Short Communications	*Curr. Appl. Sci.*, **2023**, *1*(1):51-58 DOI: 10.22034/cas.2021.144398	Current Applied Sciences

Structural and Electronic Properties of Armchair Silicon Carbide Nanoribbons

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Article Information

Received: 25 December 2022
Revised: 14 January 2023
Accepted: 19 January 2023
Published online: 06 February 2023

Keywords

Density functional theory
ASiC NRs
DOS
Bandgap

Abstract

Silicon carbide (SiC) has unique mechanical and electronic properties. SiC nanoribbons (SiCNRs) are known as outstanding inorganic counterparts of carbon-based nanostructures. The structural parameters and electronic characteristics of armchair silicon carbide nanoribbons (ASiCNRs) with edges passivated by hydrogen have been simulated. The calculated carbon-silicon bond length is in agreement with previous data. Moreover, compared to the zigzag SiCNRs with tetragonal unite cell, the proper crystal lattice for the armchair SiCNR is orthorhombic. The partial density of states (PDOS) shows that the p orbitals of carbon and silicon dominate the electronic structure of ASiCNR (w=3) near the Fermi level. In addition, the outputs show that the electronic bandgap of ASiCNRs (w=3) is larger than that of ZSiCNRs (w=3) (w stands for the width of the nanoribbon). Furthermore, the armchair nanoribbons with smaller width have a smaller bandgap due to the quantum size effects in ultra-small nanoribbon.

1. Introduction

Silicon carbide (SiC) has unique mechanical and electronic properties. It has large bandgap, high mechanical strength, low density, excellent oxidation, and corrosion resistances [1-3]. It is known as a promising material for devices operating at harsh environments, high power, and high temperature [4, 5]. SiC nanoribbons SiC NRs) have been successfully synthesized by several researchers [6-8].

Wu et al. [6] have synthesized bicrystalline SiC nanobelts exploiting a thermal evaporation and condensation process with multi-wall carbon nanotubes (MWCNTs) and silicon powder. Yushin et al. [8] reported synthesis of α-SiC micro-ribbons via a carbothermal reaction of graphite and silicon dioxide at 1,800–1,900°C. Xi et al. [7] also have studied the growth of cubic SiC (3C-SiC) nanobelts using the reaction of ethanol, lithium powder, and

tetra chlorosilane at 600°C. The ongoing research intends to simulate some of the physical properties of one of the isolated armchair silicon carbide nanoribbons and compare the data with that of other nanoribbons with different geometry and width. SiCNRs are known as outstanding inorganic counterparts of carbon-based nanostructures [9, 10].

In this paper, we investigate the structural and electronic properties of armchair SiCNRs (w=3) (w stands for the width of the nanoribbon) with edges passivated by hydrogen using density functional theory (DFT). The bandgaps of armchair and zigzag SiCNRs are also discussed.

2. Materials and Methods

2.1 *Computational details*

Our simulations are performed within DFT framework as carried out in SIESTA code [11]. We have used the generalized gradient approximation (GGA) with the Perdew-Burke-Enzerhof (PBE) method to calculate the exchange and correlation interactions [12]. The SiCNR (w=3) is optimized and the structural properties, TDOS, PDOS, and bandgaps are calculated utilizing the Monkhorst-Pack 1×1×70 k-point mesh for Brillouin zone sampling. In addition, the energy cut-off is set to 150 Ry. An orthorhombic unit cell was selected as a SiCNR (w=3) crystal lattice (Figure 1). The maximum Hellman-Feynman force on the atoms of relaxed structure was 10^{-3} eV/Å. The lattice parameters are: a=10 Å, b=14.67 Å, and c=21.6 Å. There are also 40 atoms in the unite cell.

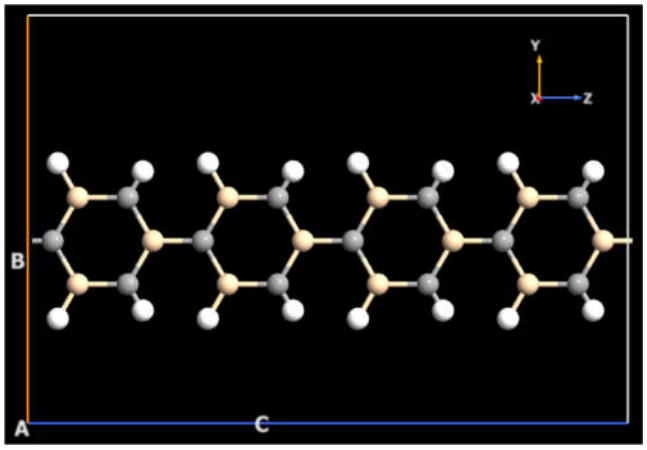


Figure 1. ASiC nanoribbon (w=3) crystal lattice with edges passivated by hydrogen. The silicon, hydrogen, and carbon elements are represented by yellow, white, and gray spheres, respectively

3. Results and Discussion

3.1 *Structural parameters*

The lattice constants and carbon-silicon bond length were calculated, and the results are compared with other reports in Table 1.

