Section A -Research paper
ISSN 2063-5346

Structural, Electronic and Transport properties of Boron and Nitrogen doped ZigzagSilicon Carbide Nanoribbons (SiCNRs): A first principle study

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Abstract

Zigzag silicon carbide nanoribbons having width of 4 atoms and doped with Boron and Nitrogen atoms have been investigated by utilizing Density Functional Theory (DFT) calculations in order to understand the effect of doping on electronic and transportproperties of nanoribbons. We considered edge and termination sites for doping to explore the effects on the electronic structure of the 4ZSiCNRs. The spin unpolarized calculation reveals that the silicon (Si) replaced by B and carbon replaced by (N) dopants introduced impurity levels in the band gap of ZSiCNRs, which affect their electronic properties. Specifically, our findings revealed that the band gap of ZSiCNR exhibits a transition from semiconductor to metallicstates. The consistency between the density of states (DOS) and transmission spectraresults suggests that both measurements exhibit similar behavior. Edge and termination site doped 4ZSiCNRshows semiconductor to metallic properties that can be useful for applications such as sensing, catalysis, nano interconnect, and nanodevices.

Keywords: Silicon carbide, Silicon carbide nanoribbon, electronic, and transport properties

1.Introduction

In 1891, American chemist Edward Goodrich Acheson revealed the first discovery of Silicon carbide.[1, 2]. Silicon carbide is a chemical compound that consists of silicon (Si) and carbon (C) atoms. The chemical formula SiC is used to represent this compound and arranged in a honeycomb-like lattice[3, 4]. Bulk Silicon carbide is widely used in the semiconductor industry, where it is used to make high-temperature, power electronic devices[5]with wide band gaps. Its high breakdown voltage, thermal conductivity, and electron mobility make it an excellent and attractive material for power electronics and other demanding applications [6-10].

The pastfew years' theoretical studies on silicon carbide nanoribbons are thin strips or ribbons of silicon carbide material that have a width on the order of nanometres (typically less than 100 nm)[11]. The unique properties and versatile potential applications such as electronics, energy conservation, and sensing of silicon carbide nanoribbons have made them a highly sought-after class of nanostructured materials in recent years [12-14]. Experimental studies, find different characterizations such as XRD, Raman spectroscopy, X-ray photoelectron spectroscopy, and SEM [15, 16]. They have been found to exhibit excellent mechanical, thermal, and electronic properties, and have the potential for use in high-performance electronic and optoelectronic devices, as well as in energy conservation and storage applications. The study focused on the structural and electronic properties of two distinct types of SiC nanoribbons with different widths: zigzag and armchair nanoribbons[17].Spin-polarised calculations were obtained apply an electric field and finding the band gap modulations [18]. Doping can also affect the electronic properties of silicon carbide nanoribbons. Boron and nitrogen doping has been found to improve the half-metallic electronic behavior of zigzag silicon carbide nanoribbons (ZSiCNR) [19].Changing the ribbon width, it is possible to tune the ZSiCNRs from a half-metallic to a semiconducting behavior, and edge magnetism in ZSiCNRS is highly sensitive to the width of the ribbon, with the wider ribbons exhibiting a lower magnetic moment due to the delocalization of the edge states[20]. The ZSiCNR exhibits a non-zero-spin polarization due to the spin-orbit coupling effect, which leads to a spin-dependent band gap, and found the spin-dependent conductance of the ZSiCNR can be changed by employing an external electric field [21]. Doping of silicon carbide nanoribbons can be achieved by introducing dopant atoms into the material during synthesis [22]. The experimental study found that nitrogen-doped silicon carbide decreases electrical conductivity[23].A previous study reported that on doping of boron and nitrogen in zigzag-shaped silicon carbide nanoribbons I-V characteristics graph indicates that the spin-down and spin-up states are selectively filtered in parallel and antiparallel arrangements, respectively. These findings hold promise for the development of spintronic device designs[24].Si atom replaced by aluminium in ZSiCNRcan reduce the material band gap and affect the electronic and spin transport properties achieved by spintronic applications such as spin filtering efficiency and NDR behaviour [25]. Recently,the study found that after boron atom doping at the center,itgives rise to additional energy bands, leading to shifts in the semiconductor properties of armchair edge-shaped silicon carbide nanoribbons towards the P-type behavior. The potential application B doped ASiCNRs in forthcoming nanoelectronic devices is worth considering [26]. In the twentieth century, most studies have been done for silicon carbide nanoribbons considering spin-polarization.

