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Exploring the Impact of Cd Doping on the Crystal Structure and Electrical Properties of ZnO Using Pymatgen-Based Simulation

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Abstract

Advances in computing technology are driving the development of advanced materials research. This study aims to model and compare the semiconductor properties of ZnO and ZnO doped with Cd (x=0.5) to form Zn0.5Cd0.5O using a computational approach based on Python Materials Genomics (Pymatgen 3.0) approach within a Python 3.10.18 environment. Modeling was carried out to analyze changes in crystal structure, band gap values, and the correlation between charge carrier concentration and temperature. BSDOS Plotter based on Density Functional Theory (DFT) calculations, was used for energy and Density of States (DOS) graph analysis. The simulation results show that the crystal structure of both materials has a wurtzite lattice shape with angles $\alpha = \beta = 90°$ and $\chi = 119°$. The band gap value of ZnO is obtained at 3.1 eV, while in Zn0.5Cd0.5O it decreases to 2.7 eV due to the influence of Cd doping which lowers the conduction band energy. The temperature ranges from 500K to 600 K the charge carrier concentration in ZnO increases from $3x10^5/cm^3$ to $10^8/cm^3$. Meanwhile, the concentrations of electron and hole Zn0.5Cd0.5O increase to $10^8/cm^3$ and $7x10^7/cm$.

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INTRODUCTION

The development of research on advanced materials is growing rapidly accompanied by technological advances such as artificial intelligence, big data, and high performance computing which accelerate the process of synthesis, characterization, and optimization of material properties (Shahzad, Mardare, & Hassel, 2024). Nanotechnology, two-dimensional (2D) materials, and new synthesis methods are now integrating, resulting in the discovery of new materials with new characteristics. Materials previously confined to laboratories are now entering the commercialization stage, marking a significant transition from basic research to industrial innovation (Arshad, 2024). Its development has also spread to the computing, where materials are now being developed through modelling and programming script.

One of the most dynamic areas in advanced materials development is semiconductors (Rimal & Comes, 2024). The need for faster, smaller, and more energy-efficient electronic devices has driven the exploration of semiconductor materials with superior properties through atomic combinations, doping, or modification of crystal structures (Moody & Islam, 2022). Although, the use of computational approaches in predicting semiconductor properties is still relatively limited compared to other materials fields, this method actually has great potential to accelerate the process of discovering and developing new, more efficient and innovative semiconductor materials (W. Zhang, Yao, & Burton, 2024).

ZnO was chosen because it has proven to be a good semiconductor material. However, it is necessary to understand the properties of ZnO when doped or composited with other materials. One material in the same group as Zn but with different covalent bonds is Cd, with Zn having 112 pm and Cd having 144 pm. Cd is an interesting material to dope with ZnO because it itself has semiconducting properties. Therefore, Cd doping in ZnO will be interesting to investigate and understand its unique properties (Singh & Keshari, 2024).

Generally, experiments only use Cd doping below x=0.2 to maintain the wurtzite crystal structure of ZnO. Synthesis with a Cd doping concentration of 50% or x=0.5 is still very rare because it usually forms two distinct phases wurtzite and rocksalt (Zaoui, Zaoui, Kacimi, Boukortt, & Bouhafs, 2010). Therefore, this research with Cd at a concentration x=0.5 doping was conducted using computational modeling to determine the crystal structure and electrical properties.

Computational approaches have been used for modeling in the last ten years. Computational modeling allows researchers to predict material properties before conducting physical experiments, thereby reducing costs, time, and the risk of synthesis failure (Chen et al., 2024). This approach serves not only as an experimental alternative, but also as a foundation of initial data that guides subsequent experimental design (Carnimeo et al., 2023). The Python environment was chosen as the language for modeling and computing because it has a module specifically designed for materials research. The Pymatgen (Python Materials Genomics) module allows researchers to model the structure and properties of materials (Rutt et al., 2022). Pymatgen has also become one of the most widely used modules by computational materials researchers this decade (Zhou & others, 2019).

This study aims to model and compare the semiconductor properties between pure ZnO and ZnO doped with Cd at a concentration (x = 0.5) to become Zn0.5Cd0.5O using the Pymatgen module in the Python programming environment. The use of a computational approach is expected to provide accurate initial predictions regarding changes in structure, band gap, and electrical properties of a material, that can be an important foundation for experimental research and development of material synthesis in the future.

METHOD

Modeling Material Structures

The Pymatgen module 3.0 in the Python environment 3.10.18 was used in this study, also the Crystal Toolkit package for visualizing atomic structures. The process of constructing material structures began by defining parameters of lattice, volume and angle in the element, molecule, and structure modules, followed by placing each atom in its position according to the predetermined crystal lattice. The input data can be displayed using a module called Crystal Toolkit, version 2022.2.11. The output of the crystal structure is a ball and stick arrangement at its coordinates and position of atoms within the crystal lattice.

