An ab-initio study of Stability Dependence on Structure of Zinc Oxide Nanowires

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Abstract

The performed study has explored structural dependence of stability for different proposed shapes for Zinc Oxide nanowires by using pseudopotentials DFT calculations. 2-atom linear, 2-atom zigzag, 4-atom square and 6-atom hexagonal nanowire are the four different shapes under consideration and the study has been performed by using ABINIT code. Our findings indicate that 2 atom zigzag shaped nanowire has shown greatest stability

Keywords: Density Function Theory, Density of State, Generalized Gradiant Approximations, Nanowires, Zinc oxide.

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1. Introduction

The present era is era of technological advancement and the world of nano dimension has played a critical role in reaching to this high level of comfort. The nanowires and the study of their electrical behaviour have come out to be an area of interest for the young researchers and the study of last 20 to 30 years are enough to show this trend. A strong deviation of properties is seen when we travel towards the smaller dimension. When the sizes of the materials are reduced to molecular dimensions they can develop exotic properties. The devices which are made from nanowires have strong dominance over the devices based on photolithography. The present work deals implication of the local density approximation to study the

stability dependence on structure for zinc oxide nanowires which has significant technical importance.

Various researchers have already sufficiently explored the silicon and germanium nanowires in theoretical as well as experimental manner [1-3]. ZnO has a wide band gap with many interesting electronic and optical properties and comes from the family of II-VI group. ZnO is used in optoelectronics and sensors [4-5]. ZnO has unique importance because of being the building blocks for coming futures. It is also used in logic circuits [6] and nanogenerators [7-8].

A lot of work has already been reported regarding synthesis of ZnO nanowire. Qing et al.[9] achieved successful synthesis of zinc oxide nanowire and fabricated gas sensors based on these nanowires. Highly densed zinc oxide nanowire array were successfully synthesized by direct oxidation of zinc substrate by Ren et al.[10]. ZnO nanowire arrays were synthesized directly on zinc foli by G. Tandra et al.[11] by using simple thermal evaporation process at critically low temperature. High purity single crystal ZnO nanowires were successfully synthesized by L. Chih and L. Yuan in 2009 by using thermal decomposition of zinc acetate dehydrates at 300 C without a catalyst [12]. Lupan O. et al.[13] synthesized and characterized the ZnO nanowires based nanosensors and highlighted their applications. Zinc oxide Nanowires with various morphologies wre synthesized by the hydrothermal method on silicon substrate coated with zinc oxide thin films by Bai S. and Wu S in 2011[14]. K. Chen et al. [15] synthesized ZnO nanostructures via hydrothermal method by using mixed solution of zinc chloride and HMTA as the precursor. Li X. et al. [16] prepared zinc oxide nanowires through reutilization of sludge from soy sauce waste water electrochemical treatment by using hydrothermal process. Zinc oxide nanowire arrays were synthesized on $ZnOTiO_2$ mixed oxide seeded FTO conducting glass plate by Marimuthu T et al. [17] in 2016 by using two step sol-gel and hydrothermal method. Zinc oxide nanowires were grown on grapheme foam with the help of hydrothermal synthesis by Yan H et al. [18] in 2017. Chen X. et al. [19] performed the IN-situ growth of zinc oxide nanowires over a sensing electrode by using facile hydrothermal route. The demonstration of rational synthesis of mono dispersed sized zinc oxide nanowires was performed by Zhao X et al. [20] in 2019. Successful synthesis for Zinc oxide nanofoam cluster was performed on zinc oxide nanowires using SiO_2/Si substrate by Chowdhary P. et al. [21].

The presented article explores the structural dependence of stability of zincoxide naowires for four different shapes 2-atom linear shaped nanowire, 2-atom zigzag shaped nanowire, 4-atom squared nanowire & six atom hexagonal nanowire, which has not been explored by any researchers in their reported work so far.

