Electronic Properties of Semiconducting Nanowires: a Comparative Study

Sanjay Prakash Kaushik[1*], Manoj Kaushik[2], Satyendra Singh[3], Ram-Krishna Thakur[4] Vivek Kumar Shukla[5] and Vijay Kaushik[6]

[1&2]State Council of Educational Research & Training, Gurugram, Haryana-122001, India
[3]Department of Physics, Seth G. B. Podar College, Nawalgarh, Rajasthan -333042, India
[4]Research and Academic Affairs, JNU Jaipur, Rajasthan-302017, India
[5]Department of Physics, Gautam Budha University, Greater Noida, U.P.-201312, India
[6]Department of Science, Scottish High International, Gurugram, Haryana – 12200, India

***CORRESPONDING AUTHOR:**

Sanjay Prakash Kaushik
Email:physicistkaushik@gmail.com

ISSN : 2382-5359(Online), 1994-1412(Print)

DOI :
https://doi.org/10.3126/njst.v21i2.67168

Date of Submission: Mar 10, 2023

Date of Acceptance: Mar 19, 2024

ABSTRACT

The presented work has explored the comparative study of electronic properties of semi conducting nanowires of different materials. These nanowires have critical role in photovoltaic and it shapes the future of new and renewable energy. The study has been performed for different shapes of nanowires. The various shapes under consideration are 2-atom Linear Nanowire, 2-atom Zigzag Nanowire, 4-atom Square Nanowire and 6-atom Hexagonal Nanowire. The findings for electronic properties reveal that 2-atom linear wire can be conducting as well semi conducting, 2-atom zigzag wire is conducting for almost all materials, 4-atom square wire is insulating for most of the materials while 6-atom hexagonal wire has come out to be insulating for all materials. Hence a semiconducting material shows conducting, semiconducting and insulating behavior depending on the proposed shape for various materials.

Keywords: Nanowire, Electronic properties, Density functional Theory, Pseudopotential, Band structure.

1. Introduction

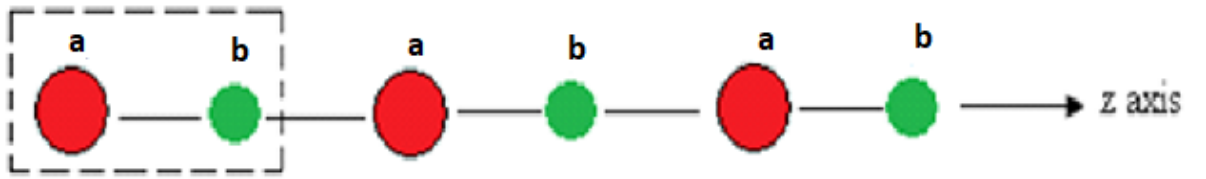
The present era is era of Science and Technology. In this technological era the behavior of electronic devices matters a lot. The photovoltaic has played its critical role in the present industrialization by bridging the gap between the demand and supply of ever-increasing demand of electricity. The efficiency of the photovoltaic cell is dependent on the semiconducting wire used for its manufacturing. The presented work revolves around this central idea of efficacy of photovoltaic cell and has explored the electrical behavior of semiconducting nanowire which are used in solar cells and has also explored other potential material for the same purpose. The electrical behavior of semiconducting nanowires plays a very critical role for the desired output efficiency of such electronic devices. The material like cadmium sulphide, zinc selenide and cadmium telluride in particular play a critical role in efficiency of solar cell.