Plotting Energy and Density Graphs

The crystal structure data obtained in the first stage were stored in a CIF or JSON format file for use in the energy and density graph plotting. When the file was loaded into the BSDOS Plotter module and plotted based on the Density of States (DOS) and energy band structure, two graphs were created. Both graphs consist of a left and right graph. The left graph displays the energy value on the Y-axis and the wave vector k in the crystal momentum space on the X-axis, while the right graph shows the density of each atom. Based on Density Functional Theory (DFT) calculations in Equation (1), the distance between the valence band and the conduction band will determine the band gap value of each material. Band structure is determined by plotting energy (∈i) value against the wave vector k, on the other DOS obtained by summing the energy within specific energy interval.

$$\in_i \psi_i(r) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V_{xc}(r) \right] \psi_i(r) \tag{1}$$

Calculating the Correlation of Charge Carriers to Temperature

The results of the band gap calculation become variables to calculate the concentration of electron (n) and hole (p) charge carriers. The temperature changes in this study were reviewed between 500 K and 600 K. Before calculating the charge carrier concentration, the effective state density value at the base of the conduction band (Nc) and at the top of the valence band (Nv) was first calculated, which was calculated using Equation (2).

$$N_c = 2\left(\frac{2\pi m_e k_B T}{h^2} \right)^{\frac{3}{2}}$$
$$N_v = 2\left(\frac{2\pi m_h k_B T}{h^2} \right)^{\frac{3}{2}} \tag{2}$$

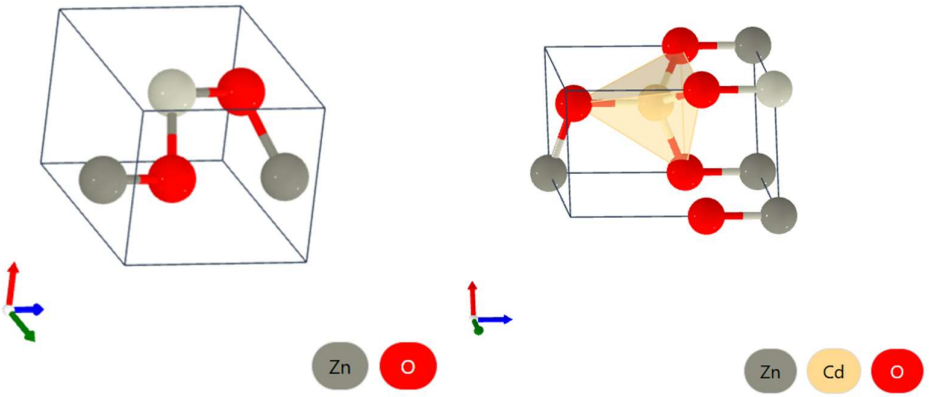
These effective state density values are then used as input in calculating the charge carrier concentration in Equation (3). This correlation enables for analyzing of the material's thermal behavior under non-equilibrium conditions, particularly regarding its conductivity response to temperature changes.

$$n = N_c . e^{-(E_c - E_F)/(k_B T)}$$
$$p = N_c . e^{-(E_F - E_v)/(k_B T)} \tag{3}$$

RESULTS AND DISCUSSION

Crystal structures are generally depicted in a lattice occupied by the bases of each constituent atom. The atoms occupy the lattice and are symbolized by solid circles , and the connecting lines between them indicate the atomic bonds within the lattice (Ardiyanti & Mustaqim, 2021). The results of modelling using the crystal toolkit module are shown in Figure 1. Figure 1a is the crystal structure

of ZnO, while Figure 1b is the crystal structure of Zn¬0.5Cd0.5O. In the crystal structure, Zn+2 ions occupy the cation site and O2- ions occupy the anion site, because Cd is an element in the same group as Zn, Cd has the same valence Cd+2. The substitutional doping process is identified by the entry of Cd atoms that replace Zn in the cation site of lattice. These modeling results correlate with experimental results using the sol-gel method, which showed that Cd doping will replace one of the Zn cation sites (Arda et al., 2023).



(a) (b)

Figure 1. a) Crystal Structure of ZnO, b) Crystal Structure of Zn¬0.5Cd0.5O.

