

# Magnetic Moment of Zigzag CuO Nanotubes at Different Temperature and Size: Ab-Initio Study

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## Abstract

Temperature and size dependence magnetic moment of zigzag (n, 0) (n= 4, 6, 8, 10) copper oxide nanotubes (CuO NTs) have been computed by using a standard density functional theory. The computational work carried out by employing spin polarized generalized gradient approximation with revised Perdew Burke Ernzerhoff type parameterization along ab-initio approach. Bond length, binding energy and total magnetic moment have been analyzed and found that the bond length decreases at first and become saturated with increasing size of the nanotube. Highest binding energy of (10, 0) confirms this as the most stable amongst all the NTs taken into consideration. The observed electronic properties of considered CuO NTs, confirms the metallic nature. The size dependence magnetic moment at room temperature is decreases around up to (8,0) beyond that magnetic moments found to be increased with the diameter of the nanotubes. The computed temperature dependence's magnetic moment of NTs first increase up to room temperature (300K) and then decreases for all NTs except (8, 0).

**Keywords:** Density Functional Theory (DFT); Bond length, Binding energy; Magnetic moment; CuO Nanotube

## Introduction

In the past few years' investigation in the magnetic properties with different aspect in nano structure have been increased rapidly because of their technological importance, lots of attractive properties like, high surface-volume ratio, electronic, optical and magnetic properties as well as for understanding the physics involved in their many unusual properties comparing with the bulk [1-5]. Since, the discovery of the high temperature superconductor in copper oxide perovskite and its unique electric and magnetic properties, Copper oxide (CuO) got more attention and made more interesting candidate for research [6-8]. Our recent ab-initio investigation on magnetism in zigzag and armchair CuO nanotubes shows remarkable magnetic properties at different diameter [9]. So, it is worthwhile to investigate the temperature and size dependent magnetic properties in zigzag CuO nano tubes as a function of temperature.

As a bulk CuO is a p-type semiconductor with band gap of 1.1-1.9 eV, unlike other transition metal oxide semiconductor, it has monoclinic structure and possesses versatile band structure, optical and magnetic properties [8,10,11].

Our work focuses on the stability analysis of zigzag CuO nanotube in terms of its binding energy, diameter along with temperature dependence of magnetic properties. Organization of this article is as follows, next section discusses the method and computational details followed by result and discussion section and conclusion of the work is presented before the references.

## Method and Computational Detail

Computational calculation has been done by Density Functional Theory (DFT), based on ab-initio code named Atomistic Toolkit (ATK-VNL) with non-equilibrium Green Function (NEGF) [12-15]. ATK-VNL is a further development of TransSIESTA-C and is based on the methodology, models, algorithms developed in academic code TransSIESTA and in part McDCal employing localized

in SIESTA [16-18]. Spin Generalized Gradient Approximation with revised Perdew Burke Eenzerrhoff used for exchange correlation energy [19,20]. Valence electrons were described by localized pseudo atomic orbital's (PAOs), with double  $\zeta$  double polarized basis set. Mesh cut-off 75 Hartree is applied in entire calculation, with K-point sampling of  $1 \times 1 \times 20$  and maximum force tolerance set at  $0.05 \text{ eV/\AA}$  [21]. Calculation was began by minimization energy, optimized geometry and further. Minimization of energy gives us stable bond length between Cu and O. The stable bond length is used to creates the CuO zigzag nanotubes using ATK-VNL tool.

## Results and Discussion

### Stability and Structural Analysis

The current work carries the analysis of diameter dependence of structural stability and electronic properties. The diameter and temperature dependence magnetic properties of zigzag CuO nanotubes also studied shown in Figure 1. The calculated magnetic properties and structure parameter have been listed in Table 1. From Table 1 for the larger diameter nanotubes, the number of atom and Binding energy ( $E_b$ ) increases, whereas bond length between Cu-O is first increased and then become saturated. The nanotube of chirality (4, 0) is found to be stable at bond length (Cu-O) of  $1.95 \text{ \AA}$ , where chirality (10, 0) is stable at  $1.90 \text{ \AA}$ . The buckle appeared on the optimized structure of nanotube decreases with increasing the diameter as shown in Figure 1. This is mainly due to well known effect of reduction of bond strain on the curvature surface with increase in the diameter of nanotube [9].

