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Electronic Properties of ZnO Nanowires: A First-Principles Analysis Using Two-Probe Methodology

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ABSTRACT

In this study, the electrical characteristics of pure ZnO nanowires are investigated using density functional theory (DFT) inside the non-equilibrium Green's function (NEGF) paradigm. We clarify the underlying electronic behaviours by a thorough analysis of I-V curves, density of states (DOS) spectra, and transmission spectra. All calculations are carefully carried out using the Quantum Wise Atomistic Tool Kit programme and the Generalised Gradient Approximation (GGA). Our results show that localised d orbitals dominantly contribute to ZnO nanowire transmission properties. We also investigate the effect of doping with copper on these characteristics. Gradual doping from pristine to 2 and 4 Cu atoms shows significant enhancements, indicating a clear relationship between electrical properties and doping concentration. Notably, the device's potential as a resistor is highlighted by the greater linearity of current with copper doping, demonstrating adherence to Ohm's law. Moving beyond basic research, we tackle real-world issues in sensing applications, including the quick identification of copper molecules in water. We provide light on the Au-ZnO-Au structure's potential for sensor applications by thoroughly discussing its electron transport properties. In conclusion, this study advances our knowledge of the electrical characteristics of ZnO nanowires and how doping modifies them, opening the door to their application in a variety of electronic and sensing devices.

Keywords: *DOS, Transmission spectrum, I-V curve, Doping, GGA, NEGF*

1. INTRODUCTION

Nanotechnology is technology which deals with manipulation of molecules and atoms. “There is plenty of room at the bottom” [1] by Nobel Prize winner Richard P. Feynman gave rise to the topic of nanotechnology, which piqued the interest of numerous researchers. The first nanotechnology term was used by Norio Taniguchi in 1974[2,3]. Nanotechnology emerged as a field in 1980 through Drexler’s theoretical and public work [2]. The bottom-up and the top-down approach are the two different sorts of approaches that have been used. Utilizing the distinct and valuable chemical, physical, and biological features of materials at the nanoscale, which are very different from those seen in bulk matter, is where nanotechnology finds its application. By harnessing nanotechnology, enhanced material devices with novel properties are being developed. Electronic devices are becoming closer to molecular electronics as the electronic industry grows in scope and speed. The goal of molecular electronics is to employ a single molecule or a small group of molecules as the fundamental building block of electrical devices. The solid-state layers of conventional semiconductor devices are replaced with materials with dimensions below 100 nm, such as organic molecules, carbon nanotubes, and nanowires. An interdisciplinary approach is employed to build up our understanding of molecules and explore their electrical characteristics. To create functioning single-molecule measuring devices at cryogenic temperatures, nanofabrication techniques are required. These devices allow researchers to more clearly comprehend the quantum mechanical properties of current passing through individual molecules. The theoretical model for such devices is also being understood with the use of computational design tools. Its potential to revolutionize various sectors such as aerospace, agriculture, biotechnology, homeland security, information technology, medicine, and transportation is widely recognized. With the temporal scale expanding linearly with the number of particles N, the spatial scale scaling as N log N, and its accuracy scale potentially scaling as high as N7 to N! with a substantial pre-factor, nanotechnology embraces a variety of length and time scales [4,5].

Lately, efforts to investigate the electrical characteristics of zinc oxide (ZnO) have persisted in applying density functional theory (DFT) methods, frequently including non-equilibrium Green's function (NEGF) formalism to give a more holistic view. ZnO in its pristine form is a compound semiconductor consisting of zinc and oxygen atoms arranged in a crystal lattice structure. Pristine ZnO exhibits unique properties such as a wide bandgap, high electron mobility, and excellent optical and electrical characteristics. These properties make it highly desirable for various applications in fields such as electronics, optoelectronics, and sensing. ZnO nanowires are one-dimensional nanostructures synthesized from pristine ZnO

through various fabrication techniques. These nanowires retain the fundamental properties of pristine ZnO while exhibiting additional characteristics due to their nano-scale dimensions and high aspect ratios. The synthesis of ZnO nanowires often involves the controlled growth of ZnO crystals along specific crystallographic axes, resulting in elongated nanostructures with unique electronic and optical properties. Studying pristine ZnO is essential for establishing a baseline understanding of its properties, which serves as a reference point for evaluating the effects of doping, modification, or nanostructuring on ZnO nanowires. By characterizing pristine ZnO comprehensively, we can better interpret the changes induced by various fabrication techniques and understand how these alterations influence the performance of ZnO nanowire-based devices. The transport characteristics of nanometer-scale molecular devices are critical in advancing nanoelectronics [6]