Data regarding lattice parameters, angles, and volumes are shown in Table 1. The angles formed are not the same on each side $\alpha=\beta= 90°$, while $\chi> 90°$. Cd doping causes changes in lattice parameters, such as at a = b there is a change from 3.237351 Å to 3.446431 Å, this is related to the atomic radius of Cd which is larger than Zn. This is in accordance with the theory which shows that Cd ions have a radius of 0.9 Å while Zn has a radius of 0.74 Å, so when Cd atoms are doped they will require a larger space (Azqhandi, Vasheghani F., Rajabi, & Keramatifarhodbonab, 2017). In addition, there is lattice distortion due to significant differences in atomic size that occurs in the c parameter which changes from 5.222061 Å to 5.705266 Å. This also affects the increase in volume which was initially 47.397148 Å3 to 58.687533 Å3. The crystal lattice in ZnO and $Zn_{0.5}Cd_{0.5}O$ is called wurtzite, a lattice that has no center of symmetry and approximates a hexagonal lattice (Mubeen et al., 2023).

Table 1. Crystal Structure Data of ZnO and Zn¬0.5Cd0.5O

	Lattice Parameters (Å) a;b;c	Angle (°) α;β;χ	Volume (Å^3)
ZnO	3.237351; 3.237351; 5.222061	90; 90; 119	47.397148
$Zn_{0.5}Cd_{0.5}O$	3.446431; 3.446431; 5.705266	90; 90; 119	58.687533

The plots generated using the BSDOSPlotter module are presented in Figures 2a and 2b. Figure 2a, shown on the left panel, illustrates the distribution of the valence band (−4.0 to 0.0 eV) and the conduction band (0.0 to 4.0 eV). The X-axis represents the wave vector k along the Brillouin zone symmetry path (Xing, Su, Shui, Qin, & Lee, 2024). The distance between the valence band and the conduction band is clearly visible, and there is no energy band touching the Fermi line, so it can be concluded that ZnO is a semiconductor material. The Maximum Valence Band Point is located at the Γ symmetry at the center of the Brillouin zone or the origin point at around -0.1 eV, while the Minimum Conduction Band is located at 3.2 eV above the Fermi line. Considering that outcome, the value of the band gap obtained is 3.1 eV. The measured band gap values range from 2.8 eV to 3.4 eV,

influenced by variations in structure and methods of synthesis (Samavati et al., 2021).

Figure 2a on the left panel shows the general distribution of electron states. In the valence band that located below the Fermi energy level, a dense distribution dominated by Zn and O atoms is observed. However, the conduction band portrays a sparse distribution, indicating only a little composition from Zn and O atoms. The larger density of states in the valence band compared to the conduction band represent the properties of a semiconductor material (H. Zhang et al., 2025).

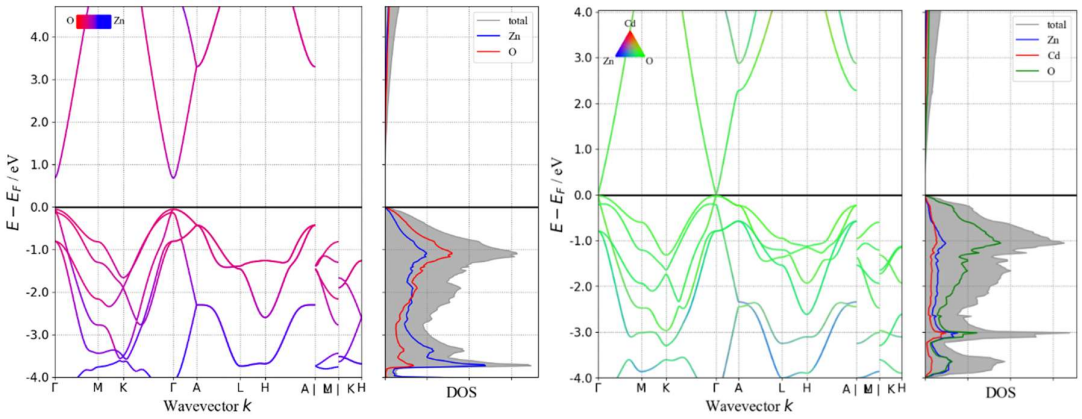
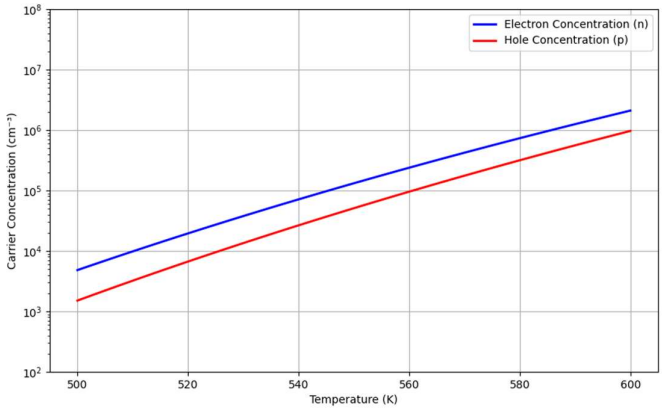


