Ab’initio studies of the structural and electronic properties for single-walled armchair MgONT, SiCNTs and ZnONTs for next generations’ optoelectronics

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1.0 Introduction
Recent advances in the field of sustainability science and technology have revealed the need for greater exploration to behaviors of metallic and nonmetallic nano structures especially nanotube materials (Meenakshi et al., 2021). This has become necessary because of greater demand to replace semiconductors made from bulk structures with 1D semiconducting chips to replace semiconductors made from bulk structures. We studied the structural and electronic properties of free (7, 0) metallic oxides and non-metallic carbide nanotubes. SWMgONT, SWZnONT and SWSiCNT were chosen as the representative model. All the quantum simulation studies were done within DFT ab’initio implemented in quantum ESPRESSO. Results obtained for structural properties revealed that the most stable bond lengths of MgONT, ZnONT and SiCNT are 1.80 Å, 1.82 Å and 1.42 Å respectively. The results obtained revealed 2.8 eV band gap for SWMgONT, 0.5 eV for SWZnONT and 0.8 eV for SWSiCNT respectively. Furthermore SWMgONT and SWZnONT are regarded as direct band gap semiconductors while SWSiCNT is regarded as an indirect semiconductor with narrow band gap. The narrow band gap of all the three systems obtained demonstrates their potential in the optoelectronic application in the next generations’ sustainability science and technology. Recent studies showed that explorations were conducted on oxide nanotubes such SiO2NT, however to the best of our knowledge, studies of the oxide nanotubes of Mg, Zn and Si have not been reported, hence few literature are available.

Abstract
Due to greater demand to use 1D semiconducting chips to replace semiconductors made from bulk structures We studied the structural and electronic properties of free (7, 0) metallic oxides and non-metallic carbide nanotubes. SWMgONT, SWZnONT and SWSiCNT were chosen as the representative model. All the quantum simulation studies were done within DFT ab’initio implemented in quantum ESPRESSO. Results obtained for structural properties revealed that the most stable bond lengths of MgONT, ZnONT and SiCNT are 1.80 Å, 1.82 Å and 1.42 Å respectively. The results obtained revealed 2.8 eV band gap for SWMgONT, 0.5 eV for SWZnONT and 0.8 eV for SWSiCNT respectively. Furthermore SWMgONT and SWZnONT are regarded as direct band gap semiconductors while SWSiCNT is regarded as an indirect semiconductor with narrow band gap. The narrow band gap of all the three systems obtained demonstrates their potential in the optoelectronic application in the next generations’ sustainability science and technology. Recent studies showed that explorations were conducted on oxide nanotubes such SiO2NT, however to the best of our knowledge, studies of the oxide nanotubes of Mg, Zn and Si have not been reported, hence few literature are available.

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Therefore there is need to explore more about this nanotube across different chirality. Magnesium oxide nanotubes (MgONTs) are types of nanotubes obtained by rolling 2D sheet of MgO this nanotube served as an efficient catalyst and has been the focus of considerable attention because it catalyzes a variety of organic reactions, such as aldol reaction, synthesis of chiral epoxy ketones and chiral nitro alcohols (Muruga et al., 2012). It is one of the metallic oxide nanotube, it can exist as armchair, zigzag or chiral depending on the orientation of rolling the hexagonal magnesium oxide mono sheet. Another type of metal oxide nanotube is Zinc oxide nanotube, just as the case of MgONT, it is prepared when hexagonal mono sheet of ZnO is rolled to form a cylindrical nanotube. This research will try to explore the electronic properties of metallic and nonmetallic oxide nanotubes by taking MgONT, ZnONT and SiO2NT as a representative samples. Recent studies showed that explorations were conducted on oxide nanotubes such SiO2NT (Ogihara, 2016), however to the best of our knowledge, studies of the oxide nanotubes of Mg, Zn and Si have not been reported, hence few literature are available.