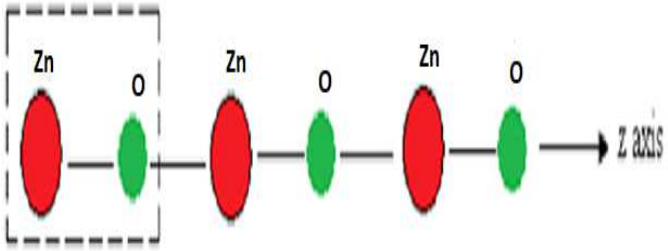
2. Computational Details

The structure of zinc oxide nanowires were investigated within the plane wave pseduopotential method by using ab-initio density functional theory calculations [22, 23]. The technique of pseduopotential has proven to be extremely useful for studying structural properties of various materials [24]. We have used ABINIT code for the proposed study [25]. The exchange correlation function of Perdew et al. [26] and generalized gradient approximation have been useful for the performed task. Troullier & Martins [27] exchange correlation has also been useful for the calculations. We received the required pseduopotential from ABINIT webpage itself. The calculations were initially applied on bulk zinc oxide material in order to test the potentials and the results so obtained were seen to be in close agreement with the already available experimental results.
The calculations were done by adopting a very self consistent manner approach.The optimization of zinc oxide structure has been performed for Hellmann-Feynman forces with a small value 10^{-3} eV/Å on each atom. The cut off energy has been considered as 30 Hartee for the performed calculations. The super cell of side 20 a.u. along XY directions were considered for positioning of nanowire. The Z axis is considered as the axis of wire and periodic boundary conditions were duely applied.

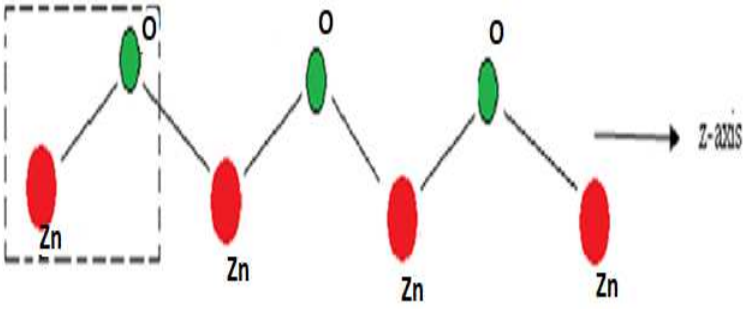
The 15k - points sampling for integration of Brillouin zone along z direction has been performed by using the Monkhorst-pack technique [28]. No constraints were imposed in order to obtain relaxation of atoms. The optimized value of lattice parameter for bulk Zinc oxide has been obtained. All the four structures are optimized to unless the lowest energy was reached.

3. Results and Discussion

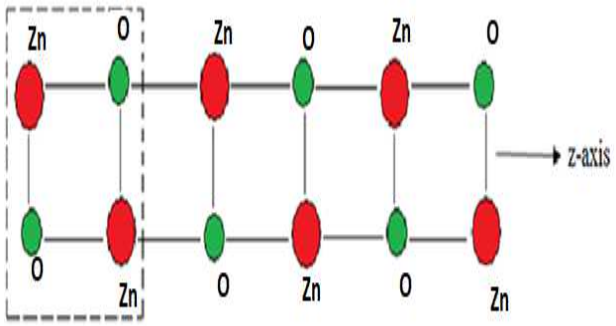
The paper covers the study of four completely different geometric structures for ZnO nanowires. The details concerned to proposed structures have been explored singnificantly in our already published work [29-39]. The various proposed structures of ZnO nanowires have been shown in Figure 1.



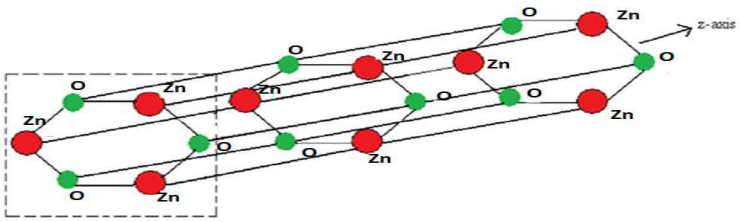
(a) 2-atom Linear Nanowire



(b) 2-atom Zigzag Nanowire



(c) 4-atom Square Nanowire



(d) 6-atom Hexagonal Nanowire

FIGURE 1. *Structures of Nanowires (a) 2-atom Linear Nanowire (b) 2-atom Zigzag Nanowire (c) 4-atom Square Nanowire (d) 6-atom Hexagonal Nanowire.*