Binding energy of the NTs are calculated through following relation;

$$E_b = \frac{[N * E_T(\text{Cu}_{iso}) + M * E_T(\text{O}_{iso}) - E_T(\text{CuONT})]}{N + M} \quad (1)$$

Where N= number of copper atoms present in SWNT

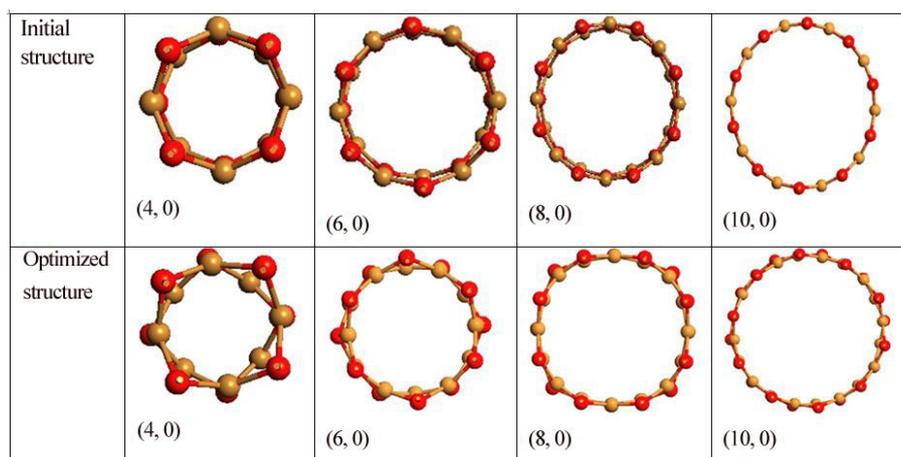
M= number of Oxygen atoms present in SWNT

$E_T$ = Total energy of Cu, O and CuO SWNTs respectively

Similarly, the binding energy is calculated through equation 1 and listed in Table 1, which concludes that the binding energy increases significantly with diameter of zigzag nano tubes for small value of diameter and after certain increase in the diameter it increase very slowly: this character of binding energy arise due to reduction in the strain.

Chirality (n,0)	No. of atom N	Bond length (Cu-O) $\text{\AA}$	Diameter $\text{\AA}$	$E_b$ (eV)	$\mu_{\text{total}}$ ( $\mu\text{B}/\text{atom}$ )
(4,0)	16	1.95	4.30	4.73	0.453
(6,0)	24	1.90	6.29	4.81	0.314
(8,0)	32	1.90	8.39	4.84	0.191
(10,0)	40	1.90	10.46	4.85	0.230

