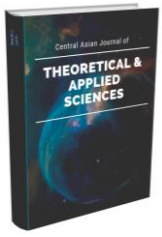

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*Article*

# A Computational Study of the Properties of Pure, Adsorbed, and Doped Zinc Oxide With Copper and Nickel Atoms

**Ghassan Rabea Hussein Abdullah[1*], Issa Z. Hassan[2]**

1,2. Department of Physics, College of Education for Pure Sciences, University of Kirkuk, Kirkuk, Iraq
* Correspondence: ephm22012@uokirkuk.edu.iq

**Abstract:** Zinc oxide (ZnO), a promising n-type semiconductor with hexagonal-layered structure, has attracted significant attention due to its versatile applications in optical and electronic devices, including field-effect transistors, nanogenerators, LEDs, laser diodes, and solar cells. Despite extensive research on pure ZnO, the effects of doping with transition metals like copper (Cu) and nickel (Ni) on its electronic properties remain underexplored. This study investigates the electronic properties of pure ZnO, ZnO doped with Cu and Ni, and ZnO co-doped with Cu and Ni using Density Functional Theory (DFT) and the GGA-PBE approximation (CASTEP). Results reveal that Cu and Ni preferentially adsorb above oxygen sites on the ZnO surface, altering its electronic structure. Pure ZnO exhibited a band gap of 1.68 eV with a bond length of 1.89 Å. Upon Cu adsorption, the gap reduced to 0.11 eV with a bond length of 1.97 Å, while Ni adsorption resulted in a 0.862 eV gap and a 2.03 Å bond length. Doping ZnO with Cu eliminated the band gap, making it conductive with a bond length of 1.888 Å, whereas Ni doping narrowed the gap to 0.369 eV with a bond length of 1.85 Å. These findings underscore the potential of Cu- and Ni-doped ZnO for enhanced electronic applications by tuning the band gap, paving the way for advances in nanoscale device engineering.

**Keywords:** ZnO, approximation (GGA, PBE), CASTEP, Electronic properties of pure, Doped and adsorbed hexagonal Zinc Oxide, Density function theory (DFT), Band gap

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## 1. Introduction

Zinc oxide (ZnO), which is an n-type semiconductor, has a wide band gap of 3.37 electron volts in its natural state and has a hexagonal crystal structure[1]. Due to its unique optical and electronic properties, it has attracted significant attention in potential applications such as solar cells, optoelectronic devices, and nanogenerators [2]. It was one of the most sensitive materials used in gas sensors [3]. In fact, due to its advantages of high sensitivity, stability, and low cost, zinc oxide nanostructures have been widely used for gas detection such as H2, NH3, CH4, CO, NO2, ethanol, and acetone [4, 5]. Recently, various two-dimensional nanostructures of zinc oxide with a thickness close to the space charge region have been fabricated. The good sensing of ZnO with a two-dimensional nanostructure led to high detection efficiency, reduced operating temperature, rapid response and recovery capability, and improved selectivity [5].

Zinc oxide is a rare mineral considered a metal and is called (zincite). It is found in the Earth's crust and is commercially produced as red zinc oxide. Most zinc oxide is synthetically manufactured. Zinc oxide is a white powder that does not completely dissolve in water. It is used in many products and additives such as ointments, plastics,

ceramics, glass, and car tires [3]. ZnO belongs to the surface-sensitive materials. When a sensing element is prepared using ZnO, the gas sensing mechanism can be summarized as adsorption - oxidation - adsorption [6, 7], which is its gas sensitivity mechanism. In the air, oxygen molecules are absorbed on the surface of ZnO and capture electrons from the conduction band of ZnO to form oxygen ions.

Many nanostructures of zinc oxide, such as nanowires, nanobelts, and nanorings, have been fabricated [8]. In recent years, there has been increased interest in zinc oxide due to its potential applications in new optical and electronic devices such as field-effect transistors and nanogenerators [9], in addition to light-emitting diodes, laser diodes, and ultraviolet wavelength detection devices [10]. Under ultraviolet light, zinc oxide is a photoconductor. The combination of the optical and semiconducting properties of doped zinc oxide makes it competitive with new generations of devices. The absorption of solar radiation in photovoltaic cells is much higher in materials composed of nanoparticles than in thin films of continuous sheets of materials, which means they increase efficiency, and the smaller the particles, the greater the absorption of solar energy [11].

## 2. Materials and Methods

Based on first principle calculations and through the density functional theory (DFT) [12] available in the CASTEP[13] program in all calculations in our current study. Where the Generalized Gradient Approximation (GGA) [14] was set to obtain accurate results for the study. The calculations were performed on a large unit supercell 3x3x1 for pure zinc oxide, doped zinc oxide with copper (Cu) and nickel (Ni) atoms, as well as adsorbed zinc oxide with copper (Cu) and nickel (Ni) atoms, with the aim of studying the electronic structure of pure, doped, and adsorbed zinc oxide.