In this investigation, the whole study is based on spin-unpolarizationusing Density functional theory (DFT) calculation. This investigation aimed to analyze the electronic and transport properties of zigzag silicon carbide nanoribbons (ZSiCNR) with 4 widths that had undergone doping at both their edge and termination sites with two distinct elements; boron (B) and nitrogen (N).

2.Computational Methods

The basis of this theoretical research is the application of density functional theory (DFT)- a quantum mechanical approach to determine the electronic structure of atoms and molecules using the ATK-VNL version 2014.1 software package[27].Double zeta double polarized basis set represents the size and complexity of the wavefunction ofelectrons in the system and sets mesh cut off 150 Rydberge. The choice ofGeneralized Gradient Approximation (GGA) utilizing the Perdew-Burke-Ernzerhof (PBE)[28] can significantly affect the accuracy of the calculation. It is a functional that describes the exchange and correlation interactions between electrons. Set K-point sampling 1*1*100, interaction maximum range 15Å, and electron temperature 300K. The bond length for Si-C, C-H, and Si-H are1.78Å, 1.09Å, and 1.42Å the whole work is to set a spin unpolarised parameter which means all systemsuse the spin-restricted formalism.

3.Result and Discussion

UsedATK VNL software andSiC (Moissanite) material in a hexagonal (Wutzites) type structure, and the space group 186 for constructing two-dimensional nanoribbonsas perFigure 1(a-e). First, we study the structural stability of a single layer of 4ZSiCNR and thenexamine the electronic band structure, electron density, the density of states (DOS), and transmission spectrum.Itis possible to analyze the behavior of electrons within a material using the same set ofparameters.

3.1.Structural stability of 4ZSiCNR

Structuralstabilityis a fundamental consideration in the design process of nanoribbons. To determine the structural stability of a nanoribbon, it is necessary to consider various factors, includingits size, shape, and material.For different constructed nanoribbons,finding the formation energy is an important concept used in solid state physics and material science to determine the stability of a crystal structure. It is defined as the energy required to form a crystal from its constituent atoms in their standard states.

From table 1a negative formation energy indicates that the material is more stable, as it requires less energy to form than the sum of the energies of its constituent atoms.The maximum formation energy represents hydrogen replaced by B in pristine 4ZSiCNR that means thematerial is least stable configuration. The minimum formation energy, represent carbon replaced by nitrogen in 4ZSiCNR that means this is the most stable configuration as it requires the least energy to form that configuration. To assess the feasibility of the pristine and modified structures, the formation energies were computed using Eq. (1) [29].

$$E_{FE} = \frac{E_{SiCNR} - ME_{Si} - NE_{C} - OE_{H} - PE_{B/N}}{M + N + O + P} \quad (1)$$

Where, E_{SiCNR} indicate the total energy of different nanoribbon and M, N, O, P represents the number of atoms and E_{Si}, E_C, E_H, and $E_{B/N}$ indicates the total energy of individual atom of Silicon(Si), Carbon(C), hydrogen(H), Boron(B)/nitrogen(N).