In order to obtain the greatest stability of the various structures of zincoxide nanowires, the primary condition is to get the configuration corresponding to maximum stability and least energy for the proposed structures. The energy variation with inter atomic distance for all geometries are mentioned in Table 1-4

and the corresponding distance for minimum energy has been highlighted in the table. Table 5 is indicating the optimized energy and corresponding distance. the independent optimization of all structural parameters was performed for each structure to achieve configuration corresponding to the least energy. The calculation of energy has been performed, for infinite linear wire, as a function of x = 'a', where 'a' is the zinc oxygen distance up to 0.01 nm and then the effective total energy is determined. The 2- atom linear nanowire shows the least energy at a distance of 0.64 nm with energy value of -1056.56 eV where as the 2- atom zigzag nanowire shows least energy of -1058.29 eV at 0.22 nm distance, i.e.. the zigzag nanowire has lower energy as compared to a linear nanowire. For 4- atom squared nanowire, the energy is least at 0.22 nm with value of –1057.89 eV. Minimum energy configuration for 6-atom hexagonal nanowire predicts another time the inter atomic distance of 0.22 nm but its total energy is found to be -1050.37 eV. The overall findings of study shows that 2-atom zigzag nanowire has the least energy and maximum stability as compared to other structures under study The graphs showing the variation between distance & energy, for all the structures, have been shown in Figure 2 to Figure 5.

Table 1. Variation of energy (eV/atom) with Interatomic distance x (nm) for 2 atom linear nanowire shape of ZnO

X (nm)	Total Energy (eV/atom)
0.06	-829.87
0.10	-1044.34
0.16	-1052.75
0.22	-1054.76
0.26	-1055.18
0.32	-1037.29
0.38	-1053.18
0.42	-1030.61
0.48	-1029.48
0.52	-995.60