All calculations were performed on a large unit cell (3x3x1), which consists of (18 atoms) distributed as follows: 9 zinc (Zn) atoms and 9 oxygen (O) atoms. The lattice parameters a-b are valued at (9.838 Å), which corresponds to the (X,Y) plane, while the parameter C is valued at (20Å) and represents the distance between two layers of the molecule along the Z-axis. The interactions between the layers can be neglected due to the large distance. Among the properties that were studied are the density of states and the energy gap. (Energy band gap).

## 3. Results and Discussion

**The best site for the adsorption of a (Cu) atom on the surface of pure zinc oxide. (ZnO)**

The geometric configuration was conducted to determine the best site for the adsorption of a copper (Cu) atom on the surface of zinc oxide (ZnO). Through the periodic boundary conditions on a large cell (3x3x1), there are three potential adsorption sites on the surface of zinc oxide.

A. Above the oxygen atom (O)
B. Above the center of the hexagonal ring of zinc oxide (ZnO)
C. Above the bond that connects oxygen (O) with zinc (ZnO)

Through conducting geometry optimization to determine the best site for the adsorption of copper (Cu) and nickel (Ni) atoms among the three sites, it was found that the preferred site for adsorption is above the oxygen (O) atom, as shown in the figure.(1). When the atoms are arranged above both the edge and the center of the hexagonal ring of zinc oxide, the adsorbed atoms shift directly above the oxygen after the geometric arrangement. This is consistent with the study conducted by Jin Chang et al. [15]

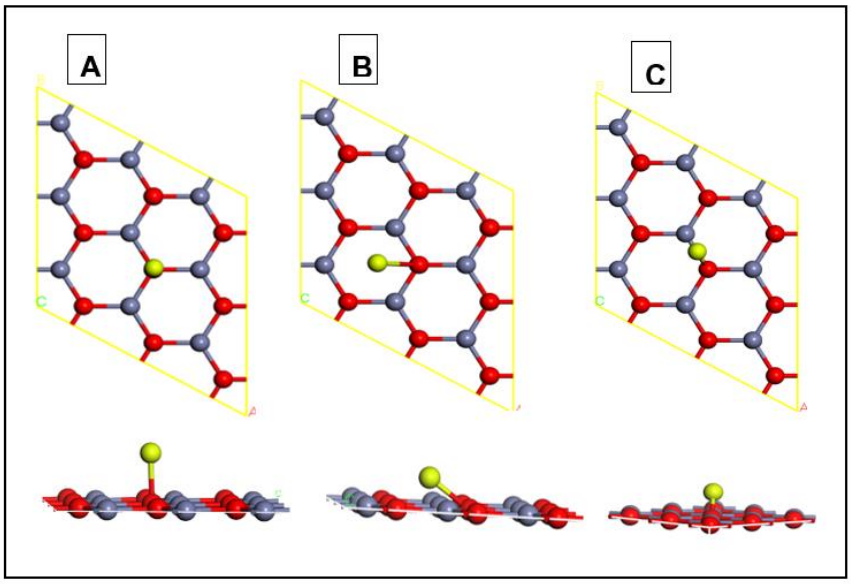



Figure 1. The three sites selected for adsorption on the surface of zinc oxide

A mathematical equation was used to calculate the binding energy of the adsorbed and doped zinc oxide with a copper seed, and the relationship was as follows.

Eb=E (ZnO+metal)-(EZnO+Emetal) (1)

EZnO+metal total energy of the compound.

EZnO Total Zinc Oxide Energy

Emetal: The total energy of the adsorbed or doped molecule (Cu,Ni)

It has been shown that the total binding energy, according to the above equation, was as per the table. (1)

Table 1. Shows the amount of binding energy and bond lengths.

| Sequence | The molecule | Binding energy | Length of the bond Å |
|---|---|---|---|
| 1 | ZnO | 2.004 eV | 1.89 |
| 2 | ZnO adsorbed Ni | 10.5 eV | 2.03 |
| 3 | ZnO doped with Ni | 5.92 eV | 1.85 |
| 4 | ZnO adsorbed Cu | 2.5 eV | 1.97 |
| 5 | ZnO doped with Cu | 6.95 eV | 1.88 |

**The electronic properties of zinc oxide (ZnO)**

In the current study, the electronic properties (band gap and total and partial density of states) were calculated using the CASTEP program. The type of band gap, whether direct or indirect, is determined by the closest points between the conduction band and the valence band. The band gap is direct if it is at the same point, and it is indirect if it falls

on different points for the (G, M, K, G) points. The band gap for pure zinc oxide (ZnO) was calculated, and it is direct at the (G) point with a value of (1.683 eV), which is close to previous studies [16].