Table 1

Calculate the value of total energyand formation energy of 4ZSiCNRs

Element	Total Energy (eV)	Formation Energy (eV)
4ZSiCNR_pristine	-704.41706	-3.13
4ZSiCNR_Si replaced by B	-603.18312	-1.74
4ZSiCNR_C replaced by N	-818.43384	-3.76
4ZSiCNR_H replaced by B	-763.45884	-1.40
4ZSiCNR_H replaced by N	-956.37300	-3.27

3.2.ElectronicBand structure analysis

Studying the electronic properties of materials requires the use of band structure analysis, which is a crucial and effective tool for this purpose. Through the analysis of band structures, one can gain a valuable understanding of how electrons behave within a crystal lattice.Figure2(a) shows pristine zigzag silicon carbide nanoribbon band structures located with a direct bandgap of 0.91 eV. From Figure 2(b)silicon atom replaced by a boron atom in zigzag silicon carbide nanoribbon (ZSiCNR) can lead to the emergence of impurity states within its band structure. Doped boron materials shift the fermi level below the Dirac point in ZSiCNR, leading to a surplus of positively charged carriers known as holes, resulting in p-type behavior.When carbon atom replaced bya nitrogen atomat the edge as shown in Figure 2(c), the doped nitrogen material shifts the Fermi level above the Dirac point in ZSiCNR, resulting in an excess of negative charge carriers, or electrons, leading to n-type behavior. The results of boron and nitrogen doping in this study are commensurate with the results of the previous studies [30, 31]. Figure 2(d) shows when H is replaced by a boron atom the conduction band comes intothe fermi level and reaches the minimum value at the fermi level, while the valence band approaches the fermi levelreaching its maximum value, which typically indicates that the material is indirect band gap semiconductor [32].Figure 2(e) shows clearly whenH replaced by nitrogen atom,the valence band crosses the fermi level and enters the conduction band and the conduction band has a minimum value band gap inthe band graph which implies that the material has metallicbehavior.

