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Ab initio density functional theory investigation of Structural and electronic properties of double-wall zinc oxide nanotubes

S. Valadbeigi[1,*], A. Fatehalian[2,3,4], S. M. Elahi[1]

[1]Plasma Physics Research Center, Science and Research Branch, Islamic. Azad University, Tehran, Iran
[2]Department of Physics, Razi University, Kermanshah, Iran
[3]Nano Science and Technology Research Center, Razi University, Kermanshah, Iran
[4]Computational Physical Science Research Laboratory, Department of Nano-Science, Institute for Studies in Theoretical Physics and Mathematics (IPM), Tehran, Iran

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Abstract

The electronic properties of double-wall zinc oxide nanotubes (DWZnONTs) are investigated via density functional theory. The DWZnONTs are separated into two categories¸ where the inner and outer nanotubes are armchair-armchair and zigzag-zigzag single-wall nanotubes. The band structure of the DWZnONTs is calculated. Our results show that the inter-wall coupling diminishes the energy gap in semiconducting nanotube. We found that the energy gap of DWZnONTs depends on the structure of the inner and outer walls.

***PACs*:** 73.22.Fg; 61.46.Mp; 81.16.Pr; 71.15.Mb
Keywords: *Znic oxide nanotube; Density function theory; Density of states*

1. Introduction

Zinc oxide (ZnO) has attracted great interest in the last few years, because its nanostructures counterparts may offer unique optical, electrical, and piezoelectric properties. Bulk ZnO is a direct wide band gap semiconductor (3.4 eV)and has a strong excitonic binding energy of 60 meV at room temperature,which makes it a promising material for high-efficiency blue and ultraviolet optical devices. Recently, 1D ZnO nanostructures have attracted much attention due to their unique physical properties as well as their applications in optoelectronic nanodevices and functional materials. For example, nanolasers, transistors, field emission display and UV detectors, fabricated by 1D ZnO nanostructures have been reported by many researchers [1-5]. Among 1D ZnO nanostructures, ZnO nanotubes with hollow structures are expected to have excellent properties. Up to now, some methods to synthesize ZnO nanotubes have been reported. Li et al. synthesized ZnO nanotubes on Au-coated silicon substrate by physical evaporation of the mixture of ZnO and graphite powders [6]. Wang et al. synthesized ZnO core shell nanobelts via a solid vapor decomposition process and obtained ZnO nanotubes by sublimation on the Zn core [7]. Hu Xu et al have investigated the structural and electronic properties of (5, 5) armchair and (9, 0) zigzag single-walled ZnONTs by using the density functional theory [8]. They found that both armchair and zigzag ZnONTs are semiconductors with direct band gaps.

In this paper, our aim is to investigate the influence of the inner-wall between two single wall zinc oxide nanotubes(SWZnONTs) on the density of states of the resulting DWZnONTs, as well as on the individual SWZnONTs within the DWZnONTs. These computations are performed via first-principles full potential linearized augmented plane-wave density functional theory, as implemented in the WIEN2k code [9]. Our calculations are done in the range of 100-200 k-points. We found that due to the overlap of the semiconducting gaps of inner and outer walls, DWZnONTs have the semiconductor behavior.

2. Computational details and results

The electronic structure calculations are performed via first principles full potential linearized augmented plane-wave density functional theory as implemented in the WIEN2K code [9]. For the exchange and correlation terms, the generalized gradient approximation (GGA) is used [10]. The total number of k-points in the whole Brillouin Zone (BZ) is taken to be equal to 200. Calculations are performed in the supercell approximation within a cubic unit cell. Figure 1 shows the structures of SWZnONT , DWZnONT and the unit cell relaxed structure of DWZnONNT.

Two possible cases are investigated. In the first case, both the inner and outer nanotubes of the DWZnONT are initially armchair SWZnONTs. Figure 2 shows the density of states of a (8, 8) and (12, 12) SWZnONT. The results show that both the inner and outer SWZnONTs are semiconductor. Figures (4) and (5) show respectively the density of states and the band structure of (8, 8) @ (12, 12). Also, these Fig-

*Corresponding author: Shahoo Valadbeigi;
E-mail: plasma_shahoo@yahoo.com
Tel: (+98) 21 44869632
Fax: (+98) 21 44869640

