Tuning the Electronic Properties of 2D Silicon Carbide Nanoribbons for Nanodevices Application

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Index-

Abstract

Silicon carbide nanoribbons (SiC NRs) are emerging as essential materials for the future of miniaturized electronic and spintronic devices due to their exceptional structural, electronic, and magnetic properties. This study explores how altering the edges of these nanoribbons by attaching hydrogen or fluorine atoms influences their stability, electrical characteristics, and electron transport behavior in both zigzag and armchair configurations. Utilizing advanced computational simulations based on density functional theory (DFT), we investigated various edge passivation techniques to understand their impact on structural robustness, electronic band structure, spin alignment, and electrical conductivity. Our results indicate that hydrogen passivation significantly enhances the stability of SiC nanoribbons while enabling precise control over their electronic properties. In zigzag nanoribbons, hydrogenation allows for a tunable transition between semiconductor and magnetic states, making them highly suitable for spintronic applications. On the other hand, fluorine passivation results in even greater structural stabilization due to fluorine's strong electron-withdrawing nature, leading to increased charge transfer and stronger chemical bonding at the edges. Additionally, fluorinated zigzag nanoribbons exhibit half-metallicity, a highly desirable property for efficient spin filtering, which is crucial for spintronic memory and logic devices. Furthermore, both hydrogenated and fluorinated nanoribbons demonstrate negative differential resistance (NDR), a phenomenon that makes them promising candidates for high-speed switching and oscillator applications. Moreover, our study evaluates how external electric fields influence the electronic and magnetic properties of SiC nanoribbons. We found that applying an electric field can modulate the band gap and magnetic behavior, enabling precise tuning of these materials for low-power electronic applications. Computational modeling of spin transport further reveals that the movement of spin-polarized charge carriers in SiC nanoribbons can be effectively controlled, providing a solid foundation for future spintronic device development. Beyond edge passivation, this research also examines the effects of nanoribbon width and edge reconstructions on their stability and electronic properties. Wider nanoribbons exhibit reduced edge effects, leading to shifts in band gap characteristics, while narrower nanoribbons show more pronounced quantum confinement effects. Additionally, our analysis suggests that specific hydrogenation configurations can stabilize distinct magnetic states, allowing transitions between ferromagnetic and antiferromagnetic behaviors depending on how the edges are functionalized. The integration of SiC nanoribbons with other two-dimensional (2D) materials, such as graphene and MoS_2, could further enhance their electronic properties, opening new avenues for high-mobility hybrid electronic devices. However, validating these theoretical predictions experimentally remains a significant challenge, requiring advancements in nanofabrication techniques to achieve controlled synthesis and precise edge engineering. Furthermore, understanding the thermal stability, defect tolerance, and long-term performance of SiC nanoribbons is crucial for their successful implementation in commercial electronic, spintronic, and quantum computing technologies.

Overall, this study underscores the vital role of edge functionalization in tailoring the electronic and magnetic properties of silicon carbide nanoribbons. The observed half-metallicity, negative differential resistance, and spin-filtering effects make these materials highly promising for applications in nanoscale transistors, high-speed electronic switches, and energy-efficient spintronic circuits. By achieving precise control over edge chemistry and leveraging external electric fields, SiC nanoribbons hold great potential to revolutionize the next generation of semiconductor technologies, paving the way for ultra-fast, energy-efficient, and multifunctional nanodevices.

Key Words – Nanoribbons, Spintronics, Hydrogenation, Antiferromagnetism

1. Introduction –

Silicon carbide (SiC) is a wide-bandgap semiconductor known for its exceptional mechanical strength, thermal conductivity, and chemical stability, making it highly suitable for high-power electronic devices and harsh-environment applications. Its outstanding electronic properties, including high electron mobility and tunable band structure, have spurred extensive research into its low-dimensional forms, such as nanowires, nanotubes, and nanoribbons [1–10]. Among these, zigzag silicon carbide nanoribbons (ZSiCNRs) have attracted considerable attention for applications in nanoelectronics and spintronics due to their unique quantum confinement and edge effects that significantly influence their electronic and magnetic properties. Density functional theory (DFT) studies using exchange-correlation functionals like the Perdew–Burke–Ernzerhof (PBE) under generalized gradient approximation (GGA) or local density approximation (LDA-PZ) reveal insights into their structural stability, bandgap modulation, and charge transport. Narrow ZSiCNRs display enhanced quantum confinement effects, and edge passivation—commonly with hydrogen or fluorine—further tailors their band structures and improves stability. Edge-modified ZSiCNRs exhibit distinct electronic behavior; while bare ZSiCNRs tend to show metallic or semi-metallic character due to localized edge states, hydrogenation stabilizes the electronic structure by suppressing these states, and fluorination enhances electron localization, significantly affecting conductivity. Spin-polarized DFT calculations demonstrate the presence of ferromagnetic (FM) and antiferromagnetic (AFM) ground states based on edge termination, with some configurations exhibiting half-metallicity, thus making ZSiCNRs promising for spin-filtering applications.