**Table 1:** Bond length, Binding energy, Diameter and Total Magnetic Moment at room temperature of CuO SWNTs

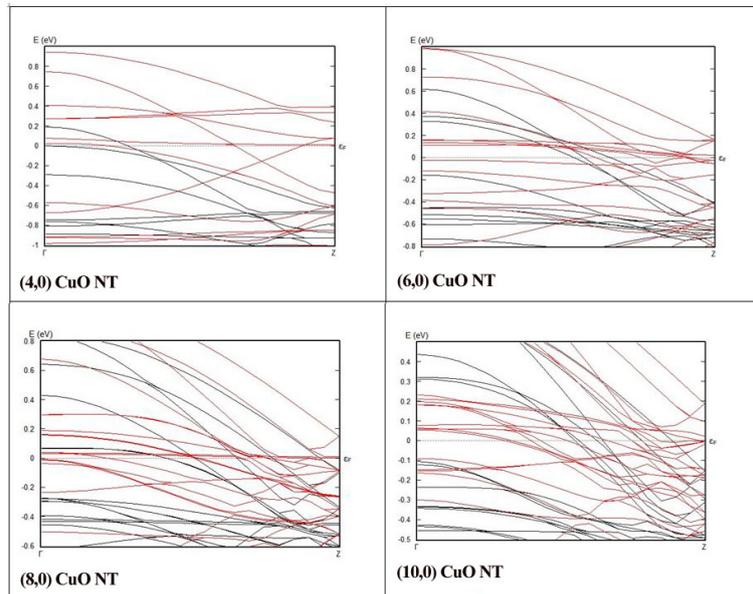


**Figure 1:** (color online) Initial and optimized geometries of CuO NTs

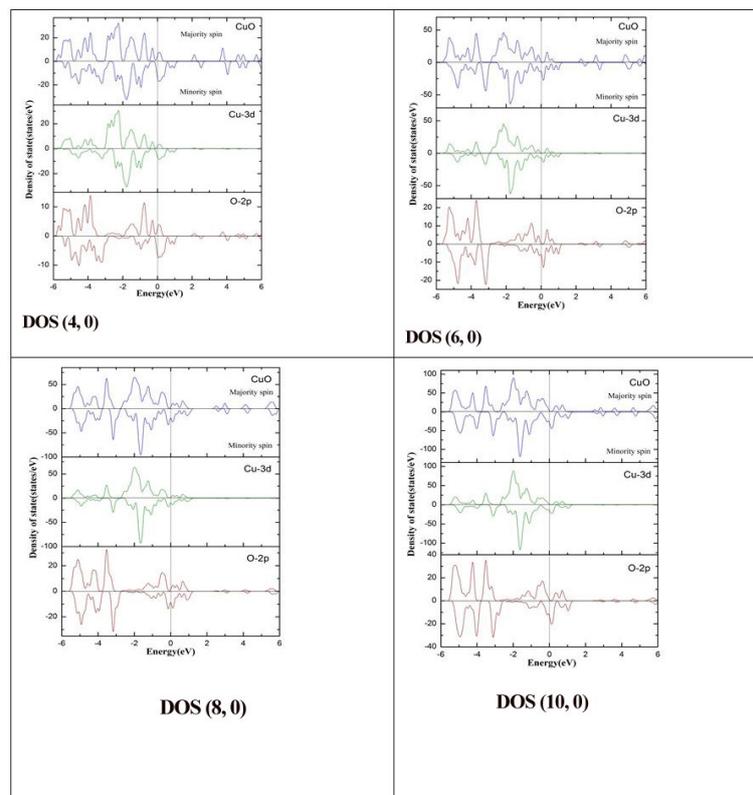
### Electronic Property

Band structure of CuO zigzag nanotubes with majority and minority spin at room temperature are plotted in Figure 2. Where black lines indicate the majority spin and red lines indicates the minority spin. Our work shows that zigzag CuO nanotubes are metallic in nature, but the bulk CuO is a p-type semiconductor. This is responsible due to hybridization between O-2p and Cu-3d states near the Fermi level. This nature observed here in our case is in line with that reported earlier [22,23].

At different diameter, and at room temperature, the density of state (DOS) of zigzag CuO nanotubes have also been observed using spin polarization DFT calculation and plotted at Figure 3. The peaks appear near the Fermi levels in valance band are because of Cu-3d and O-2p states, while the peak in conduction band is due to 4s state of Cu. The finite contribution of O atom to the density of state at Fermi level might be a reason for the metallic nature of nanotube, besides the hybridization on of Cu-3d and O-2p states.



**Figure 2:** (color online) Band structure of CuO NTs with majority(black) and minority (red)Spin



**Figure 3:** (color online) Spin Polarized DOS of CuO NTs at room temperature

## Magnetic moment

It would be exciting to analyze the magnetic properties because of the metallic nature of CuO nanotubes. Magnetic moment of zigzag CuO nanotube at room temperature listed in Table 1 on which we observe that the magnetic moment is high for (4, 0) (1.95 Å), after increasing in diameter magnetic moment is decreases but at for (10, 0) (1.90 Å) structure, it starts increases (Figure 4). The

magnetic moment of bulk CuO is  $0.86 \mu\text{B}/\text{atom}$  and individual Cu, O atoms values are  $0.68 \mu\text{B}/\text{atom}$  and  $0.18 \mu\text{B}/\text{atom}$  respectively [8]. Magnetic moment is induced due to the exchange-splitting between states, here exchange splitting of the Cu-3d and O-2p states provide magnetic moment to CuO NTs. The fluctuation on magnetic moment on increasing diameter are due to increase in number and decrease in bond length between Cu and O atom. According to Hund's rule of magnetism if the bond length is decrease and number of atom increased that means the atom coming together and interaction between them increases, here this is responsible for decreasing magnetic moment [24]. The total magnetic moment  $\mu_{\text{total}}$  ( $\mu\text{B}/\text{atom}$ ) of CuO nanotubes are linked directly to the individual magnetic moment of Cu and O atoms, strong interaction decrease their individual magnetic moment and affect the total magnetic moment of CuO nanotubes.

