International Journal of Physics and Mathematical Research *http://www.wrpjournals.com/IJPMR*
Vol. 1, No. 1, pp. 009-010, November 2012

Research Article

Ab-Initio Analysis of Electronic Properties of Linear Zno Nanowire of 0.4nm, 0.64nm and 0.8nm Diameter

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Received Article 15th October 2012; Published Article 30th November 2012

First principle density function theory based approach has been used to analyze the structural stability and electronic properties of ZnO nanowire in the zincblende (B3) type phase. The stability of the material has been analyzed using local density approximation (**LDA**) with the Perdew-Zunger (PZ) parameterization. The study found that the B3 type phase of ZnO nanowire is stable at different diameters and in comparison to its bulk semiconducting counterpart, the nanowire of the same is metallic in all the three diameters 0.4nm, 0.6nm and 0.8nm, taken into consideration.

Key words: ZnO, Nanowire, ab-initio, Zincblende

INTRODUCTION

semiconducting nanowires (NWs) with a onsymmetric crystal structure have recently drawn significant research interest[1] ZnO being wide band gap semiconductor interesting electronic, piezoelectric, and photoconducting properties [1].One-dimensional ZnO nanostructures have been synthesized in various morphologies like nanorods, nanowires, nanobelts, nanorings and nanohelices [2] ZnO nanowires (NWs) have been extensively studied over the past several years for their potential aplications in fabricating electronic, optoelectronic, electrochemical and electromechanical devices such as solar cells, ultraviolet(UV) lasers, piezonanogenerators, light-emitting diodes, and field emission devices [3] ZnO NW photodetectors and optical switches have been the subject of extensive investigations [4]

Computational method

We are performed our calculation by using Atomistix toolkit (ATK) based on the first-principles density-functional theory with the Localized density approximation (LDA-PZ) for exchange and correlation. The Steepest descent geometric optimization technique with Pulay algorithm for iteration mixing. The of special *k*-points of 1x1x50 used with energy cutoff of 100 Ryd the irreducible Brillouin zone integration The electronic structures and the quantum transport propertiesare calculated by using the density-functional theory (DFT) and the nonequilibrium Green's function (NEGF) formalism implemented in the Atomistix ToolKit (ATK) package (version 2008.02).[5]

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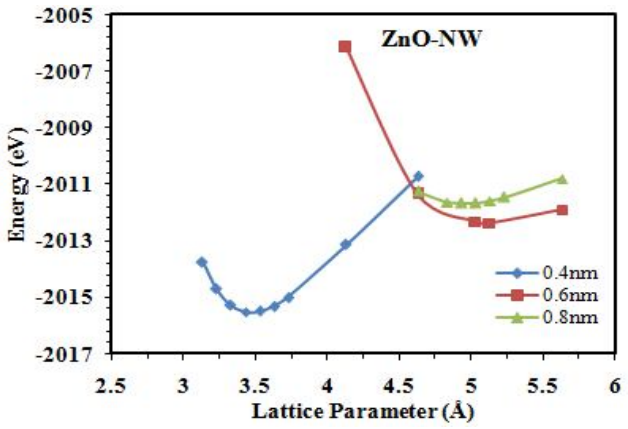
RESULTS

The study confirms the stability of B3 type hase of linear shaped ZnO nanowire at different diameters.ZnO nanowire at 0.8nm can be considered as the most stable structure as it posses the lowest total energy and higheat binding energy.The energy as a function of lattice parameter has been plotted for all the considered ZnO NWs and shown in Fig-1. The lattice parameter of ZnO NWs at 0.6nm and 0.8nm are larger than its bulk counterpart . The lattice parameters for the bulk ZnO in B3 phase is 4.63 Å shows a close match with its experimental counterpart [5].The electronic band structures shows that the present linear geometries are metallic in nature at all the three diameters 0.4nm, 0.6nm and 0.8nmand shiw in the Fig-2. The study observed the semiconducting (bulk ZnO) to metallic (ZnO NW) transition. The study shows that as the size increases the number of bands increases.The density of states clearly shows localization of states near the Fermi level, which clearly defends its metallic behavior.