A noteworthy advancement in these investigations is the examination of new doping strategies and how they affect the electronic characteristics of ZnO. Although the previously described work concentrated on copper doping, more recent studies have investigated a larger variety of dopants, including as nitrogen, rare earth elements, and transition metals [7]. These dopants are carefully selected in order to modify ZnO's conductivity, band structure, and carrier concentration in order to maximise its performance in electrical devices. Recent research has broadened the focus of practical applications beyond basic device characterisation to tackle real-world problems. For example, there has been a lot of interest in the quick identification of certain chemicals in water, such copper ions, utilising ZnO-based sensors [8]. To increase the sensitivity, selectivity, and reaction time of ZnO-based sensors for environmental monitoring and water quality evaluation, researchers are looking into novel sensor designs, surface functionalization methods, and signal processing algorithms.

2. THEORETICAL BACKGROUND

One-dimensional (1D) nanomaterials, in particular, are the fundamental building blocks for a broad range of possible utilizations in optoelectronics, sensors, biomedical engineering etc. Nanotubes stand out among the different 1D nanostructures for their special significance and range of potential uses. In 1985, the first stage in the development of carbon nanotubes became known, and in 1991, Iijima used the arc discharge method to create multiwall carbon nanotubes[9]. In 1993, Bethune broadened the field by investigating materials other than carbon, which resulted in the development of ZnO nanotubes. ZnO, a semiconductor, has a wide and direct bandgap, high thermal conductivity, high electron mobility and high exciton binding energy making it useful for several types of devices [9]. ZnO has a substantial exciton binding energy and a wide and direct bandgap in the near-UV spectral region[10]. ZnO exhibits significant piezoelectric and pyroelectric properties. Its discovery can be traced back to the 1930s, gaining prominence in the 1950s. Subsequently, ZnO experienced a peak in 1974 and a resurgence in the 1990s. Notably, the synthesis of n-type ZnO has been extensively pursued, as the production of p-type ZnO poses considerable challenges. The formation of ZnO involves structural defects in oxygen, such as zinc interstitials and antisites. When a nucleus of a particular species occupies a lattice position usually reserved for another species, such as a zinc atom occupying an oxygen site, this is known as an antisite defect. Interstitial defects arise when an atom occupies a position within the lattice that is not part of the regular lattice sites. Hall studies conducted on electron-irradiated ZnO indicate that zinc is the most probable candidate for a shallow donor predominantly associated with lattice-related effects, exhibiting an activation energy ranging from 30-50 eV. Various methods have been employed to produce nanostructured ZnO, including hydrothermal synthesis, bulk epitaxial film growth, sputtering, reactive evaporation, chemical vapors, and pulse aqueous chemical methods. In summary, although the basic ideas presented in the first research are still applicable, further developments have clarified ZnO's electrical characteristics and increased the range of possible uses.

Current research initiatives continue to push the frontiers of knowledge in this sector and open the door for the creation of next-generation ZnO-based devices by using sophisticated computational approaches, investigating novel doping tactics, and addressing real-world issues. Recently, the influence of Fe_3O_4 nanoparticles (NPs) on dielectric properties of planar and homeotropic oriented nematic liquid crystals (NLCs) were studied during the temperature interval of 298–322 °K. It was found that the dielectric permittivity was considerably increased by adding NPs mass percentages. These results were assigned to the strong dipole–dipole interaction between the superparamagnetic particles and the surrounding liquid crystal molecules[11]. The effects of Co doping on the structural and optical properties of ZnO:Co nanoparticles were investigated using X-ray diffraction (XRD), scanning electron microscopy, fourier transform infrared (FTIR) spectroscopy, ultraviolet–visible spectroscopy, photoluminescence spectroscopy and vibrating sample magnetometer (VSM) [12]. The purpose of this study is to employ a two-probe setup to explore the electronic transport characteristics of the ZnO molecule.