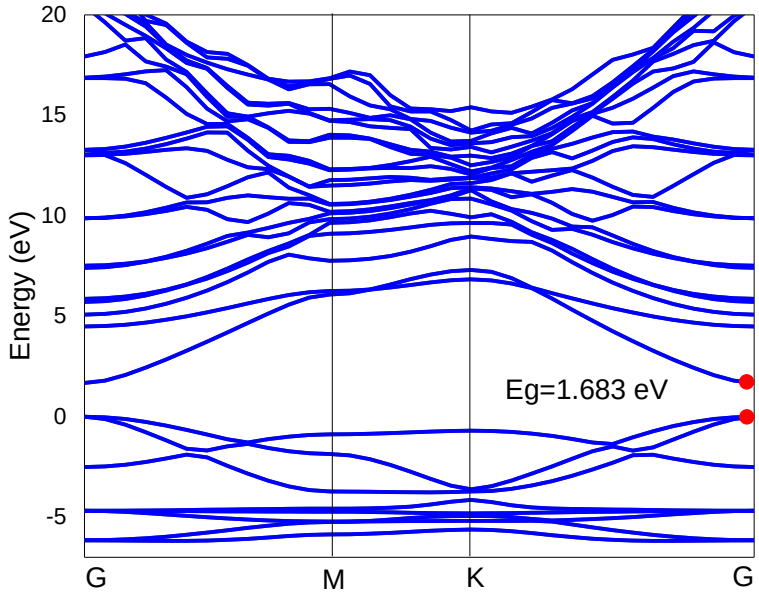
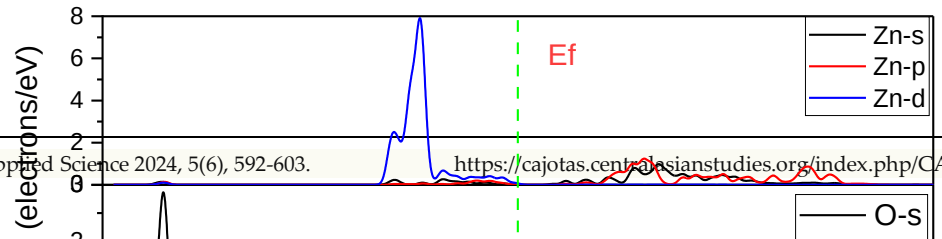



Figure 2. Illustrates the direct energy gap of pure zinc oxide

The density of partial and total states was calculated using the Generalized Gradient Approximation (GGA-PBE) on a large cell unit (3x3x1) of pure zinc oxide (ZnO) with an energy cutoff of 10 eV. The maximum force was 0.03 eV/Å, the maximum stress was 0.05 GPa, and the maximum displacement was 0.0010 Å. In the current study, a plot containing the density of all states (total and partial) was used to obtain an accurate electronic structure diagram of zinc oxide (ZnO). The figure shows that the color  The black color indicates the s orbital, the red color indicates the p orbital, and the blue color indicates the d orbital. The electronic distribution for the element zinc(_ ^30)Zn=1s^2  2s^2 2p^6 3s^2 3p^6 4s^2 3d^10 . In the valence band, the highest density of states was recorded at the d orbital, reaching (8 electrons/eV) at (-4.79 eV), which dominated the valence band.

The density of states gradually decreased at the energy gap. As for the conduction band, the p orbital had the highest peak of density of states, reaching (1.25 electrons/eV) at (6 eV), indicating the presence of free-moving electrons, with the s and p orbitals dominating the conduction band. The electronic distribution of the oxygen element (_ ^8)O=1s^2 2s^2 2p^4  in the valence band recorded the highest density of states for the s orbital, which reached (2.8 electrons/eV) at (-17 eV). Additionally, the highest density of states for the p orbital was recorded at (2 electrons/eV) at (-0.94 eV). The s and p orbitals dominate the valence band, and the density of states is zero at the Fermi level (the zero level), which is free of electrons. In the conduction band, the p-orbital is dominant in the conduction band and gradually diminishes.

As for the calculation of the total density of states for zinc oxide (ZnO) shown in the figure, the first valence band extends from -17.7 eV to -16.5 eV, with a value of 3.17 electrons/eV. The second density of states extends from -6.5 eV to 0 eV, with a value of 8.2 electrons/eV. The density of states vanishes at the Fermi level. As for the conduction band, the density of states extends from 20 eV to 1.9 eV, with the highest peak value being 5.4 electrons/eV at (14 eV). The largest contribution comes from the (d, p) orbitals of the zinc and oxygen atoms respectively (Zn, O), and the hybridization is clear and strong between the d orbital of the Zn atom and the s orbital of the O atom as in (3).



**For the electronic properties of copper-doped zinc oxide (ZnO) (Cu)**

The energy gap of zinc oxide (ZnO) adsorbed with a copper atom (Cu) on a (3x3x1) unit cell was calculated using the (GGA-PBE) approximation. The preferred site for the adsorption of the copper atom was above the oxygen atom in the zinc oxide molecule. The energy gap between the closest points of the conduction and valence bands was indirect, occurring at both the (K,G) point with a value of (0.110 eV), as shown in (4).