Many researchers have shown their keen interest in the electrical properties of the nanowires since around 1980 and have come out with significant conclusions. If we compare the bulk form with the

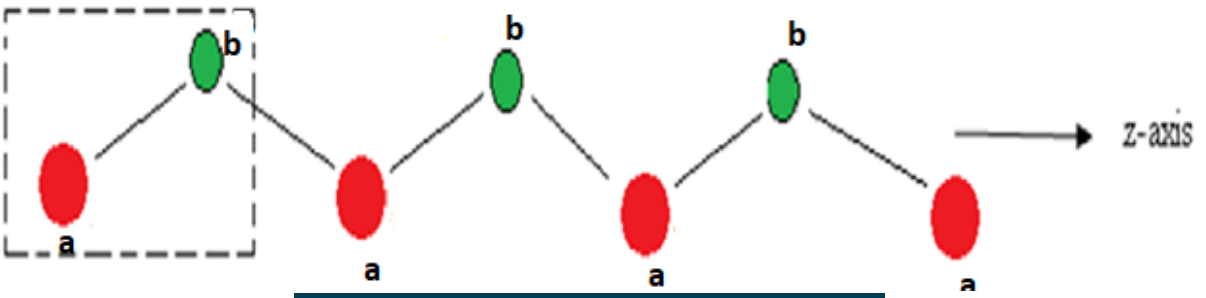
nano dimension of these materials then a variation in electrical as well as other properties is noticed. Exotic properties were reflected by these miniature structures at nano-scale and because of this there has been an urgent need for exploration and investigation of such structures. The devices made on this technique are seen to have technical advantages over other devices based on photolithography. The Review on structural dependence of electronic behavior of various nanowires as reported by the researchers in past around thirty years is the outcome of this proposed work.

From the early eighties of 20th Century, the germanium and silicon nanowires have been the central spot for the researchers and thus sufficient experimental work on these nanowires have already been performed by various researchers (Li *et al.* 2003; Tian 2007; Greytak 2004). The work has explored review of electronic properties of various semiconducting materials as proposed by many researchers and it also includes our work in which we have performed the study for cadmium sulphide, zinc selenide and cadmium telluride. Cadmium Sulphide is used as buffer layer in the cell (Kapadnis *et al.* 2020) and is also used in designing the photovoltaic cell, Zinc Selenide, which may be used to improve the absorption coefficient which affects solar cell (Nisreen *et al.* 2020) and Cadmium Telluride which can be used for increasing the efficiency of Solar Cell (Fardi *et al*. 2013). The semiconducting nanowires play a significant role in efficiency of present-day devices and hence are the material under much explored study. This has attracted us to explore these materials in terms of electronic properties and hence we have performed the review which shall be very critical for future researchers.

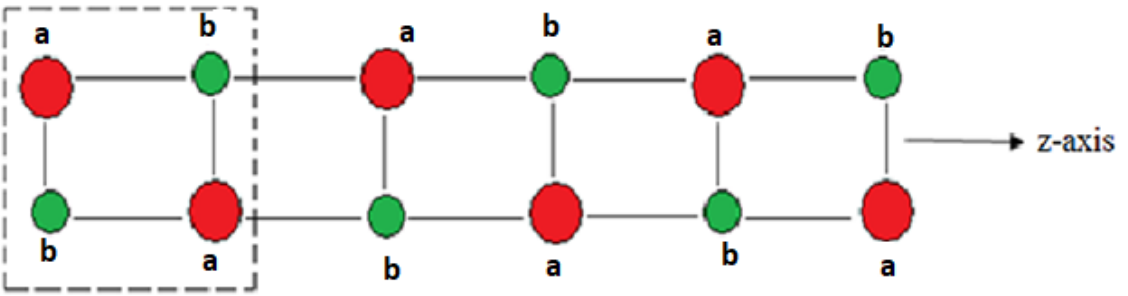
The different atomic arrangements are discussed in the performed study. The various shapes explored by the different researchers in this review are: 2-atom linear, 2-atom zigzag, 4-atom square and 6-atom hexagonal shapes as shown below in Fig. 1.