3. METHODOLOGY

Using the Quantum Wise Atomistic Tool Kit software, density functional theory (DFT) with a basis set was used to computationally investigate the ZnO nanostructures [13]. Due to its great accuracy, the DFT-NEGF technique was used to account for the coupling between the expanded molecule and the electrode. For developing quantitative models of quantum transport, the non-equilibrium Green's function (NEGF) formalism provided a strong conceptual framework. [14]. The generalized gradient approximation (GGA) was used to calculate the exchange and correlation energy function [15]. One advantage of employing GGA is its ability to mitigate spurious scattering effects, aligning well with the benefits of NEGF. Sampling of the Brillouin Zone was achieved using a mesh of 1×1×100. Open boundary conditions were implemented in the transport direction for the transport

calculations. The current flowing through the conducting channel was evaluated using the Landauer formula. With the adoption of open boundary conditions, electrons were conveniently scattered, partially in the central region and partially in the donor region. The two-probe system comprised a left electrode, right electrode, and a scattering region. Referred to as the scattering region, the central region introduced variations in the physical and chemical environment, causing charge carriers traveling between the electrodes to undergo scattering. Sulphur has been used as linker atom due to the fact that sulphur can make stable chemical interactions with both zinc (Zn) and oxygen (O) atoms on the nanowire surface, it is frequently utilised as a linker element in ZnO nanowires. Because of this, sulphur may function as a passivation agent more effectively, preventing the emergence of surface flaws and enhancing the stability and electrical characteristics of the nanowire. In this variable bias voltage of -1V to 1V has been taken. Also extension regions are present for numerical stability. It is exact replica of electrode and are not allowed to change during the geometry optimization of device. In general the number of atoms and bias voltage cause significant change in transmission spectra. The current of device can be calculated by Lanunder-Buttiker formula [16] given by equation(1).

$$I=\frac{2e^2}{h}\int_{-\infty}^{\infty} T(E)[n_f(E-\mu_L)-n_f(E-\mu_R)] \quad (1)$$

where e=charge on electron, h is planck constant and T(E) is transmission cofficient,$n_f$are Fermi level,E is energy and μ_L ,μ_R are electrochemical potential of two electrodes. The transmission coefficient determines the probability of electron transferring between the two semi-infinite electrode [17]. The Virtual Nano Lab (VNL) interface of Atomistix Toolkit (ATK) was used for all modeling and simulation tasks [18]. Fig.1 shows the two-probe structure of ZnO sandwiched between two gold electrodes with oxygen atoms represented by red and zinc atoms represented by blue with sulphur acting as anchoring element whose reason has been already discussed above.

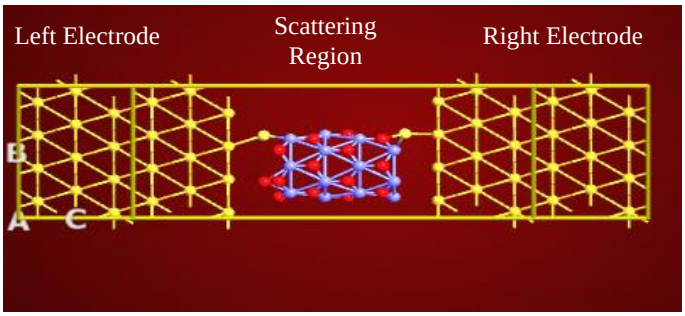

Figure 1. Two-probe structure of ZnO sandwiched between two gold electrodes.