Fig. 1. The structure and unit cell of DWZnONT

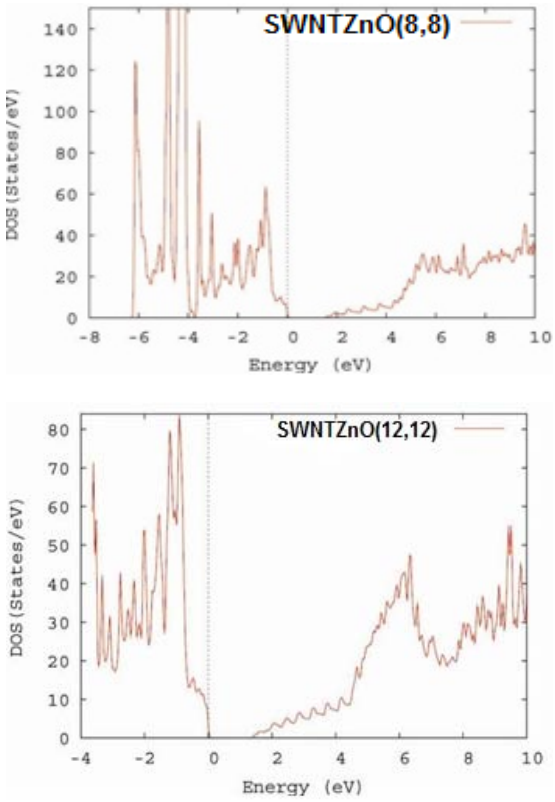

Fig. 2. The density of states of (8, 8) and (12, 12) SWZnONTs.

ures show the density of states of SWZnONTs , when they are parts of the DWZnONT. The results show that both the inner and outer SWZnONTs remain semiconductor and the DWCNT is also semiconductor.

In the second case, the inner and outer SWZnONTs are zigzag. Figures 3 show respectively the density of states of (5, 0) and (12, 0) SWZnONT. The results show that both the inner and outer SWZnONTs are semiconductor. Figures (6) and (7) show the density of states and the band structure for these DWZnONTs. The results show that both the inner and outer SWZnONTs remain semiconductor and the DWZnONT is also semiconductor.

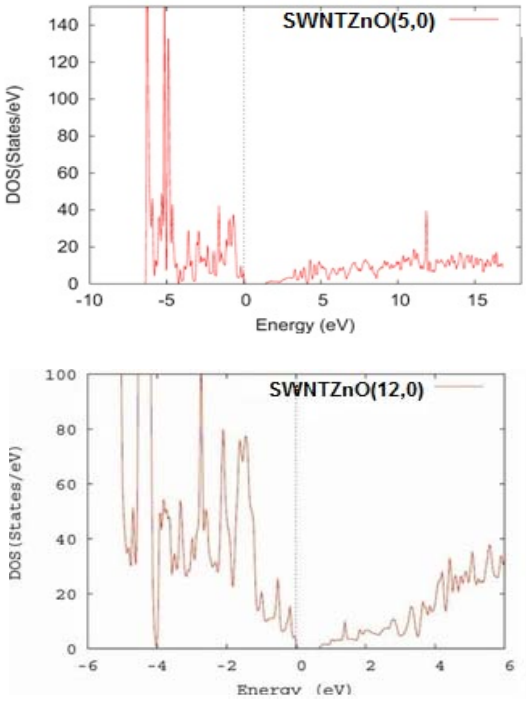

Fig. 3. The density of states of (5, 0) and (12, 0) SWZnONTs.

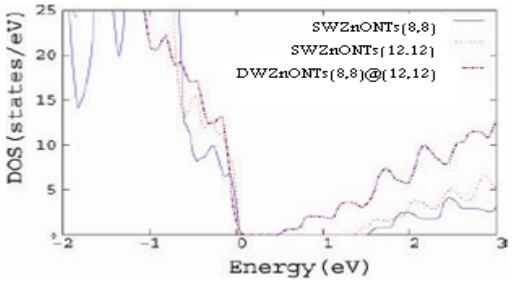

Fig. 4. The density of states of (8, 8) @ (12, 12) DWZnONTs.

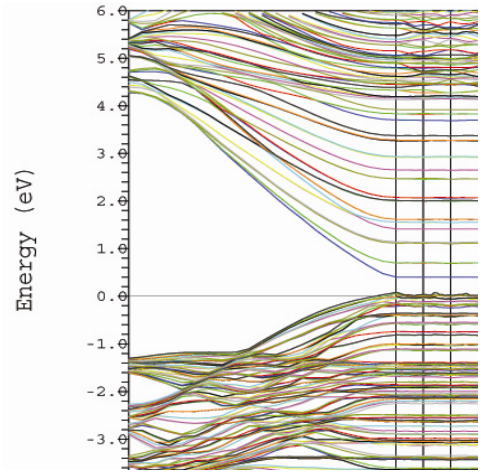

Fig. 5. The band structures of (8, 8) @ (12, 12) DWZnONTs.