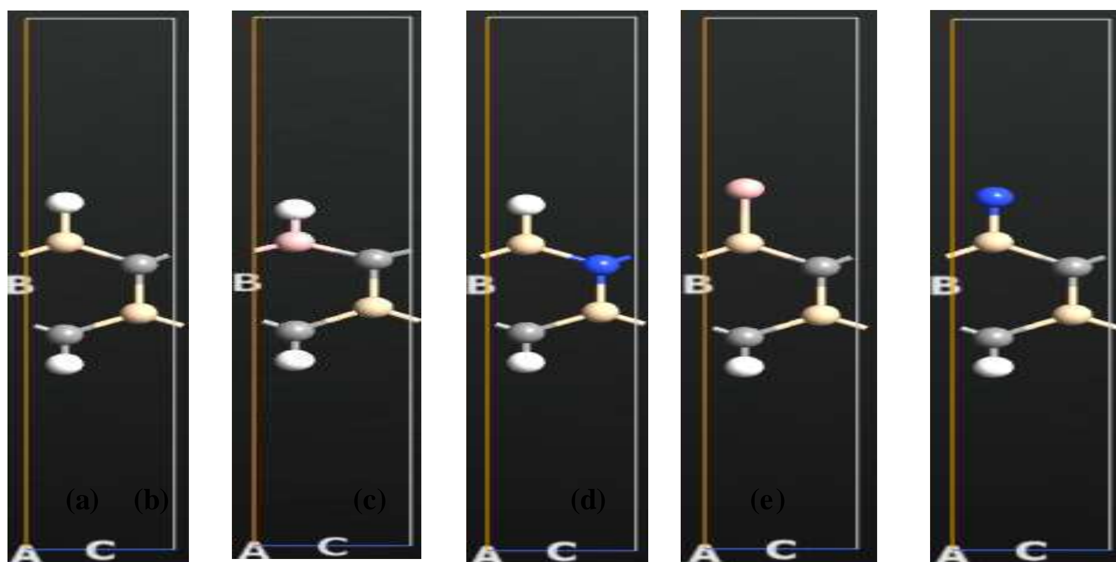
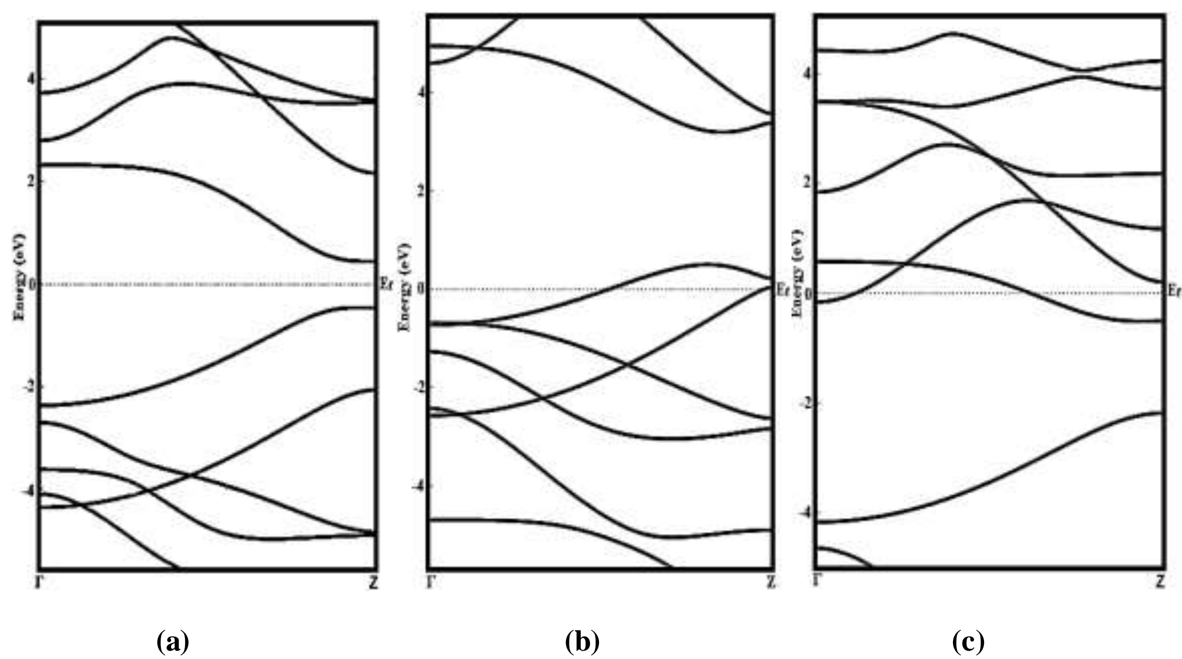


Figure 1. Geometrical electronic structure of 4ZSiCNR (a) pristine (b) Si replaced by B (c) C replaced by N (d) H replaced by B (c) H replaced by N.