3.1. Mechanism of Charge Transport

In this study, the phenomenon of charge transport is described as ohmic. In 1961, Harden Mc Connell gave a mathematical equation for electron transfer rate constant across a bridge, denoted by equation (2)

$$K_{ET}=Ae^{-\beta l}, \quad (2)$$

where l represents the length of the bridge and β is an energy-dependent parameter characterizing the voltage molecule. The electron transport process involves three types of processes [19]. The first type involves donor and acceptor sites acting as a single molecule, while the second type involves components with the lowest unoccupied sites separated by a bridging element, possessing molecular orbitals of different energy levels. Electrons tunnel through the right electrode towards the acceptor side during this procedure, also referred to as electron-type super exchange. Hoping is the last step, in which an electron is excited thermally or electrically and hops from the donor to the acceptor. In this case, ohmic charge flow causes incoherent diffusive processes, with tunneling playing a prominent role. Two cases can be considered:

1. When the particle's total energy (E) exceeds the voltage (Vo) (E > Vo).
2. When the particle's total energy (E) is lower than the voltage (Vo) (E < Vo). [20-22]

The particle will unquestionably overcome the potential barrier in the first scenario (E > Vo), showing a unity transmission coefficient and a zero-reflection coefficient. The particle will unquestionably be reflected from the barrier in the second scenario (E < Vo), producing a transmission coefficient of zero and a reflection coefficient of one. The Theory of Resonant Tunnelling via Molecules explains how molecular orbitals are used for electron transport. Electron transport through molecular orbitals is made possible when there is enough energy close to the Fermi level. Applying a bias to the acceptor and donor metallic terminals will result in the necessary alignment.
It has been noted that the distance between the donor and acceptor sites affects the rate of charge transport [23]. Equation $k_{CT}(R) = k_0 e^{-\beta R}$ can be used to calculate the charge transport rate $k_{CT}(R)$, where k_0 stands for the pre-exponential factor and β is the decay parameter that can be used to distinguish between the various charge transport processes present in DNA.

Each chemical orbital has a certain energy value, and the occupancy of these orbitals defines a molecule. In contrast to vacant molecular orbitals, occupied molecular orbitals have electrons. The energy difference between highest occupied molecular orbitals and lowest unoccupied molecular orbitals is denoted by the HOMO-LUMO gap (HLG). The Fermi level of the terminals is situated in the center of the HOMO-LUMO gap when no bias is applied. When a positive voltage is applied to the donor side, the terminal loses electrons, lowering the Fermi level for the source terminal while maintaining the donor's Fermi level in the center of the HLG. When a potential difference is present, current begins to flow, indicating either p-type or n-type conduction. As the voltage value increases, the current further intensifies. Applying a negative potential to the acceptor causes electron injection, leading to an increased current flow and an elevated Fermi level. This establishes a bridge and results in n-type conduction."

4. DATA COLLECTION AND ANALYSIS

4.1. DOS

Density of state basically tells the probability of presence of electron. DOS is number of electronic energies calculated per volume. If there is presence of high DOS it means there are high energy electrons with higher probability of transmission. If DOS is less, it is observed that the probability of transmission is less in terms of presence of less numbers of electrons. The mathematical formula for DOS is given by equation (3)

$$D(E)=dN(E)/d(E) \text{ [24]} \quad (3)$$

The quantity N represents the count of electrons possessing energy E that exist within a specific energy range dE, with the number of electrons being energy-dependent [3].

4.2. Transmission Spectra

The calculation of the transmission spectra is very interesting. Fermi level is the location where the transmission peak is at its highest. The transmission spectrum compares the electron energies and the HOMO LUMO gap. The type of peaks in the transmission spectra defines the type of tunneling whether it is through-bond tunneling or through space resonance tunneling. If the through bond tunneling is happening then it is characterized by broad peaks, and if there is space resonance tunneling happening then it is characterized by sharp narrow peaks. Through-bond tunneling is done through delocalized orbitals and space tunneling is done through localized orbitals. Through integration of the bias window, a finite portion of the transmission spectrum, we can also determine the current.

4.3. Molecular Energy Spectrum

Molecular energy spectrum is a spectrum of radiation which is formed due to transitions and other quantum charges consisting of few lines. It helps to find HOMO-LUMO gap at 0 eV. Through HOMO-LUMO chemical stability is calculated.