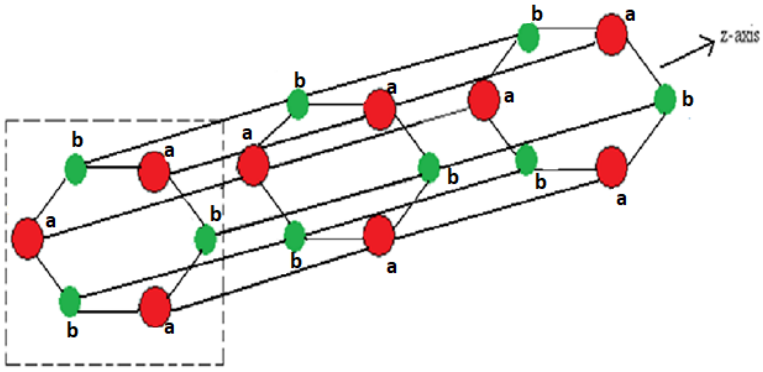
(a) 2-atom Linear Nanowire



(b) 2-atom Zigzag Nanowire



(c) 4-atom Square Nanowire



(d) 6-atom Hexagonal Nanowire

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

Srivastava (Srivastava *et al.* 2008) studied Gallium Nitride by pseudopotential density functional by using generalized gradient approximation (Perdew *et al.* 1996) and proposed that the 2-atom linear wire reflected semi conducting nature, 2-atom zigzag & 4-atom square wires reflected metallic nature and 6-atom hexagonal wire showed insulating nature. Materials at lower dimension show different behavior for Gallium Arsenide was established by a group of researchers and it was also proposed in their findings that for 2-atom linear and 2-atom zigzag shapes are conducting for GaAs whereas 4-atom square and 6-atom hexagonal shapes are insulating (Singh *et al.* 2009). The same group of researchers employed ab-initio DFT calculations (Hohonberg *et al.* 1964; Kohn *et al.* 1965) on Gallium Antimonide and proposed that the 2-atom linear and 2-atom zigzag shapes are conducting here also whereas 4-atom square and 6-atom hexagonal shapes are insulating in nature for GaSb. In 2011, Srivastva (Srivastva *et al.* 2011) used exchange correlation potential of Trouiller– Martin (Troullier et al. 1991) and performed the study on Gallium Phosphide and proposed that the 2-atom linear & 2-atom zigzag wires are reflecting metallic nature whereas 4-atom square and 6-atom hexagonal wires are insulating in nature. Srivastva (Srivastva *et al.* 2011) performed the structural dependence of aluminum nitride and predicted the electronic behaviour of the material by stating that 2-atom linear, 2-atom zigzag & 4-atom square shape is conducting in nature whereas 6-atom hexagonal wire have shown insulating character. Singh (Singh *et al.* 2015) by employing 15-k point sampling for integration of Brillouin Zone by Monkhorst-pack method (Monkhorst *et al.* 1976) on Zinc Oxide (ZnO) performed the ab-initio study for electronic behavior, his study for band structure indicated that 2-atom linear shape is semiconducting, 2-atom zigzag shape is semiconducting while 4-atom square and 6-atom hexagonal shapes are insulating in nature.

We have also performed the ab-initio DFT calculations and decided to extend the work for II-VI semiconducting nanowires and choose Cadmium Sulphide (CdS), Zinc Selenide (ZnSe) and Cadmium Telluride (CdTe). The selected wires have their unique applications like ZnSe semiconductor has its unique application as light emitting diodes (Chen *et al.* 2005), photo detector (Vigue *et al.* 200) & scintillator (Nasieka *et al.* 2014) while CdS semiconductor has its unique application as field emitter (Yi *et al.* 2007), logic gate (Ma *et al.* 2007) and CdTe has its application of being used in solar cells (Amin *et al.* 2007).

Our findings for cadmium telluride (CdTe) revealed that for various shapes the electronic behavior is also different. The electronic behavior reflected that for cadmium telluride the 2-atom linear and 2-atom zigzag wires are semi-conducting in nature while 4-atom square & 6-atom hexagonal shapes are insulating in nature (Kaushik *et al.* 2020). The study for cadmium Sulphide (CdS) nanowires by us established that 2-atom linear shape is conducting, 2-atom zigzag shape is semiconducting and 4-atom square shape & 6-atom hexagonal shapes are reflecting insulating characters (Singh et al. 2020). The ab-initio study for Zinc Selenide by us (Kaushik *et al.* 2020) for electronic properties reflected that the 2-atom zigzag wire is conducting, 2-atom linear wire is semiconducting whereas 4-atom square & 6-atom hexagonal shapes are coming out to be insulating here also. We (Kaushik *et al.* 2022) have also reviewed structural dependence for semiconducting material and the stability has also shown variation with