ISSN 2063-5346

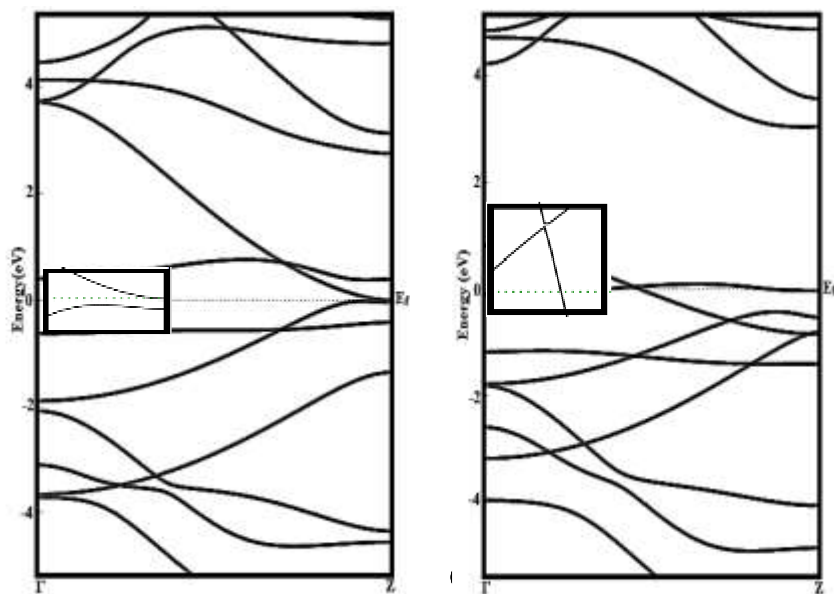


Figure 2. Band structure of 4SiCNR(a) Pristine (b) Si replaced by B (c) C replaced by N (d) H replaced by B (e) H replaced by N.

3.3.Electron Density

The concept of electron density in density functional theory (DFT) calculations is based on the probability of detecting an electron at a specific location within space. FromFigure 3(a) the lack of clear visibility of the silicon atom in hydrogen-passivated zigzag silicon carbide nanoribbons (ZSiCNR) is likely since the silicon atoms are less reactive than the carbon atoms in the material, which makes them more strongly likely to bind with hydrogen atoms during passivation. From Figure 3(b) the silicon atom may not be visible when replaced by a boron atom in a 4ZSiCNR with hydrogen passivation could be due to differences in electron density. When boron replaces silicon, it creates a hole in the electron structure because boron has one less electron than silicon.As a result, the boron atom surrounding electron density affects its visibility while the carbon atoms may be more visible because they have similar electron density to the silicon atoms they are replacing. Therefore, in the electron density picture, it is possible that the boron atom may appear less visible while the carbon atoms are still visible.Figure 3(c) Carbon is replaced by the nitrogen atom and the nitrogen atom is more visible than the carbon atom, which is only slightly visible because nitrogen and carbon have higher electronegativities than hydrogen and silicon, which means they have a greater tendency to attract electrons towards themselves. From Figure3(d) Carbon has a higher electronegativity than silicon and hydrogen, which means that it tends to attract electrons more strongly and electron density around the atom may be higher than that around a silicon or hydrogen atom, making it more visible. From Figure 3(e) hydrogen replaced by a nitrogen atom has more visible in the figure because of higher electronegativity than hydrogen, which means it attracts electrons more strongly.