4.4. I-V Characteristics at Different Bias Voltages

It is apparent that relying solely on the transmission spectra is insufficient to fully characterize the transport characteristics of ZnO. Therefore, it becomes imperative to examine the current-voltage (I-V) curve, which provides insights into electron transport behavior under varying bias voltages.

5. RESULTS AND DISCUSSION

5.1. DOS Analysis

The DOS, which is inversely proportional to the slope of energy [25], can be integrated with respect to energy in order to calculate the total number of energy levels. Energy levels decrease with energy band steepness whereas energy levels increase with energy band height. In this electron flow take place by effect of super exchange technique. The electrons flow from one side to another and exhibit tunneling process. From figs. 2(a),(b) and (c), it is evident that the first peak of HOMO is at approximately 0.3 eV and LUMO peak is at approximately at 0.2 eV. There is a very small amount current present at 1.5 V. The HOMO-LUMO gap for the pristine form of ZnO nanowire is very narrow, indicating a small energy difference between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO). This suggests that the pristine form may have relatively high electron mobility and conductivity. With the introduction of 2 Cu dopants, there is a noticeable increase in the HOMO-LUMO gap compared to the pristine form. Interestingly, with 4 Cu dopants, there is a slight decrease in the HOMO-LUMO gap compared to 2 Cu dopants, but it remains higher than the pristine form. This indicates that increasing the doping concentration may have complex effects on the electronic structure of the nanowire, possibly influencing its conductivity.

5.2. Analysis of Transmission Spectra

The energy within the bias window is between Fermi levels -EV/2 and EV/2. As it has been seen in figs.3(a),(b) and(c) that transmission is fully based on valence bands and it has been observed that the peaks are sharping at -1V and as we increase the number of doped Cu atoms, as a result there is an increase in transmission rate. The transmission rate for pure Au-ZnO-Au is 0.176, 0.719 for Au-ZnO-Au with two doped Cu atoms, and 1.088 for Au-ZnO-Au with four doped Cu atoms. This is a very high transmission rate since the electron excitation at that point is very strong. At 1V, the majority of the conduction takes place.

5.3 Analysis of Molecular Energy spectrum

The HOMO represents donor electrons and LUMO represents acceptor electrons and gap between them define molecular stability. Energy of HOMO is directly related to ionization potential and LUMO define electron affinity and in this case HOMO was found to be -0.0219 and LUMO to be 0.189 as is evident from figs.4(a),(b)and(c).

5.4. Analysis of I-V Characteristics at Different Bias Voltage

To conduct a more in-depth analysis, we examined the I-V curve of our device, noting its highly symmetric nature when subjected to applied voltage. As the voltage is increased the value of current is increased. As we have shown in transmission peak that high conductance is around 1V, so the maximum current is also around the same voltage for all the three devices. It can be observed from the fig.5(c) that the graph for Au-ZnO-Au with 4 doped atoms of Cu, after 0V is a linear graph. It is obeying Ohm's Law. In case of Au-ZnO-Au with 2 doped Cu atoms in fig.5(b) the slope of the graph changes at around 0.6V which is the same voltage where we can observe the peak in the transmission spectra depicting a sudden increase in conduction. In case of the pristine form Au-Zn-Au device changes in conduction are seen at -0.6V, -0.4V, -0.2 V, 0.4V and 0.8V which are in agreement with the peaks of the transmission curve as is evident from Fig.5(a).