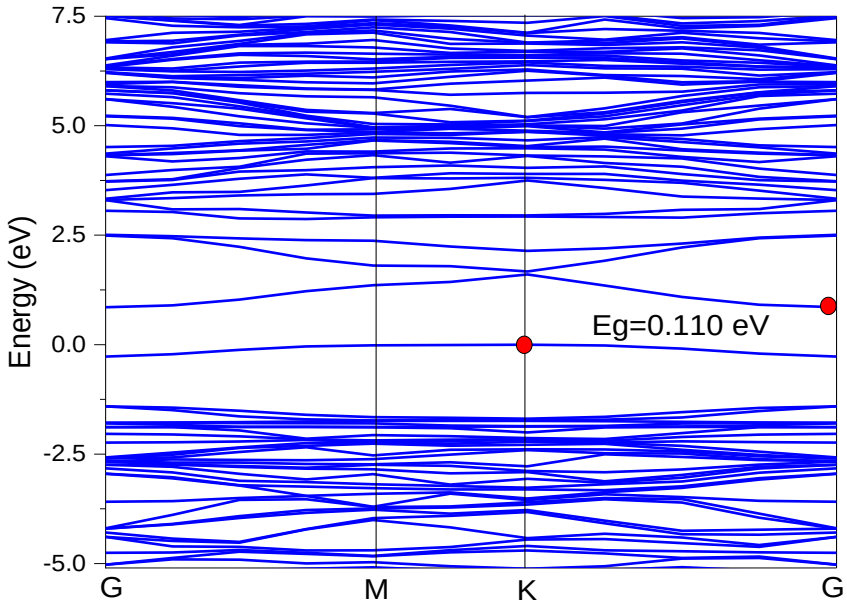



Figure 4. Illustrates the adsorption of Cu on the surface of pure zinc oxide.

The partial and total density of states were calculated using the Generalized Gradient Approximation (GGA-PBE) on a large cell unit (3x3x1) of zinc oxide doped with copper (ZnO-Cu). A plot containing the total and partial density of states was used to obtain an accurate electronic structure diagram of copper-doped zinc oxide. The figure shows that the black color indicates the s orbital, the red color indicates the p orbital, and the blue color indicates the d orbital. In the zinc (Zn) atom, the valence band shows the highest density of states at the d orbital, reaching (68 electron/eV) at (-6 eV), which dominated the valence band. The density of states gradually decreased at the energy gap. The conduction

band shows the highest peak of density of states at the s orbital, reaching (8.59 electron/eV) at (5.3 eV), and the highest peak of density of states at the p orbital reached (9.6). electron/eV) at (4.7 eV), meaning it contains free-moving electrons where the (s,p) orbitals dominate the conduction band. In the oxygen atom (O), the valence band gives the highest density of states at the s orbital, which reached (23 electrons/eV) at (-18.4 eV).

Additionally, the highest density of states in the p orbital was recorded at (16.6 electrons/eV) at (-2.6 eV). The s and p orbitals dominate the valence band, and the density of states is zero at the Fermi level (the zero level), which is free of electrons. In the conduction band, the p-orbital is dominant in the conduction band and gradually diminishes. In a (Cu) atom, the valence band gives the highest density of states at the d orbital, which reached (13.5 electron/eV) at (-1.72 eV). The d orbital dominates the valence band, and the density of states becomes zero at the Fermi level (the zero level), which is free of electrons. In the conduction band, both p orbitals dominate the conduction band, where the p orbital records the highest density of states (2.1 electrons/eV) at .(3 eV).

As for the calculation of the total density of states of zinc oxide doped with copper (ZnO-Cu) in Figure (12-3), the first valence band extends from (eV 17.9 to -19.4 eV), with a peak density of (25.77 electrons/eV). The second density of states extends from (0 eV to -7.9 eV), with a peak density of (71 electrons/eV) at (-6.1 eV), and the density of states vanishes at the Fermi level. The conduction band density of states extends from (2 eV to -16.6 eV), with a peak density of (54.6 electrons/eV) at (15.4 eV). The largest contributions are between the d and p orbitals of the atoms (Zn and O) respectively, and another contribution between the d and p orbitals of the atoms (Cu and O) respectively. Hybridization is clear and strong at the s orbital of the atom (O)".

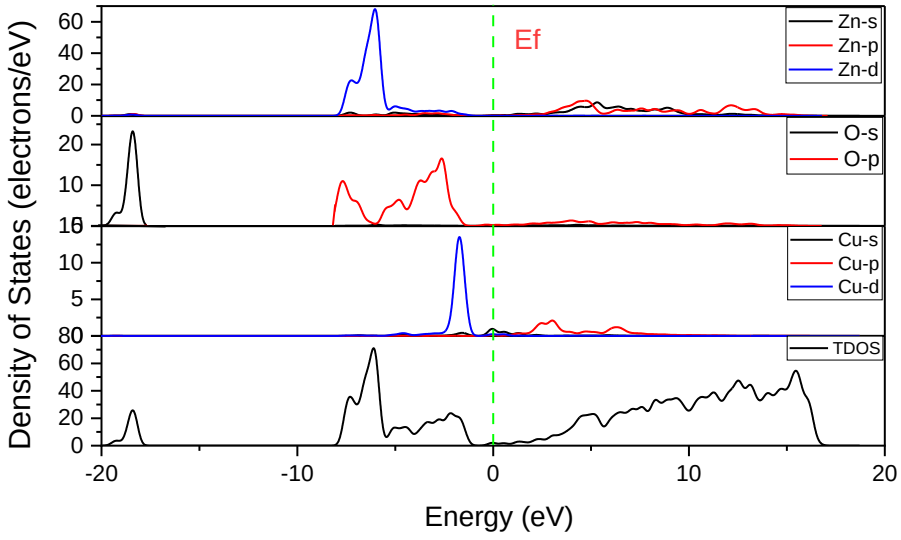



Figure 5. The density of total and partial cases of zinc oxide adsorbed with copper (Cu)