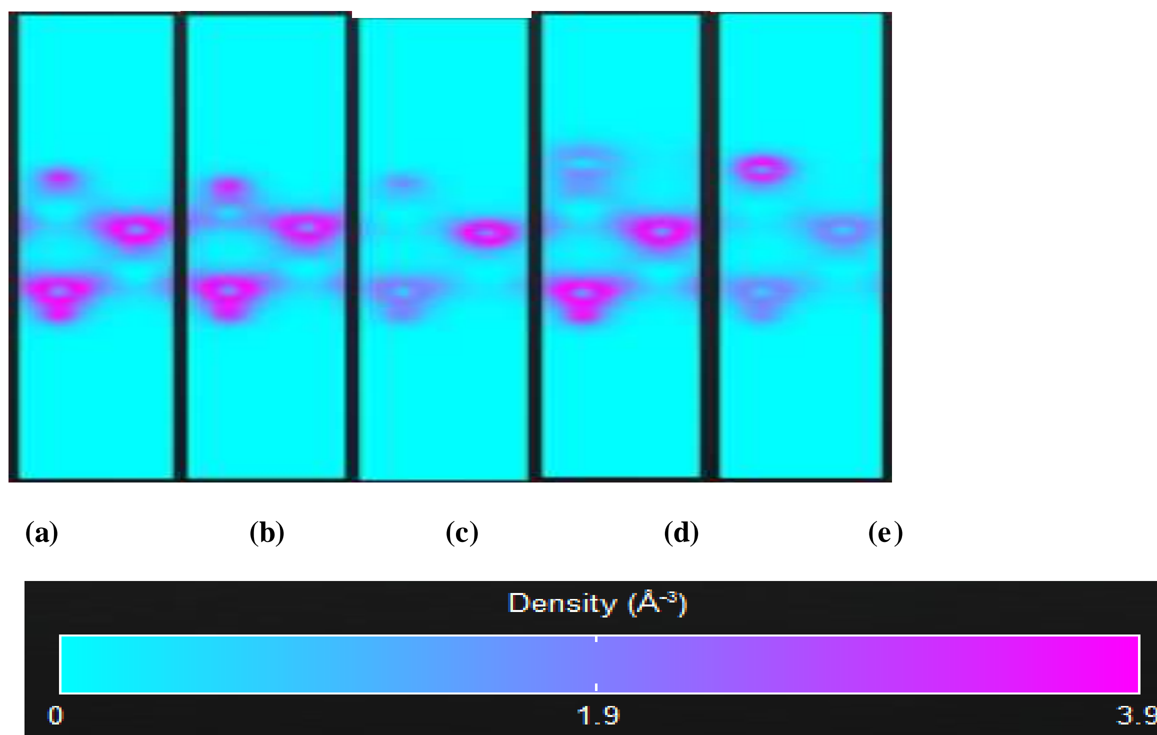


Figure 3. Electron density of 4ZSiCNR (a) pristine (b) Si replaced by B (c) C replaced by N (d) H replaced by B (e) H replaced by N.

3.4 Density of states(DOS)

The Density of states (DOS) can be calculated using the theoretical method of DFT. The DOS is an important analysis of electronic structure, as it provides information about their electronic behavior. It is a measure of how many energy states are available for electrons to occupy at a particular energy level in a material. It is typically expressed as an energy function.Figure4 (a-e)displays all graphs depicting the density of states,energy versus density of states (DOS), all graphsshowthe same behavior of band structure, which means semiconductor to a metallic behavior.