2.0 Materials and methods

The microscopic structure of zigzag (7, 0) SWMgONT, SWZnONT and SWSiCNT is closely related to that of zigzag SWCNT (Yuqing et al., 2019), therefore the tubes are usually levelled in terms of the graphene hexagonal lattice vectors. Furthermore, comparing structure of all the systems to graphene lattice gives room for theoretical derivation of many properties of the materials under study. The structures of the CNTs are described in terms of the chirality of the tube otherwise helicity. This is defined by the chiral vector \( C_h \) and the chiral angle \( \theta \), the chiral vector can be described in terms of the lattice translational indices \((n, m)\) and the unit vectors \(a_1\) and \(a_2\). Structural optimizations of all systems were done by considering the lattice parameters of each atom, bond length and chiral angles were also considered. The zigzag SWMgONT, SWZnONT and SWSiCNT were all considered to be of \((7, 0)\) configurations. The calculated chirality were obtained by implementing the equation

\[
C_h = ma_1 + n a_2
\]  

Where \(m\) and \(n\) are the integers which denote the number of steps of the zigzag Mg-O, Zn-O and Si-C bonds along the hexagonal lattice. The degree of twisting the tube is determined by the chiral angle \( \theta \) between \( C_0 \) and \( a_1 \) (Chang et al., 2007).

The structural and electronic responses of the system of \((7, 0)\) SWMgONT, SWZnONT and SWSiCNT were computed using the DFT ab initio as implemented in quantum ESPRESSO (Maigari et al., 2022) (Sushant et al., 2018). The maximum number of atoms in each case is 28. The nanotubes were built by rolling up a considerably relaxed 2D sheets of MgO, ZnO and SiC respectively. The oxygen atom protrudes from the Mg, Zn and Si planes in an alternate direction by 0.38 Å. The nanotube bond length was ensured to be 1.82 Å, 1.80 and 1.52 for MgO, ZnO and SiC respectively. Kohn-Sham equations were applied by implementing the DFT ab initio quantum computing (Chien et al., 2021) framework within the Perdew-Burke-Emzahope (PBE) exchange functional. The energy cut-off value for the construction of the plane-wave basis was achieved at 60 Ry, and the k-point value which correlates to the ecut value was 1 x 1 x 40 k-mesh. This gives a total of 40 nk-points in the first Brillouin zone (BZ). The norm-conserving pseudo potentials were used to calculate the ion-electrons attractive interactions. The maximum force, stress, and displacements were set at 0.06 eV/Å, 0.06 GPa, and 6 x 10^-4 Å, respectively. The unit cell volume is 5515.67Å³ with lattice parameters \(a = 16.68\) Å and \(c = 7.68\) Å.

3.0 Results and discussion

3.1 Structural properties

The optimal and equilibrium structure of the model \((7, 0)\) SWMgONT, SWZnONT and SWSiCNT were studied, the results were outlined in Figure 1. All the structures were optimized by rolling 2D monolayers of their corresponding MgO, ZnO and SiC respectively. The materials were highly stable by ensuring that the bond length of MgO were ensured at 1.80 Å, a 1.82 Å bond length was also ensured for ZnO while 1.42 bond length was ensured for SiC. Therefore, it can be reported that the bond lengths of metallic oxide nanotubes is greater than the bond length of organic oxide nanotubes. Consequently, the Mg-O bond length is found to be the unique quantity to calculate percentage errors in the present study. It has been noted that the MgONT chirality demonstrates significant effects on the bond length, the direction of the bond length along the nanotubes axis is different from their direction along the tube circumference. The results of the structural properties of all the three systems revealed that the bond lengths decrease with diameter.

3.2 Electronic properties

In order to understand well about the physical characteristics of these three nanotubes, there is need to have better explanations about their electronic interactions between energy states, relationships between the HOMO and LUMO and the amount of charge carriers per energy state. Electronic properties are those parameters which fully demonstrates the state and electronic behavior in the material (Itas et al., 2022). In terms of nanotubes, band structure calculations determine the behavior of nanotubes in terms of their energy (E) and momentum (k) (Itas et al., 2020).
These are strongly coupled with quantities such as electrical conductivity and dielectric response. This section explains the electronic behaviors of SWMgONT, SWZnONT and SWSiCNT materials for applications to sustainability science and technology. The electronic bands structure and DOS for SWMgONT were presented in Figure 2. As can be seen in Figure 2 (a), there were empty band in conduction band up to 1.8 eV, similarly zero bands were seen in the conduction band from -1.7 up to Fermi level, there were no cross bands at the Fermi level and no any intersection at the Dirac point. This region is called the empty states for SWMgONT, as such it is regarded as the band gap. The band gap created as a result of electronic behavior of MgONT is 2.8 eV. This value agreed well with the range of bands obtained for MgONT and other nanotubes (Badar et al., 2012). The band gap obtained is a direct band gap because of amplitude correlation between HOMOLUMO (Itas et al., 2022), on the other hand they are at the same momentum. The narrow band gap of SWMgONT reported in this work reveals it potential in the next generation’s optoelectronic applications (Itas et al., 2022). To further confirm the reported band structure for SWMgONT, electronic density of states were studied. The result is presented in Figure 2 (b). There is higher intensity of electronic states in the conduction band than in the valence band. Presence of electronic states in the conduction bands is because of presence of delocalized electrons which are highly mobile and are responsible for electrical conductivity in SWMgONT. To justify the band gap obtained, empty electronic states can be seen from -1.8 up 1.8 eV.
Figure 2. Electronic bands and DOS for (7, 0) SWMgONT