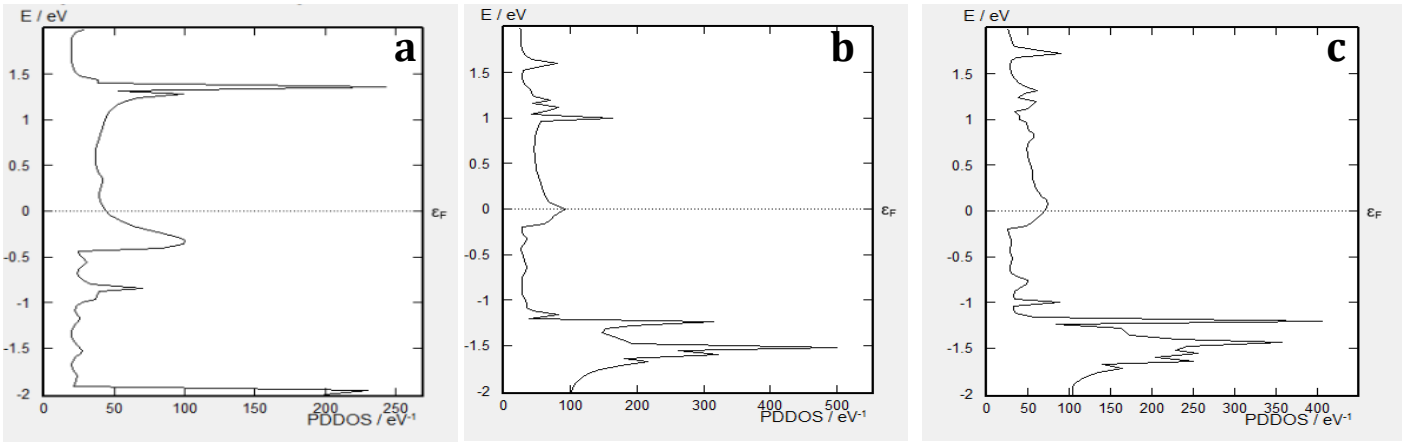

Figure 2. Density of states for (a) Pristine ZnO structure (b) Au-ZnO-Au structure with 2 doped atoms of Cu (c) Au-ZnO-Au structure with 4 doped atoms of Cu

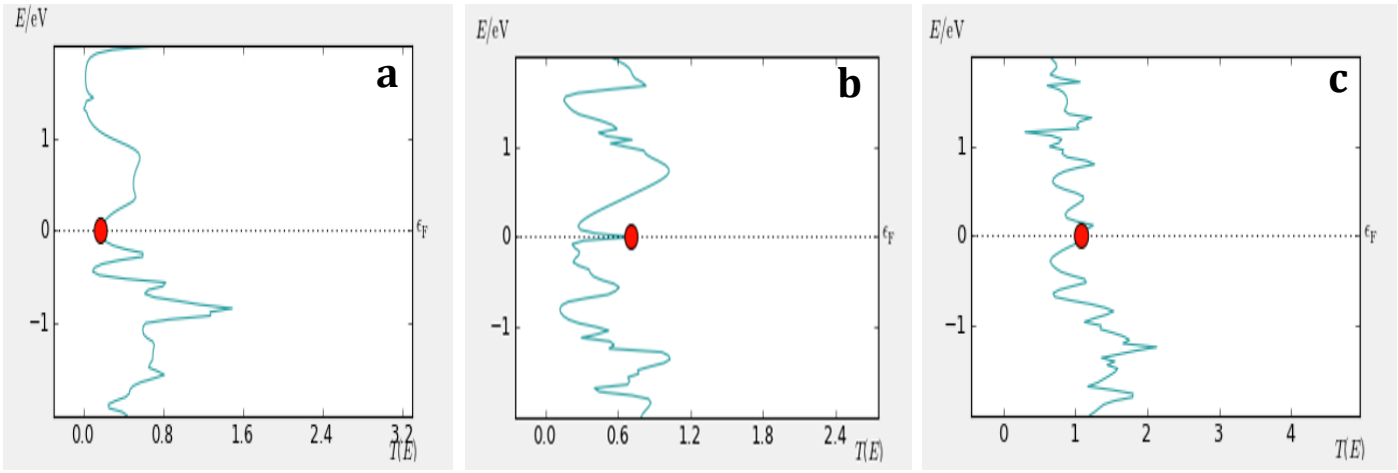

Figure 3. Transmission spectra for (a) Pristine ZnO structure (b) Au-ZnO-Au structure with 2 doped atoms of Cu (c) Au-ZnO-Au structure with 4 doped atoms of Cu