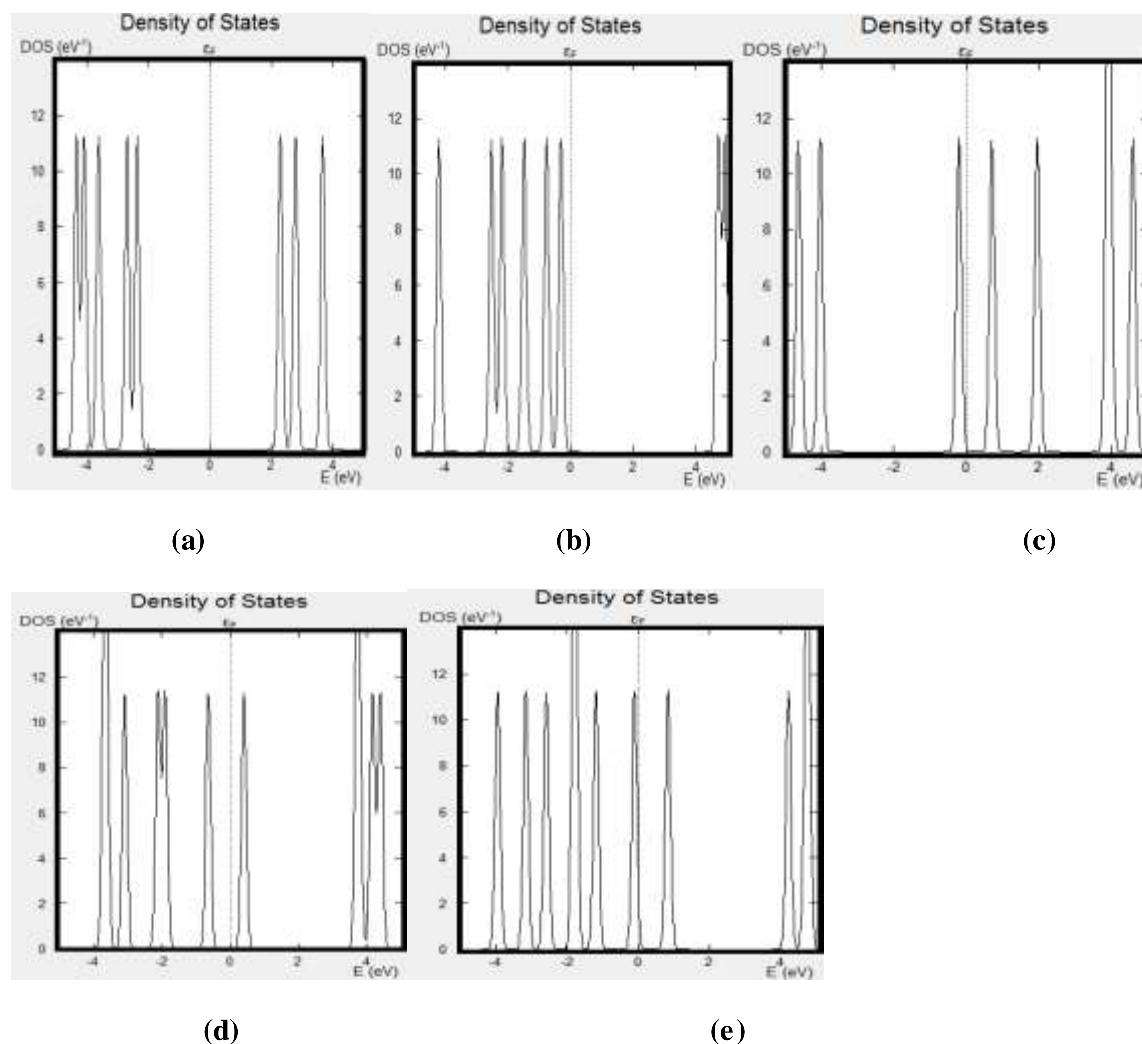


Figure4. Density of states of 4ZSiCNR(a) Pristine (b) Si replaced by B (c) C replaced by N (d) H replaced by B (e) H replaced by N.

3.5 Transmission Spectrum

In the computational analysis, the Non-equilibrium Green's function (NEGF) technique is a highly effective theoretical tool for carrying out calculations of the electronic transmission spectrum of material in a nanoscale device. The NEGF method is a highly sophisticated theoretical technique requiring advanced knowledge of quantum mechanics, quantum mechanics, and computational methods. A transmission spectrum is a valuable tool for understanding and usingproperties for the electronic behavior of different device applications, such as in electronic circuits. The transmission spectrum is a property of a material's electronic structure that describes the number of electrons that are transmitted through the material at different energies. In theoretical calculations, the transmission spectrum is often displayed as a graph that shows the transmission coefficient plotted versus energy. All graphs of transmission spectra as shown in

ISSN 2063-5346

Figure5 (a-e) exhibit the behaviour commensurate to band graphs, which means semiconductor to metallic behavior.