0.58	-1019.83
0.64	**-1056.56**
0.68	-1054.96
0.74	-1042.52
0.80	-1047.33

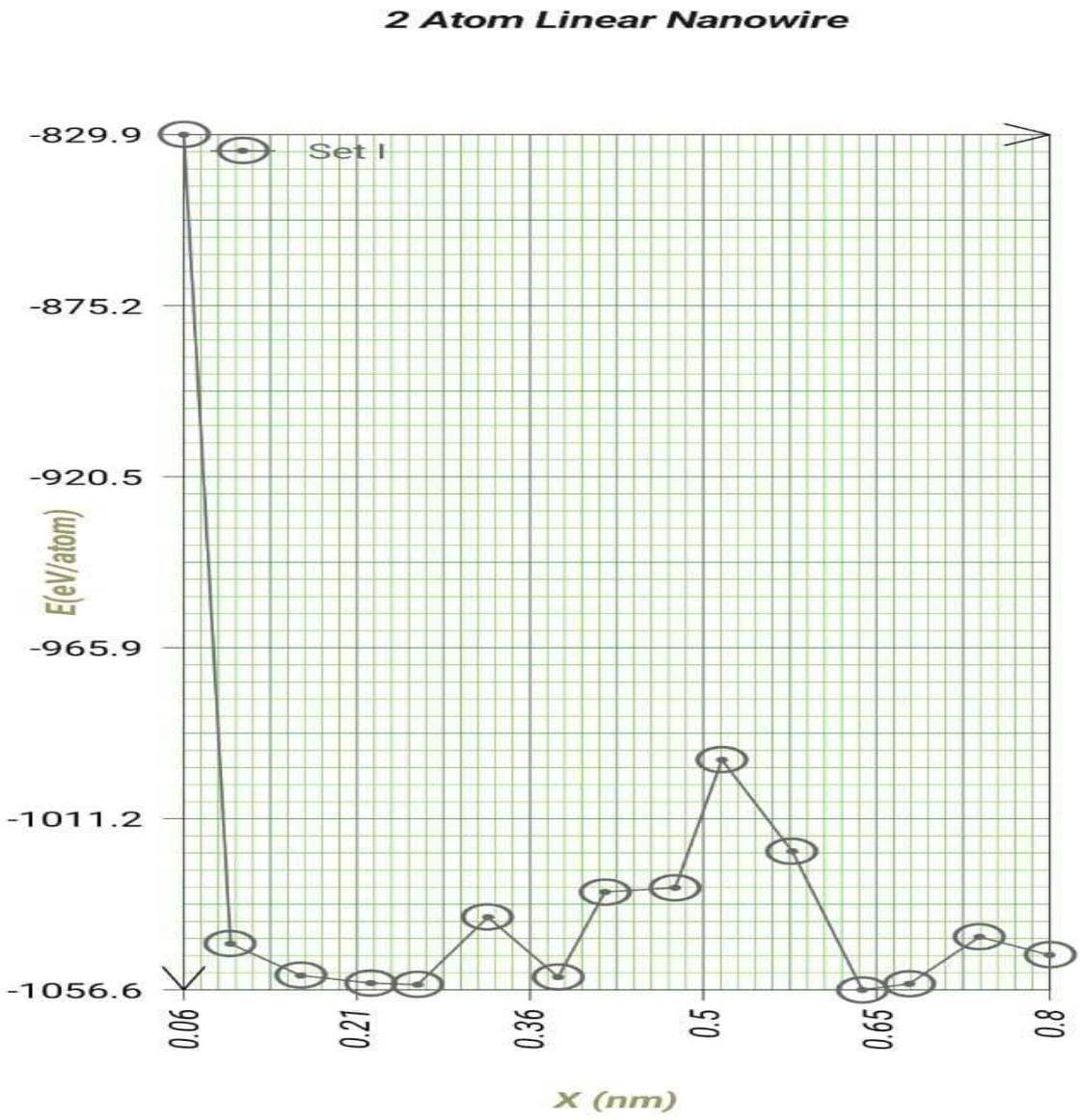


FIGURE 2. The variation between distance and energy for 2 atom linear nanowire

Table 2. Variation of energy (eV/atom) with Interatomic distance x (nm) for 2 atom Zigzag nanowire shape of ZnO

X (nm)	Total Energy (eV/atom)
0.06	-787.13
0.10	-1020.18
0.16	-1053.06
0.22	-1058.29
0.26	-1053.81
0.32	-1057.33
0.38	-1055.76
0.42	-1057.24
0.48	-1056.85
0.52	-1048.98
0.58	-1055.58
0.64	-1027.27
0.68	-1052.53
0.74	-1050.56
0.80	-1056.49