**The electronic properties of copper-doped zinc oxide (ZnO) (Cu)**

The energy gap of zinc oxide (ZnO) doped with a copper atom (Cu) instead of a zinc atom (Zn) on the surface of pure zinc oxide (ZnO) and on the large unit cell (3x3x1) was calculated using the (GGA-PBE) approximation. The changes in the electronic properties of the zinc oxide molecule after doping with a copper atom were studied, and the energy gap was found to be negligible due to the overlap of the conduction and valence bands and the transition of electrons to the conduction band through the energy gap, indicating that the material transformed from a semiconductor to a metal, as shown in (6)

"The density of states, both partial and total, was calculated using the generalized gradient approximation (GGA-PBE) on a large unit cell (3x3x1) of copper-doped zinc oxide (ZnO_Cu). A plot containing the density of all states (total and partial) was used to obtain an accurate electronic structure diagram of copper-doped zinc oxide. The figure shows that the black color indicates the s orbital, the red color indicates the p orbital, and the blue color indicates the d orbital. In the zinc (Zn) atom, the valence band gives the highest density of states at the d orbital, reaching (61.7 electron/eV) at (-5.32 eV), which dominated the valence band and became negligible.

The density of states gradually increases at the energy gap, while the conduction band has the highest peak of the density of states at the s orbital, reaching (8.3 electron/eV) at (6.2 eV), and the highest peak of the density of states at the p orbital, reaching (10.3 electron/eV) at (5.2 eV). This means it contains free-moving electrons in both orbitals. (s,p) dominate the delivery bundle. In the oxygen (O) atom, the valence band gives the highest density of states at the s orbital, which reached (24.75 electron/eV) at (-17.64 eV). Additionally, the p orbital recorded the highest density of states at (15.15 electrons/eV) at (2.09 eV). The s and p orbitals dominate the valence band, and the density of states is zero at the Fermi level (the zero level), which is free of electrons.

In the conduction band, the p-orbital is dominant in the conduction band and has gradually diminished. In a copper (Cu) atom, the valence band extends from -6.5 eV to -0.66 eV, providing the highest density of states at the d orbital, which reached 4.3 electrons/eV at -0.59 eV. It is observed that the d orbital has transitioned from the valence band to the conduction band through the energy gap. In the conduction band, both the s and p orbitals dominate the conduction band, with the p orbital recording the highest density of states (1.84 electrons/eV).) 5.8 eV) .

As for the calculation of the total density of states of zinc oxide doped with copper (ZnO_Cu), shown in Figure (7), the first valence band extends from (18.3 eV to -17 eV), reaching a peak of (27.3 electrons/eV). The second density of states extends from (0.32 eV to -7.15 eV), with the highest peak reaching (65.1 electrons/eV) at (-5.37 eV). We observe that the density of states has transitioned from the valence band to the conduction band across the energy gap, indicating that the material has transformed from a semiconductor to a metal. As for the conduction band, the density of states extends from (1.6 eV to 17.3 eV), with the highest peak reaching (50.9 electrons/eV) at (13.4 eV). The largest contribution is between the d and p orbitals of the atoms (Zn and O, respectively). Another

contribution occurs between the p and d orbitals of the atoms (O and Cu, respectively). Hybridization is clear and strong at the s orbital of the atom. (O)".

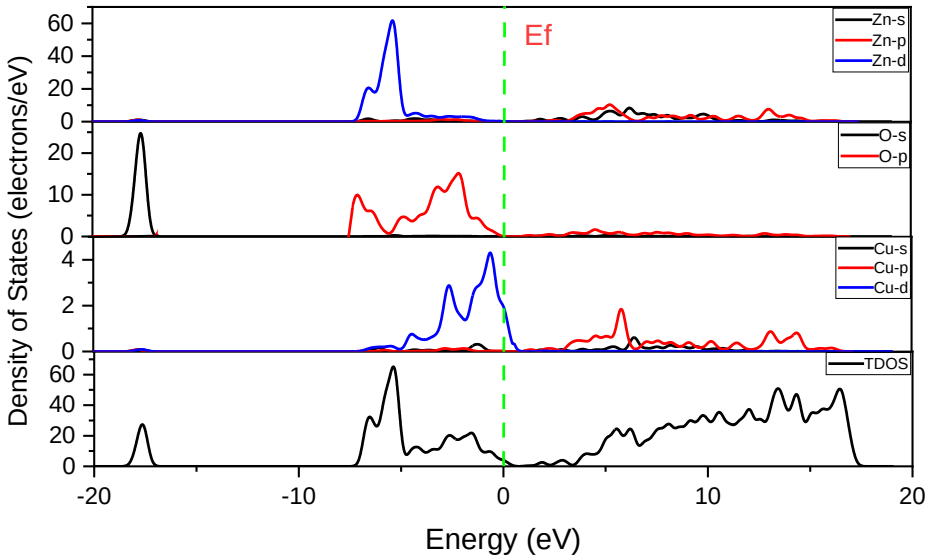



Figure 7. The density of total and partial cases of copper-doped zinc oxide (Cu)

