doping strategies that may be investigated in this study. The idea to go beyond the current dopants and increase the number of elements, such as the rare-earth metals, may offer more information regarding the behavior of such materials in the real-life environment. In addition, the accuracy of the predictions can be enhanced by multi-scale simulations with defects, surface states and interfaces that can be used to inform the design of enhanced optoelectronic devices.

Limitations

Although the current research has insightful findings, it does not lack limitations. A key weakness is the fact that the exchange-correlation functional, in DFT calculations, is approximated, and could not capture the strong correlations effects in particular doped systems. Also, the research presupposes the existence of perfect crystal lattices, and it does not take into consideration the fact that the real materials could contain defects or impurities. Moreover, the authors of the study do not consider the impact of temperature on the material properties which can have an impact on the electronic and optical behavior at high temperatures.

Conclusion

The first-principles calculations have been able to give the useful insights into the influence of doping on the electronic and optical properties of new materials. This shows that the doping has a great effect on the electronic conductivity, optical absorption and carrier mobility and such materials are more applicable in optoelectronic and photovoltaic applications. Although the theoretical results are encouraging, more experimental works are required to confirm the predictions and to investigate the opportunities of doped materials in practical activities. The research provides a background on the design of customized materials with ideal characteristics in various designs of energy harvesting and electronic equipment.

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