The Fermi energy (8, 8) @ (12, 12) and (5, 0) @ (12, 0) DWZnONTs are equal to -0.197 (Ry) and -0.277 (Ry) respectively.
The behavior of the (8, 8)@(12,12) and (5,0)@(12,0) DWZnONTs is explained in terms of two factors which influence its electronic conduction properties. First, there is the overlap of the semiconducting gaps of individual SWZnONTs. Second, the interaction between the walls of the inner and outer SWZnONTs.

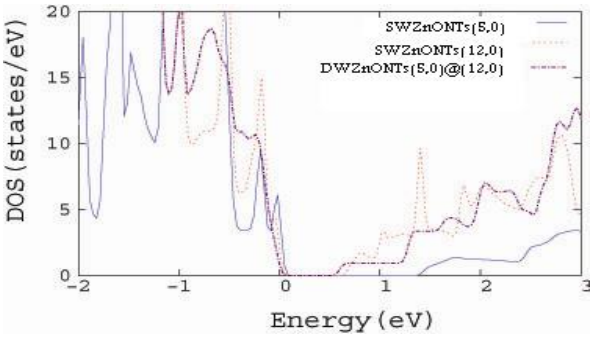

Fig. 6. The density of states of (5, 0) @ (12,0) WZnONTs.

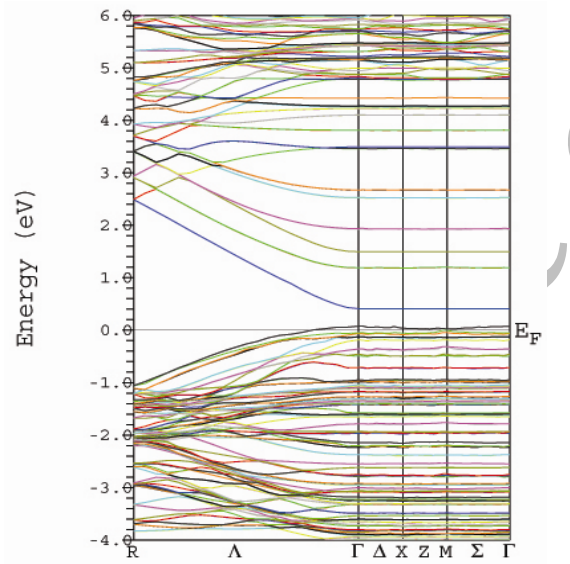

Fig. 7. The band structures of (5, 0)@(12,0) DWZnONTs.

3. Conclusion

We have investigated the electronic conduction properties of DWZnONTs via density functional theory as implemented in the code WIEN2k. All possible combinations of SWZnONTs making up a DWZnONT are considered. For DWZnONTs where both SWZnONTs are armchair or zigzag semiconductors, we found that due to overlap of the semiconducting gaps of inner and outer walls, DWZnONTs have the semiconductor behavior. Our results can open interesting avenues in research concerned with the use of zinc oxide nanotubes in the emerging field of nano-electronics.

References

[1] W. I. Park, G. C. Yi, J. W. Kim, S. M. Park 2003 Appl. Phys. Lett. **82** (4358).
[2] Y. W. Heo, L. C. Tien, Y. Kwon, D. P. Norton, S. J. Pearton, B. S. Kang, F. Ren, Appl. Phys. Lett. **85**, 3468 (2004).
[3] W. I. Park, J. s. Kim, G-C. Yi, M. H. Bae, H-J. Lee, Appl. Phys. Lett. **85**, 5052 (2004).
[4] C. S. Rout, S. H. SKrishna, S. R. C. Vivekchand, A. Govindaraj, C, Rao, NR. Chem. Phys. Lett. **418**, 586 (2006).
[5] Q. H. Li, Q. Wan, Y. X. Liang, T. H. Wang, Appl. Phys. Lett. **84**, 4556 (2004).
[6] X. H. Kong, X. M. Sun, X. L. Li, Y. D. Li Mater. Chem. Phys. **82**, 997 (2003).
[7] X. Y. Kong, Y. Ding, Z. L. Wang, J. Phys. Chem. B **108**, 570 (2004)
[8] Hu Xu, R. Q. Zhang, X. Zhang, A. L. Rosa, T. Frauenheim, Nanotechnology **18**, 485713 (2007).
[9] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Luitz, WIEN2k Karlheinz Schwarz, Tech.Universitat Wien, Austria ISBN 3-9501031-1-2.
[10] J. P. Perdew, S. Burke, M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).