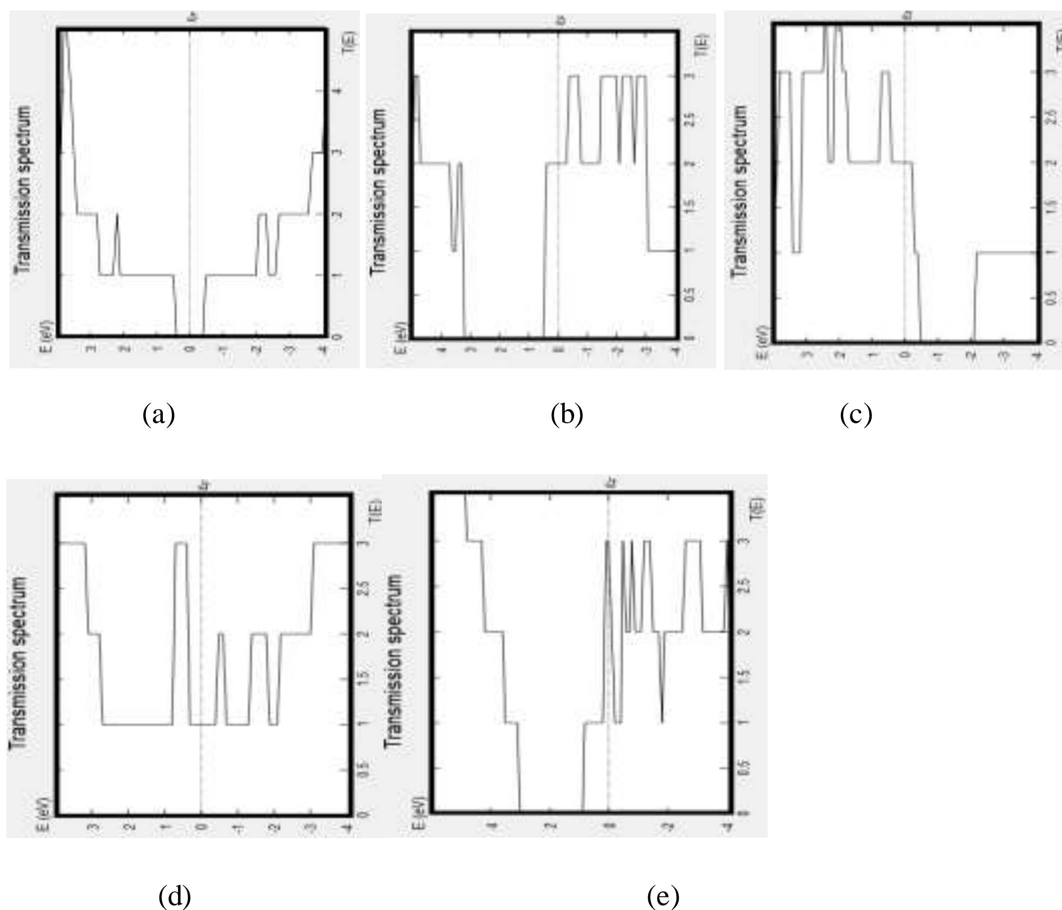


Figure 5. Transmission Spectrum of 4ZSiCNR (a) pristine (b) Si replaced by B (c) C replaced by C (d) H replaced by B (e) H replaced by N.

4Conclusions

The effects of doping of Boron (B) and Nitrogen (N) at the edge and hydrogen termination sites in zigzag silicon carbide nanoribbon (ZSiCNR) with 4 widths have been analyzed by studying the electronic and transport properties of the system. Constructedtheoretical nanoribbon of pristine 4ZSiCNR in which silicon is replaced by boron, carbon is replaced by nitrogen, hydrogen is replaced by boron, and hydrogen is replaced by nitrogen.Employed DFT framework to obtain brand graph, electron density, and density of states. The Non-equilibrium Green's function (NEGF) method was used to obtain and study transmission spectra. The following are the conclusions of the study:-

1. Band graph analysis reveals that pristine 4ZSiCNR has semiconducting behavior.
2. Behavior changes when Si is replaced by B or C is replaced by N exhibiting a P type and N type.
3. When H is substituted by B or N, the nanoribbonsshows the transition of electronic behaviour from semiconductingto metallic.
4. Analysis of electron density, the density of states (DOS), and transmission spectra confirm the same electronic behavior as revealed by band graph analysis.

The resulting behavior found in the study can be used in future nano-electronicdevices and nano interconnects.

Acknowledgments

The authors are grateful to the Computational Nanoscience and Technology Lab (CNTL), located at the ABV-Indian Institute of Information Technology & Management (IIITM) in Gwalior, Madhya Pradesh, Indiafor generously providing computational resources that were essential for carrying out this study.

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