varying atomic arrangement. The electronic properties of Organic-Inorganic mixed halides-based perovskites have been analyzed by density functional theory is also being performed by us (Sharma *et al.* 2023) and found that addition of halogen shifts the energy bands in band structure which results in change of bandgap for of Solar Energy Material $CH_3NH_3PbX_3$ (X= I, Br and Cl) Perovskites. A model developed to study the effect of size and shape on the bandgap of semiconductor nanomaterials has found that bandgap increases by decreasing the size and depends on the shape considered (Paneru *et al*. 2023). The bandgap variation are reported (Singh *et al.* 2023) for spherical, thin film, nanowire, regular tetrahedral and regular octahedral shapes of semiconductor nanosolids. According to the study shape effect becomes prominent as the form changes from spherical to regular tetrahedral shape up to the size limit of 20 nm and concluded that the bandgap increases on decreasing size to the nanoscale.

2. Computational Details

The structures of the mentioned nanowires have been explored through Density Functional Theory calculations (Hohonberg *et al.* 1964; Kohn *et al.*1965). The pseudopotential technique has proven to be a very dynamic tool for studying electronic properties for different materials (Martin *et al.* 2009). Most of the above studies are performed by using ABINIT Code (Gonze *et al.* 2002).

3. Results

We have performed the extensive review with the available existing studies for electronic behavior for various semiconducting materials. The electronic properties show a drastic variation when the atomic arrangement is varied. The behavior of the semi conducting material under observation has shown all possible behavior. The detailed findings of the reviewed literature for electronic behavior are of critical importance.

The findings for electronic behavior for various materials as shown below in Table I reflect that 2-atom linear wire has come out to be conducting as well semiconducting for various materials depending on the nature of material, 2 atom zigzag wire has come out to be conducting for almost all materials other than cadmium sulphide and cadmium sulphide where it has shown semiconducting nature, 4-atom square shape has come out to be insulating for all materials other than gallium nitride and aluminum nitride where it has shown conducting nature but 6-atom hexagonal wire has come out to be insulating in all cases.

Table 1: Electronic Behavior Table for various Materials.

Material	Electronic Behavior of Material for Different Shapes			
	2-atom linear	2-atom zigzag	4-atom square	6-atom hexagonal
Gallium Nitride (GaN)	Semi-conducting	Conducting	Conducting	Insulating
Gallium Arsenide (GaAs)	Conducting	Conducting	Insulating	Insulating
Gallium Antimonide (GaSb)	Conducting	Conducting	Insulating	Insulating
Gallium Phosphide (GaP)	Conducting	Conducting	Insulating	Insulating
Aluminum Nitride (AlN)	Conducting	Conducting	Conducting	Insulating
Zinc Oxide (ZnO)	Semi-conducting	Conducting	Insulating	Insulating
Cadmium Sulphide (CdS)	Conducting	Semi-conducting	Insulating	Insulating
Zinc Selenide (ZnSe)	Semi-conducting	Conducting	Insulating	Insulating
Cadmium Telluride (CdTe)	Semi-conducting	Semi-conducting	Insulating	Insulating

4. Conclusion

The review on electronic properties of semiconducting nanowires has been performed. The structural dependence of electronic properties for different material by using ab initio DFT calculations have been analyzed. It is concluded that the electrical behavior of the nanowire is critically dependent on shape. A semiconducting nanowire may possess the conducting, semi conducting and insulating nature by varying the atomic arrangement i.e., the electronic behavior can be changed by changing the atomic arrangement for the materials under study. The present findings can be very carefully utilized while using these materials for designing various scientific devices.

Acknowledgements

We are also thankful to all researchers cited in the review. It is because of their reported work because of which we could perform the study and reach to such an important conclusion. We also express our gratitude for SCERT Gurugram, for providing infrastructural facilities because of which we could carry out our experimental work.

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