Figure 3. Electronic bands and DOS for (7, 0) SWZnONT

Figure 4. Electronic bands and DOS for (7, 0) SWSiCNT
In the case of (7, 0) ZnONT, a very narrow band gap of 0.5 eV was realized (Figure 3(a)), just like SWMgONT, it is also a direct band gap. The band gap of SWZnONT is narrower than SWMgONT because Zn is more electron negative than Mg. The 0.5 band gap of ZnONT demonstrates its candidacy for thermoelectric device fabrication, it also revealed ZnONT as having a high potential for efficient power generation and cooling. The DOS spectrum of Figure 3(a) show the highest electronic state at 31, therefore it can be stated that there are more energy states in SWMgONT than SWZnONT. Unlike SWMgONT, fairly equal states can be seen between conduction band and the valence band. The electronic bands structure for (7, 0) SWSiCNT showed entirely different shape with those of SWMgONT and SWZnONT, this is enough to explain that bands for metallic oxide nanotubes are not the same with bands of organic nanotubes. As shown in Figure 4(a), an indirect band of 0.8 eV has been obtained for SWSiCNT, the bands are called indirect because the amplitude of HOMO are not at the same momentum with the amplitude of LUMO. Another reason for this is the carbon ability to form covalent bonding with a non-carbon compound. Furthermore, bands gaps for SiCNT decreases with chirality because it is indirect. It has also been established that zigzag SiCNT with n = 5 and 6 are metallic while zigzag SiCNT with n = 7-9 are semiconductors (Larina et al., 2008), our 0.8 eV result for this (7, 0) SWSiCNT confirms this claim. In the DOS spectrum of SWSiCNT shown in Figure 4(b), two sub bands can be seen in the valence band, these are called intra-bands. This intra–bands transition are as a result of excitations of carbon electrons from one band to another band in the same valence band.

4.0 Conclusion
In this study, the structural and electronic properties of metallic oxides nanotubes and organic nanotubes were studied within DFT ab initio approach. Structural properties revealed the most stable form of SWMgONT, SWZnONT and SWSiCNT are those with bond lengths of 1.80 Å, 1.82 Å and 1.42 Å respectively. Base on this results, the three systems studied can be regarded as good candidates for high elastic moduli applications such as automobiles shock springs. In terms of the electronic properties, it can be reported that zigzag form of metallic oxide nanotubes are semi conducting from n = 7-9, in the case of SiCNT, the results showed that is it semiconducting irrespective of chirality. The electronic bands structure and DOS for SWMgONT obtained revealed that there were empty band in conduction band up to 1.8 eV, similarly zero bands were seen in the conduction band from -1.7 up to Fermi level, there were no cross bands at the Fermi level and no any intersection at the Dirac point. This region is called the empty states for SWMgONT, as such it is regarded as the band gap. The band gap created as a result of electronic behavior of MgONT is 2.8 eV. This value agreed well with the range of bands obtained for MgONT and other nanotubes.

List of abbreviations
MgONT = Magnesium Oxide Nanotube
SiCNTs = Silicon Carbide Nanotubes
SWMgONT = Single Walled Magnesium Oxide Nanotubes
ZnONTs = Zinc Oxide Nanotubes

Declarations
Ethics approval and consent to participate
Not Applicable
Consent for publication
All authors have read and consented to the submission of the manuscript.
Availability of data and material
Not Applicable.
Competing interests
The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.
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