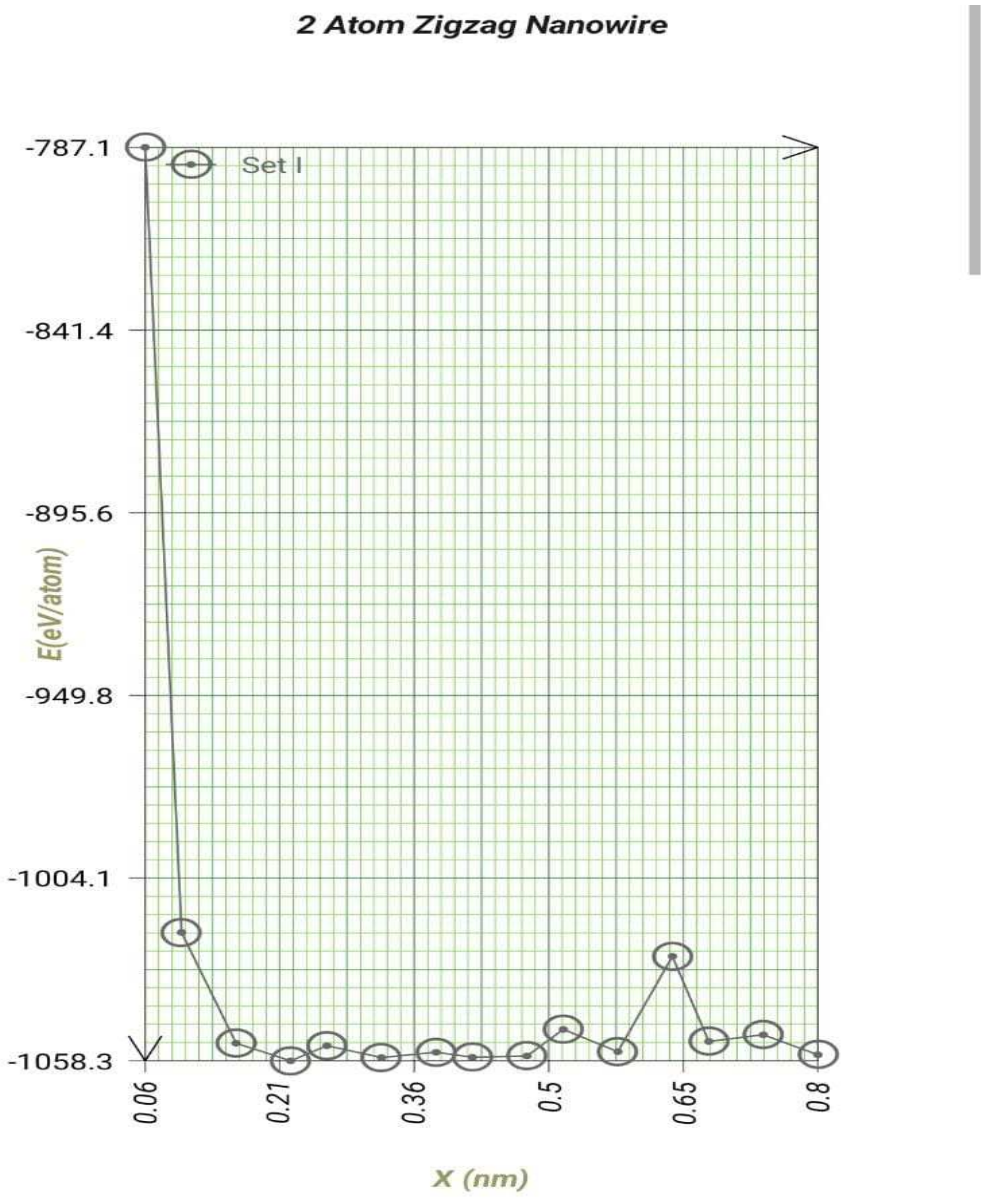


FIGURE 3. *The variation between distance and energy for 2 atom Zigzag nanowire*

Table 3. Variation of energy (eV/atom) with Interatomic distance x (nm) for 4 atom square nanowire shape of ZnO.

X (nm)	Total Energy (eV/atom)
0.06	-244.19
0.10	-1013.91

0.16	-1056.99
0.22	**-1057.89**
0.26	-1052.96
0.32	-1053.21
0.38	-1054.53
0.42	-1055.99
0.48	-1050.01
0.52	-1042.65
0.58	-1055.45
0.64	-1055.38
0.68	-1056.27
0.74	-1047.78
0.80	-1057.04

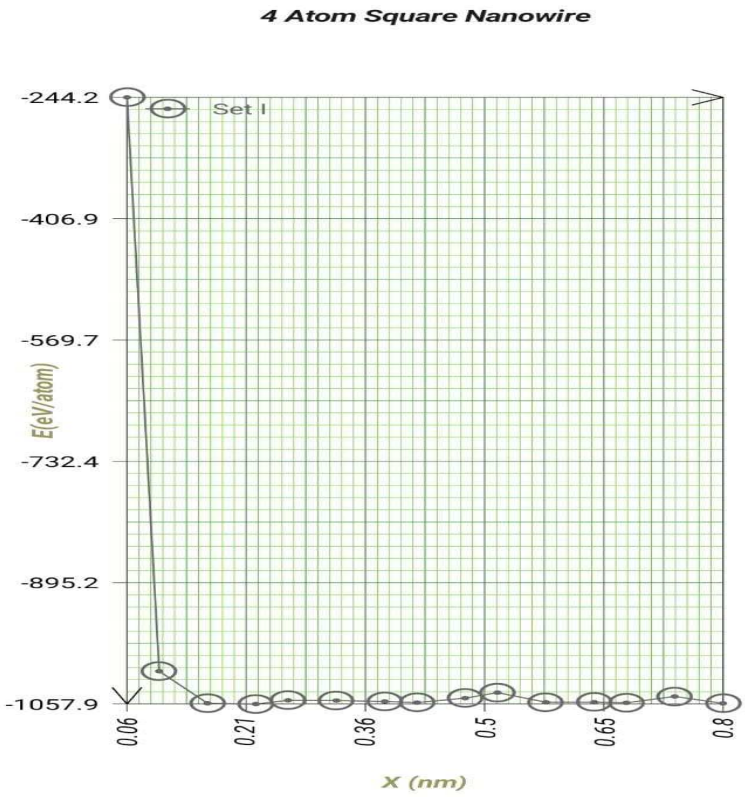


FIGURE 4. The variation between distance and energy for 4 atom square nanowire.