**The electronic properties of copper-doped zinc oxide (ZnO) (Ni)**

The energy gap of nickel-adsorbed zinc oxide (ZnO) on the unit cell (3x3x1) was calculated using the (GGA-PBE) approximation. The preferred site for nickel atom adsorption was above the oxygen atom in the zinc oxide molecule. The energy gap between the nearest points of the conduction and valence bands was indirect, occurring at both the (M,G) point, with a value equal to (0.862 eV)

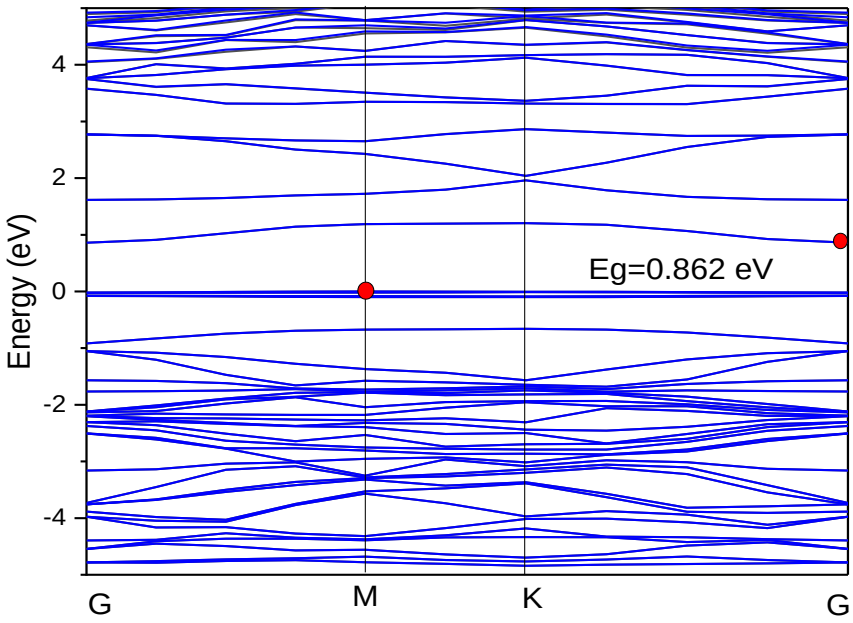



Figure 8. The energy gap for the adsorption of Ni on the surface of pure zinc oxide.

The density of partial and total states was calculated using the Generalized Gradient Approximation (GGA-PBE) on a large unit cell (3x3x1) of zinc oxide doped with nickel (ZnO-Ni). A plot containing the density of all states (total and partial) was used to obtain an accurate electronic structure diagram for nickel-doped zinc oxide. The figure shows

that the black color indicates the s orbital, the red color indicates the p orbital, and the blue color indicates the d orbital. In the zinc (Zn) atom, the valence band gives the highest state density at the d orbital, reaching (70.5 electron/eV) at (-5.57 eV), which dominated the valence band, and the density dropped to zero.

The states gradually appear at the energy gap, while the conduction band has the highest peak of density of states at the s orbital, reaching (9.19 electron/eV) at (5.68 eV), and the highest peak of density of states at the p orbital, reaching (10.57 electron/eV) at (5.05 eV). This means it contains free-moving electrons, with the (s,p) orbitals dominating the conduction band. In the oxygen atom (O), the valence band exhibits the highest density of states at the s orbital, reaching (23.5 electrons/eV) at (-17.9 eV). Additionally, the p orbital recorded the highest density of states at (17.29 electrons/eV) at (-2.07 eV). The s and p orbitals dominate the valence band, and the density of states is zero at the Fermi level (the zero level), which is devoid of electrons.

In the conduction band, the p-orbital is dominant in the conduction band and gradually diminishes. In the Ni atom, the valence band gives the highest density of states at the d orbital, which reached (0.8 electron/eV) at (-0.7 eV). The d orbital dominates the valence band, and the density of states becomes zero at the Fermi level (the zero level), which is free of electrons. In the conduction band, the d orbital dominates the conduction band, where the d orbital records the highest density of states (14.13 electrons/eV) at (0.78eV), while the p orbital records a peak value of (2 electrons/eV) at (0.78eV).3.26 eV).

As for the calculation of the total density of states for zinc oxide adsorbed with nickel atoms (ZnO-Ni) in Figure (3-16), the first valence band extends from (-17.3 eV to -18.4 eV), with a peak density of (26 electrons/eV). The second density of states extends from (-1.2 eV to -7.4 eV), with the highest peak reaching (73.4 electrons/eV) at (-5.6 eV). The density of states vanishes at the Fermi level. The conduction band density of states extends to (17.2 eV), with the highest peak reaching (50 electrons/eV) at (15.6 eV), and the largest contribution is between The d and p orbitals of the atoms (Zn, O) respectively, and hybridization is clear and strong at the s orbital of the (O) atom and the d orbital of the atom. (Ni).