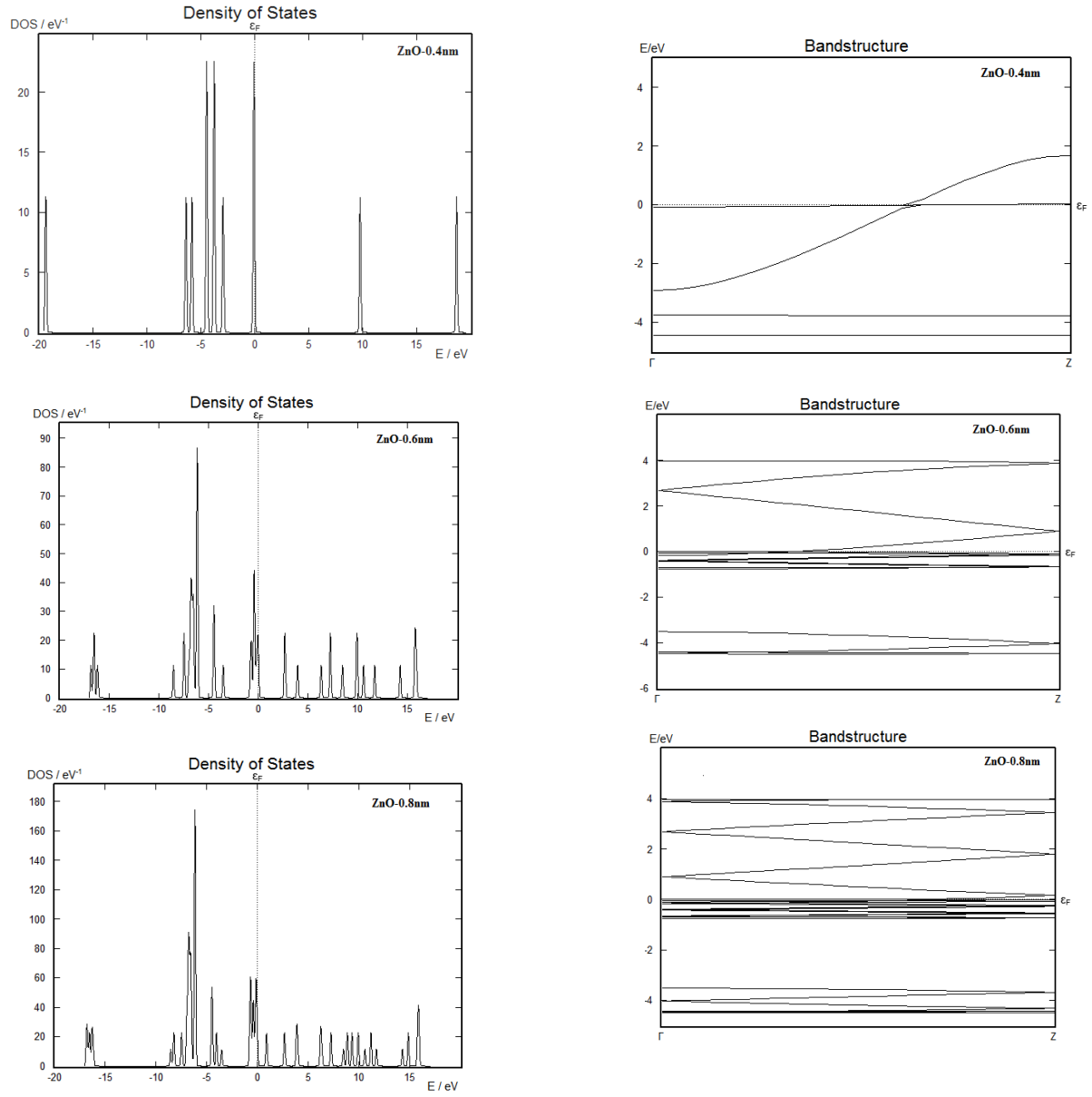


Fig.2 , 3 and 4 Electronic band structures and DOS of ZnO NWs of different diameters

Table-1: The lattice parameter (a), total energy and binding energy for different size ZnO nanowires

ture	Lattice Parameter (Å)	Total Energy (eV)	Binding Energy/atom (eV)
ZnO-0.4nm	3.43	-2015.52	-0.73
ZnO-0.6nm	5.13	-2012.37	-0.39
ZnO-0.8nm	4.93	-2011.68	-4.57

Conclusion

We have presented a first principle study of structural stability of linear shaped ZnO NWs with different diameters and found that all the ZnO NWs are metallic in nature. The metallic nature of these nanowires makes them useful in sensing and device applications.

Acknowledgement

Authors are thankful for we wish to thank Atomistix for the use of the trial version of Atomistix ToolKit 2.3 (ATK 2.3).

And Atal Bihari Vajpaiee institute of Information Technology and Management, Gwalior to providing the computational facilities in CNTL research Lab.

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