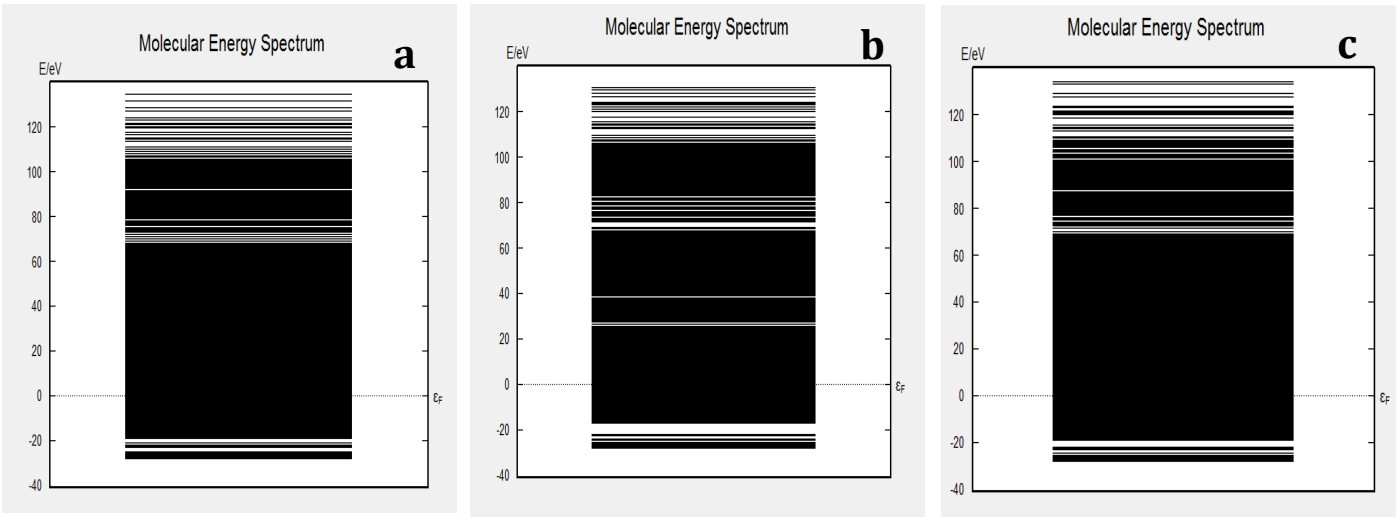

Figure 4. Molecular Spectrum for (a) Pristine ZnO Structure (b) Au-ZnO-Au with 2 doped atoms of Cu (c) Au-ZnO-Au with 4 doped atoms of Cu