Table 4. Variation of energy (eV/atom) with Interatomic distance x (nm) for 6 atom hexagonal nanowire shape of ZnO

X (nm)	Total Energy (eV/atom)
0.06	-159.88
0.10	-921.81
0.16	-1024.95
0.22	**-1050.37**
0.26	-1042.78
0.32	-993.76
0.38	-1037.96

0.42	-1037.18
0.48	-1006.86
0.52	-1041.60
0.58	-1047.54
0.64	-1034.06
0.68	-941.69
0.74	-865.61
0.80	-1044.49

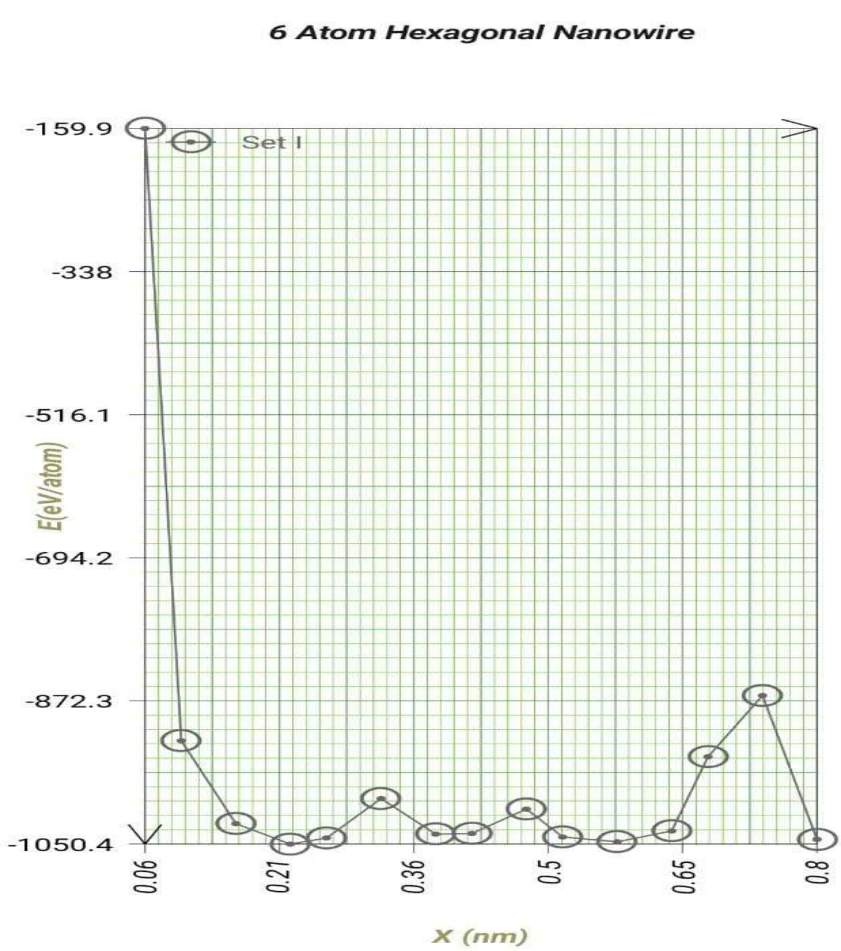


FIGURE 5. The variation between distance and energy for 6 atom hexagonal nanowire

Table 5. The interatomic distances and Total energy of Optimized Structures

Structure	Zn-O Distance (nm)	Zn-Zn Distance (nm)	Total Energy(eV/atom)
2 atom Linear	0.64	1.28	-1056.56
2 atom Zigzag	0.22	0.44	-1058.29
4 atom Square	0.22	0.44	-1057.89
6 atom Hexagonal	0.22	0.44	-1050.37

4. Conclusion

The study has performed plane wave pseduopotential DFT calculations for four different structures of Zinc oxide nanowires by using ABINIT code. Our study has reflected that 2- atom zigzag shape has come out to be more stable as compared to other shapes under consideration.

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Declaration of Conflict of Interest

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

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