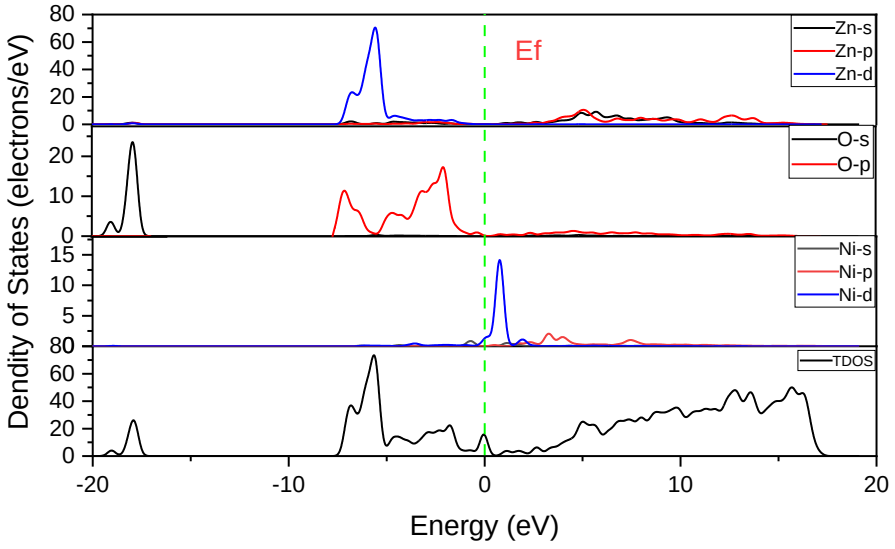



Figure 9. The density of total and partial states of nickel-adsorbed zinc oxide (Ni)

**Electronic properties of nickel-doped zinc oxide (ZnO) (Ni)**

The energy gap of zinc oxide (ZnO) doped with a nickel (Ni) atom instead of a zinc (Zn) atom on the surface of pure zinc oxide (ZnO) and on the large unit cell (3x3x1) was calculated using the (GGA-PBE) approximation. The changes in the electronic properties of the zinc oxide molecule after doping with a copper atom were studied, and the energy gap was found to be between the closest points of the conduction and valence bands directly, where it was located at both the (G) point with a value equal to (0.369 eV).

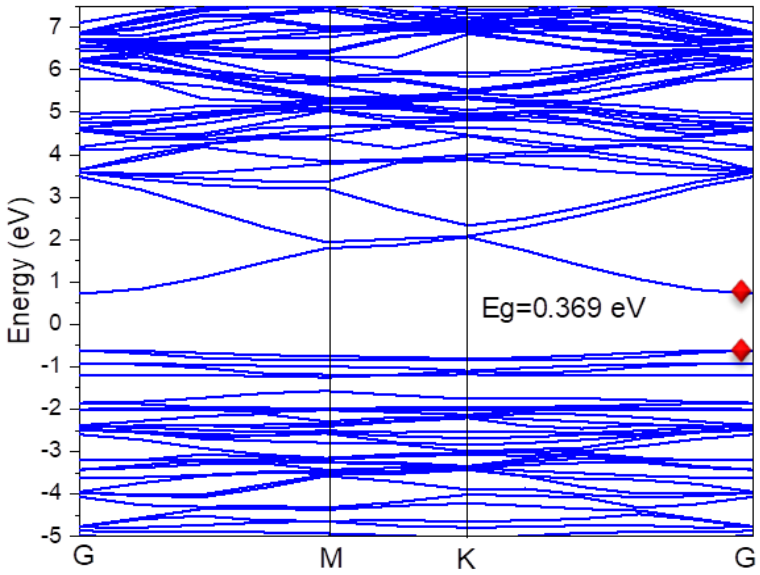



Figure 10. Energy gap for doping Ni instead of Zn in zinc oxide.

The partial and total density of states were calculated using the generalized gradient approximation (GGA-PBE) on a large unit cell (3x3x1) of nickel-doped zinc oxide (ZnO_Ni). A plot containing the total and partial density of states was used to obtain an accurate electronic structure diagram of copper-doped zinc oxide. The figure shows that the black color indicates the s orbital, the red color indicates the p orbital, and the blue color indicates the d orbital. In the zinc (Zn) atom, the valence band shows the highest density of states at the d orbital, reaching (61 electron/eV) at (-5.85 eV), which dominated the valence band. The density of states gradually decreased at the energy gap.

The conduction band shows the highest peak of the density of states at the s orbital, reaching (7.9 electron/eV) at (-5.69 eV), and the highest peak of the density of states at the p orbital. It reached (10.37 electron/eV) at (-4.79 eV), meaning it contains free-moving electrons where the (s,p) orbitals dominate the conduction band. In the oxygen atom (O), the valence band shows the highest density of states at the s orbital, reaching (25 electrons/eV) at (-15.2 eV). Additionally, the p orbital recorded the highest density of states at (15.3 electrons/eV) at (-2.68 eV).