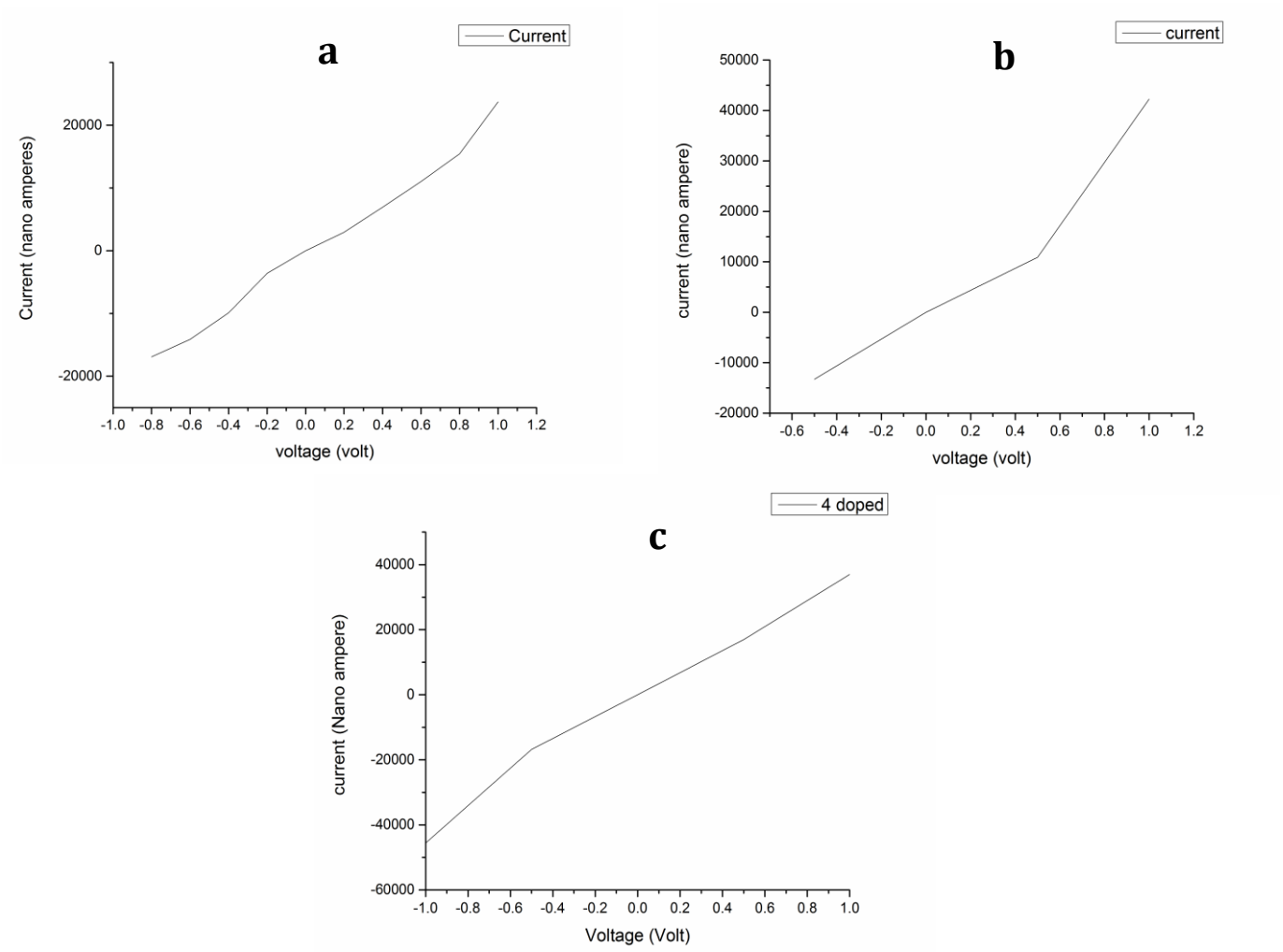

Figure 5. I-V Curve for (a) Pristine ZnO structure (b) Au-ZnO-Au structure with 2 doped atoms of Cu (c) Au-ZnO-Au structure with 4 doped atoms of Cu

Table 1: HOMO-LUMO Gap

Molecule	HOMO	LUMO	HOMO-LUMO
Pristine form	-0.0219	0.0189	0.003
2 doped of Cu	-0.0414	0.094	0.032
4 doped of Cu	-0.0268	0.065	0.038

6. CONCLUSION

In conclusion, our study employed a combination of Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) methods to investigate ZnO devices, focusing on Density of States (DOS), transmission spectra, and current-voltage (I-V) curves. Through our research, we observed that the contact surfaces between Au and ZnO considerable impact on how the current-voltage characteristics are calculated. Furthermore, our investigation revealed that valence band electrons play a crucial role in the majority of electron transmission. This finding provides valuable insights into the charge transport mechanism within the ZnO devices. Moreover, the introduction of Cu-doped atoms demonstrated significant improvements in the linearity, conductance, and electron transmission of the I-V graph. The resulting device with 4 doped Cu atoms exhibited characteristics consistent with Ohm's Law, suggesting its potential utility as a resistor. To further enhance the device's conductive qualities, future research could explore the effects of employing a greater number of Cu atoms, as well as switching the electrode material between Cu and Ag. A comparative study between these configurations would provide valuable information for optimizing the device's performance. Our work demonstrates the effectiveness of combining DFT and NEGF methods to gain a comprehensive understanding of ZnO devices and their electron transport properties. The findings not only shed light on the role of valence band electrons but also underscore the significance of Cu-doped atoms in enhancing the device's conductive behavior. This research opens up exciting possibilities for developing advanced electronic devices based on ZnO and highlights potential avenues for future investigations in the field.

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