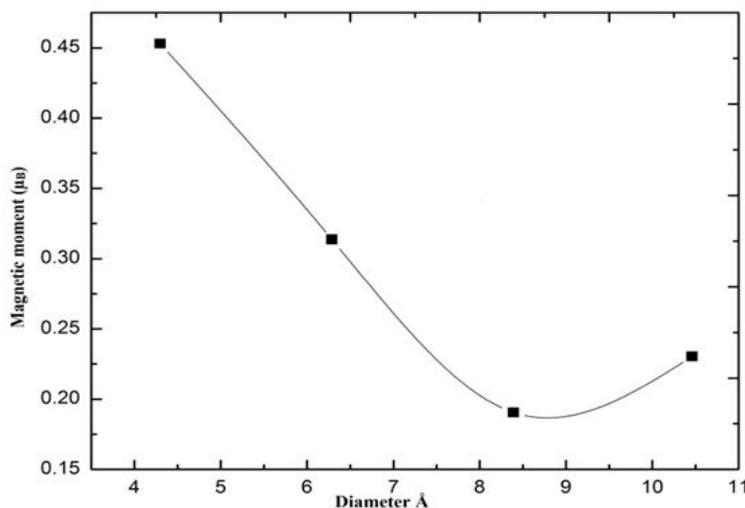


Figure 4: (color online) Magnetic moment as a function of diameter at room temperature.

Further we analyzed magnetic moment with different temperature. The temperature variation of the nano tubes is performed manually; it actually represents the temperature under which calculations are performed. We found that magnetic moment have high value at room temperature (300K) then decrease with increasing temperature which is shown at Figure 5. But for (8, 0) NT magnetic moment is increasing with increasing temperature. In our result maximum magnetic moment is observed at  $4.30 \text{ \AA}$  [(4,0) NT] and minimum at  $8.39 \text{ \AA}$  [(8,0)NT].

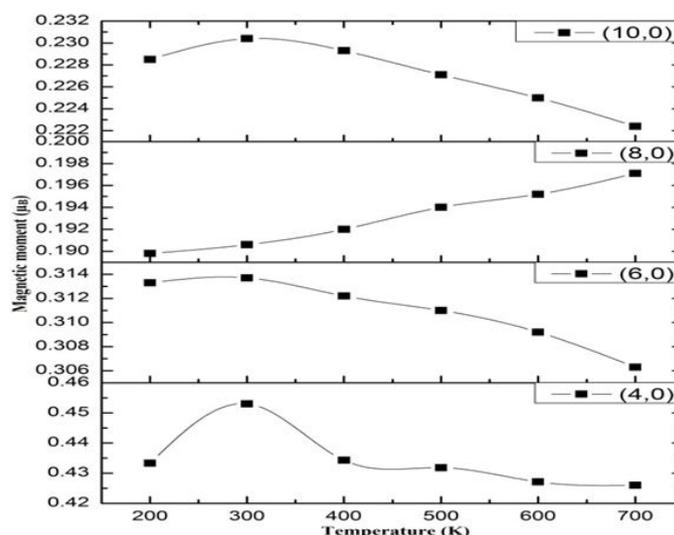


Figure 5: (color online) Magnetic moment as function of Temperature (K).

## Conclusion

Structural, electronic and magnetic properties of zigzag nano tube of (4, 0), (6, 0), (8, 0) and (10, 0) NT were analyzed by density function theory based on ab-initio code ATK-VNL. Buckling has been occurred on optimized geometry structure. The magnitude of buckling is decreases on increasing diameter of tube. Furthermore as diameter increases the number of atoms are also increases, however binding energy of CuO nano tube increases at first and tends towards the saturation with increasing number of atoms. The hybridization of Cu 3p state and O 2p state make CuO nanotube metallic. Magnetic moments were calculated through Mulliken population analysis of CuO nanotube. Magnetic moments with respect to different diameter and different temperature were investigated. Highest value of magnetic moment  $0.453 \mu\text{B}$  was observed for (4, 0) at 300 K, which continuously decreases for higher

diameter nanotubes which attains minimum value at (10, 0) beyond that it is found to be increased. We were also analyzed relation of temperature and magnetic moment. All study show peak value at room temperature except (8, 0). In (8, 0) nanotube magnetic moment is increase with temperature. As our findings are first in series, it would certainly be of great importance to the theoretical as well as experimental workers of this area. CuO show remarkable magnetic moment indicating that we can use it in spintronics devices, memory devices and magnetic sensors. We are seeking the experimental verification of these data. If verified CuO can be used as binary analog to other CNT with novel magnetic properties.

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