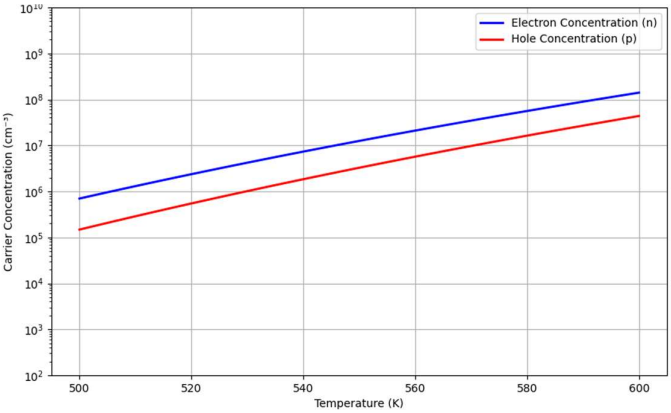
Figure 2. a) Energy Band and Density of ZnO, b) Energy Band and Density of Zn¬0.5Cd0.5O

Figure 2b shows the energy band and Density of State Zn¬0.5Cd0.5O, there is difference from Figure 2a. This difference is due to the presence of Cd doping, which has a higher orbital energy than Zn (Khan et al., 2021). The effect of Cd doping is dominance in the conduction band which shows that Cd has a lower ionization energy than Zn. The Maximum Valence Band point is observed at the first Γ symmetry point along the wavevector path on the X-axis at approximately -0.1 eV, while the Minimum Conduction Band is found at the second Γ symmetry point along the wavevector path on the X-axis at approximately 2.8 eV above the Fermi level. The correlation of the two information obtained a band gap value of 2.7 eV. The difference in band gap values apart from the Cd doping effect can also be caused by Oxygen vacancies and Zn interstitials (Abdulrahman, Barzinjy, Hamad, & Almessiere, 2021).

Further identification of the conductivity properties of both materials is using an activation graph plot through increasing temperature. Figure 3a shows a graph of the increase in electron and hole concentrations at a temperature increase of 500-600 K. At a temperature of 500K the concentration of electron carriers begins to increase at a concentration of 6x103/cm3 while the concentration of holes is at 2x103/cm3. As the temperature increases the concentration of each carrier also increases until it reaches 106/cm3 and 4x106/cm3 for holes and electrons, respectively.



(a)



(b)

Figure 3. a) The Effect of Temperature on ZnO Charge Carrier Concentration, b) The Effect of Temperature on Zn¬0.5Cd0.5O Charge Carrier Concentration

Figure 3b shows the same trend as Figure 3a, with the concentrations of electron and hole carriers increasing with increasing temperature. Zn¬0.5Cd0.5O have higher concentrations carriers than ZnO because of doping of Cd. At 500K, the electron carrier concentration is $9x10^5/cm^3$, while the hole carrier concentration is $3x10^5/cm^3$. Meanwhile at 600K, the concentrations of electron and hole increase to $10^8/cm^3$ and $7x10^7/cm^3$, respectively. These values were obtained follows Equation 2, The increase in the concentration of charge carriers indicates the conductivity properties of the material and its sensitivity to temperature (Gullu, Isik, Gasanly, & Parlak, 2021). Both graphs show that the concentration of electron carriers is always higher than hole carriers, this property is closely related to n-type semiconductors (Colas et al., 2025). The change in charge carrier concentration due to increasing temperature is also related to the role of oxygen vacancies. As the temperature increases, more oxygen is adsorbed, creating oxygen vacancies to donate electrons. This process increases the concentration of electrons and holes, thereby increasing electrical conduction (Petrov, Varzarev, & Abdullin, 2019).

CONCLUSION

Simulation using the Pymatgen module successfully modeled the crystal structure and electrical properties of ZnO and Zn¬0.5Cd0.5O. The results showed that both materials have a

wurtzite crystal structure, with the Cd-doped material exhibiting increased lattice parameters due to the larger ionic radius of Cd2+. The doping process caused a decrease in the ZnO band gap value from 3.1 eV to 2.7 eV. This implies that Cd doping reduces the band gap and increases electrical conductivity. Based on the graph of the correlation between carrier concentration and temperature, it shows that the charge carrier concentration increases with increasing temperature. Further oxygen is absorbed as the temperature rises, resulting in oxygen vacancies that contribute electrons. Electrical conduction increases as a result of this action, which increases the concentration of electrons and holes. This computational approach using Pymatgen is able to provide data from semiconductor materials as a basis for experimental research.

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