Looking at the data, it is clear that the calculated carbon-silicon bond length is in agreement with other structural results. Moreover, compared to the zigzag SiCNRs with tetragonal unite cell, the proper crystal lattice for the armchair SiCNR is orthorhombic.

Table 1: structural parameters and electronic bandgap of different SiCNRs

SiCNR	Crystal lattice	a, b, c (Å)	Carbon-silicon bond length (Å)	Bandgap (eV)
ASiCNR (w=3) (this work)	Orthorhombic	a=10.0 b=14.6 c=21.6	1.84	2.3
ASiCNR (w=4) [13]	-	-	1.73	2.35
ASiCNR (w=5) [13]	-	-	1.73	2.5
ZSiCNRs (w =3) [14]	Tetragonal	a =3.11 b=c=20	1.78	
ZSiCNR (w=14) [15]	Tetragonal	a=b=32 c=3.10	1.82	0.07
ZSiCNR (w=16) [15]	Tetragonal	a=b=34 c=3.10	1.82	0.00
ZSiCNR (w=18) [15]	Tetragonal	a=b=36 c=3.10	1.82	0.00
ZSiCNR (w=20) [15]	Tetragonal	a=b=38 c=3.10	1.82	0.00

3.2 *Electronic properties*

The partial density of states (PDOS) and total density of states (TDOS) of ASiCNR (w=3) are represented in Figures 2 and 3.

The partial density of states (PDOS) shows that the p orbitals of carbon and silicon dominate the electronic structure of ASiCNR (w=3) near the Fermi level.

The band structure of the simulated nanoribbon is represented in Figure 4. The band structure is in agreement with the TDOS.

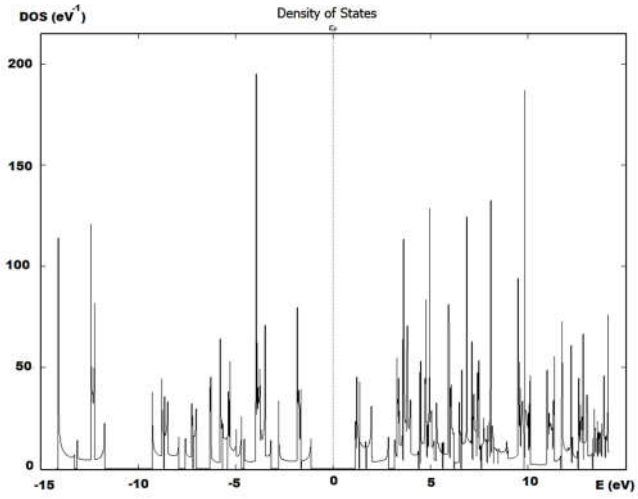
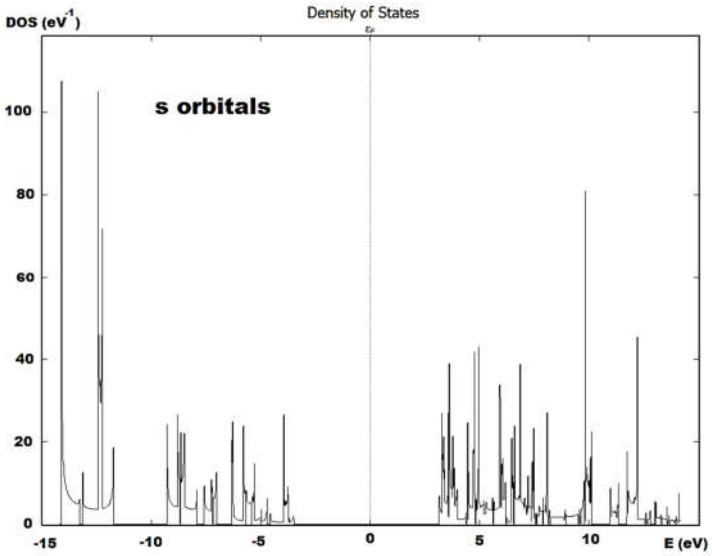
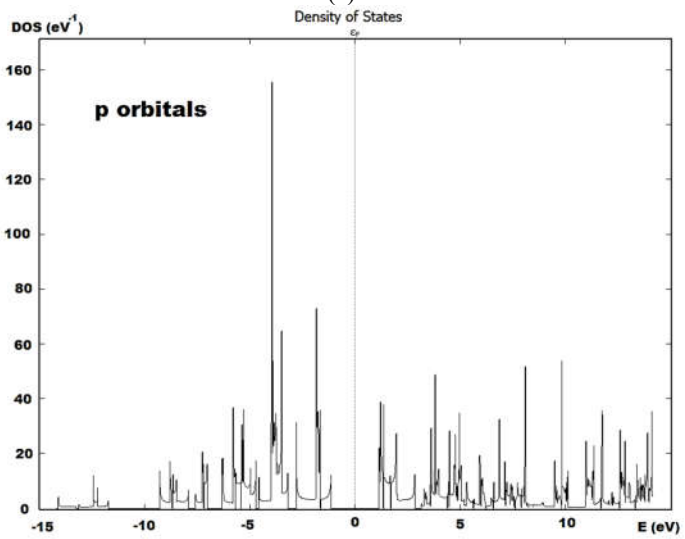