The s and p orbitals dominate the valence band, and the density of states is zero at the Fermi level (the zero level), which is free of electrons. In the conduction band, the p-orbital is dominant over the conduction band and has gradually diminished. In a (Ni) atom, the valence band extends from (-7.1 eV to -1.16 eV), giving the highest density of states at the d orbital, which reached (4.12 electron/eV) at (0.02 eV). It is observed that the d orbital has transitioned from the valence band to the conduction band through the energy gap. In the conduction band, both the s and p orbitals dominate the conduction band, with the p orbital recording the highest density of states (1.9 electrons/eV) at (5.7 eV).

As for the calculation of the total density of states for nickel-doped zinc oxide (ZnO_Ni) shown in Figure (11), the first valence band extends from (-18.8 eV to -17.6 eV) with a peak density of (27.66 electrons/eV). The second density of states extends from (-7.6 eV to 1.5

eV) with a peak density of (64.5 electrons/eV). (-5.9 eV). As for the conduction band, the density of states extends from (3 eV to 16.77 eV), with the highest peak reaching (50.2 electrons/eV) at (15.9 eV). The largest contribution is between the d and p orbitals for the atoms respectively (Zn, O), another contribution is between the p and d orbitals for the two atoms respectively (O, Ni), and hybridization is clear and strong at the s orbital of the O atom and the d orbital of the atom. (Ni).

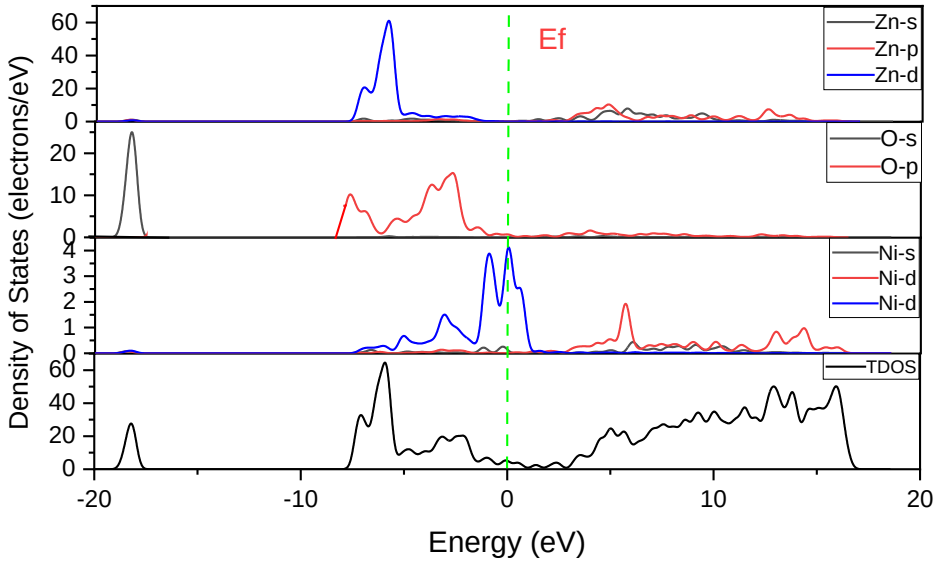



Figure 11. The density of total and partial states of nickel-doped zinc oxide (Ni)

## 4. Conclusion

In the current study, a large cell unit (3x3x1) was used with the Generalized Gradient Approximation (GGA-PBE) for zinc oxide (ZnO), where the electronic properties (band gap and total and partial density of states) of pure, doped, and copper (Cu)-doped zinc oxide were calculated. The band gap of pure zinc oxide (ZnO) that was deduced was (1.683 eV), which is a direct band gap and lies at the G point using the Generalized Gradient Approximation (GGA-PBE). The band gap of zinc oxide (ZnO) doped with copper (Cu) that was deduced was (0.11 eV), which is an indirect band gap and lies at the K and G points. As for the band gap of zinc oxide (ZnO) doped with copper (Cu) that was deduced, it disappeared due to the overlap of the conduction and valence bands, and the semiconductor material transformed into a conductor.

When nickel was adsorbed, the energy gap of zinc oxide (ZnO) adsorbed with nickel atom (Ni) became (0.862 eV), which is a direct gap and lies at point G. The nickel-doped (Ni) energy gap was (0.369 eV), which is also a direct gap and lies at point G. As for the total state density of pure zinc oxide (ZnO), its highest peak reached (8.2 electrons/eV) at (-4.72 eV). The largest contribution comes from the (d, p) orbitals of the atoms (Zn, O) respectively, and the hybridization is clear and strong between the d orbital of the Zn atom and the s orbital of the O atom. Calculation of the total density of states for zinc oxide adsorbed on a copper atom (ZnO-Cu) shows a peak of 71 electrons/eV at -6.1 eV, and the density of states vanishes at the Fermi level. The largest contribution between the d and p orbitals of the atoms respectively (Zn, O) and another contribution between the d and p orbitals of the atoms respectively (Cu, O) is observed, and hybridization is evident. When nickel was adsorbed, the energy gap of zinc oxide (ZnO) adsorbed with nickel atom (Ni) became (0.862 eV), which is a direct gap and lies at point G. The nickel-doped (Ni) energy gap was (0.369 eV), which is also a direct gap and lies at point G. As for the total state

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