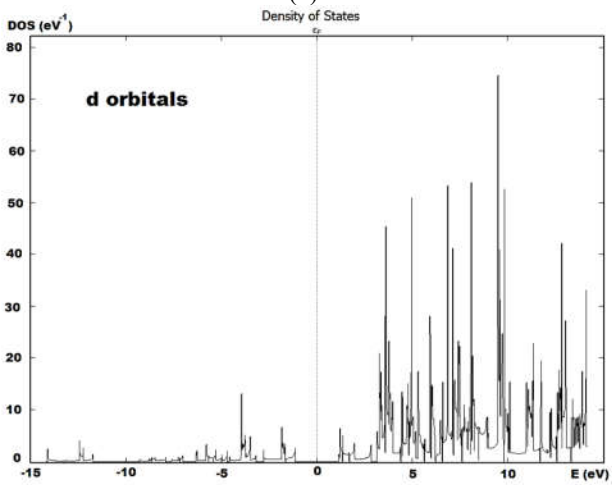
Figure 2. TDOS of ASiCNR (w=3). Fermi level is set to zero



(a)



(b)



(c)

Figure 3. PDOS of ASiCNR (w=3): (a) s orbitals, (b) p orbitals, (c) d orbitals. Fermi level is set to zero

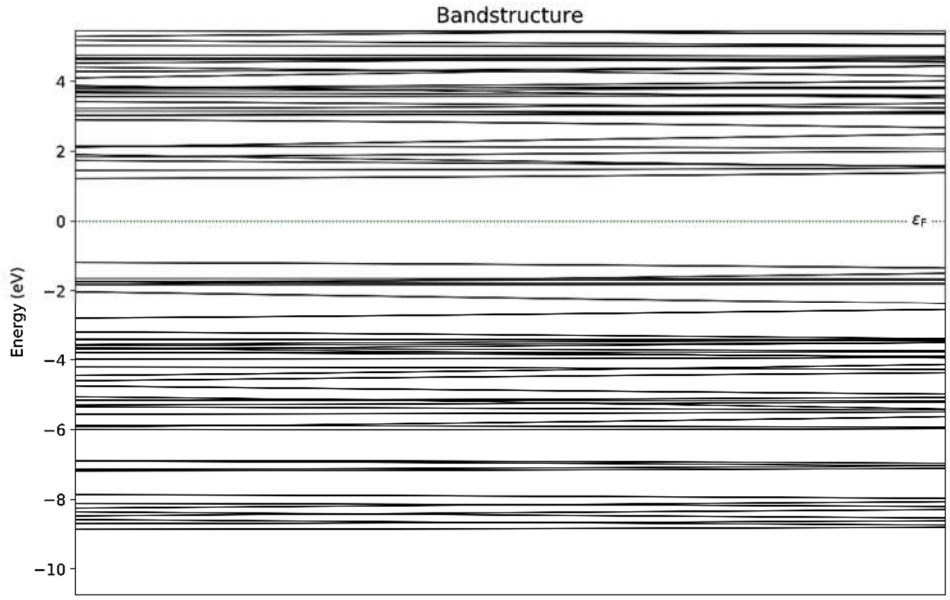


Figure 4. Band structure of ASiCNR (w=3). The Fermi level is set to zero

Table 1 compares the electronic bandgap of armchair and zigzag silicon carbide nanoribbons. The outputs show that the electronic bandgap of ASiCNRs (w=3) is larger than that of ZSiCNRs (w=3). Furthermore, the bandgap of zigzag SiCNRs is smaller than the bandgap of the simulated armchair silicon carbide nanoribbon.

Table 1: Structural parameters and electronic bandgap of different SiCNRs

SiCNR	**Crystal lattice**	**a, b, c (Å)**	**Carbon-silicon bond length (Å)**	**Bandgap (eV)**
ASiCNR (w=3) (this work)	Orthorhombic	a=10.0 b=14.6 c=21.6	1.84	2.3
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From the table it is clear that the ASiCNRs are semiconducting while ZSiCNRs are metallic. The main reason for this is the different geometry and different hybridization through these nanoribbons. In addition, the armchair nanoribbons with smaller width have a smaller bandgap due to the quantum size effects in ultra-small nanoribbons. It should be noted that there is no experimental data to compare the bandgap of these structures with.

4. Conclusions

FP-LAPW calculation via GGA approach for the exchange-correlation potential has been exploited to compute the of the SiC nanoribbons. The calculations showed that the p orbitals of carbon and silicon dominate the electronic structure of ASiCNR (w=3) near the Fermi level. In addition, the outputs showed that the electronic bandgap of ASiCNRs (w=3) is larger than that of ZSiCNRs (w=3).

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding this article.

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How to cite this article: Badehian HA, Badehian Z, Sharifirad R. Structural and Electronic Properties of Armchair Silicon Carbide Nanoribbons. *Curr. Appl. Sci.*, 2023, 1(1):51-58. https://doi.org/10.22034/cas.2021.144398