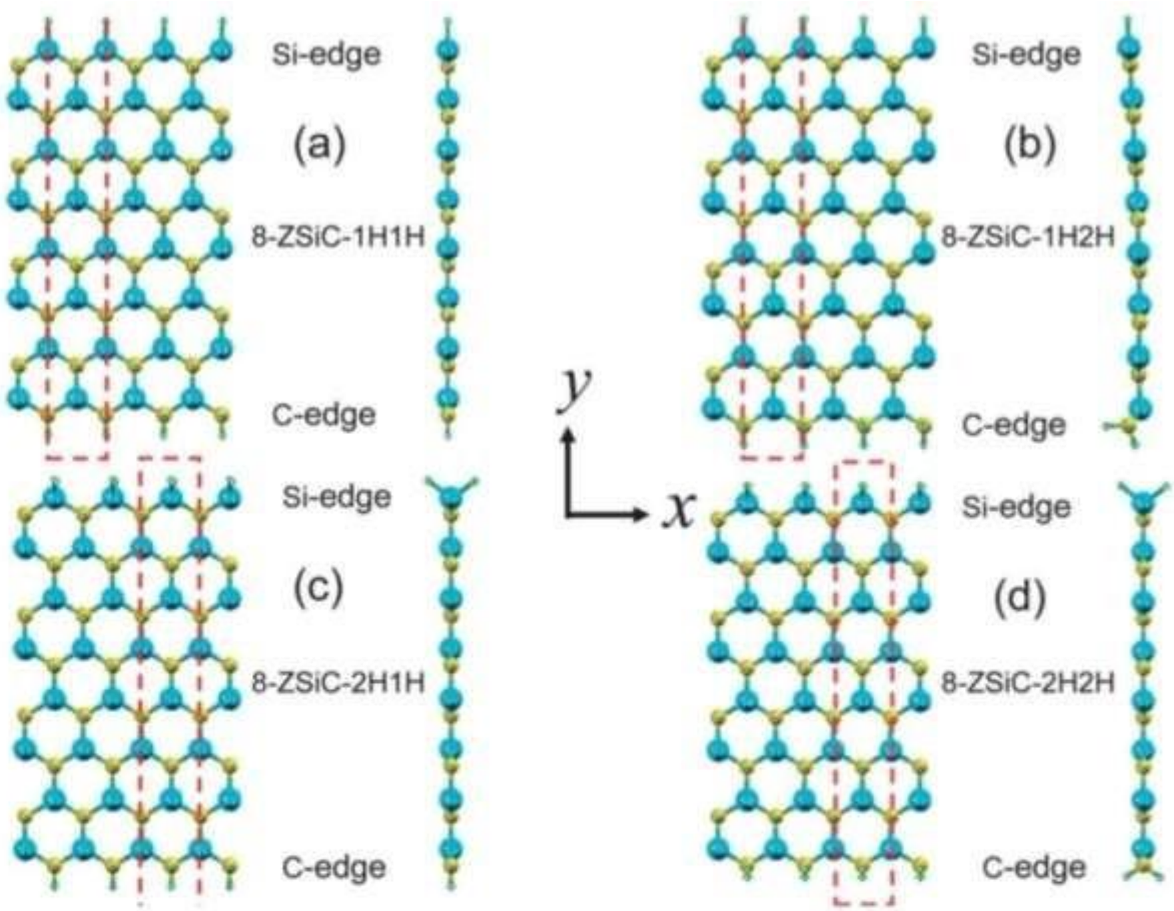
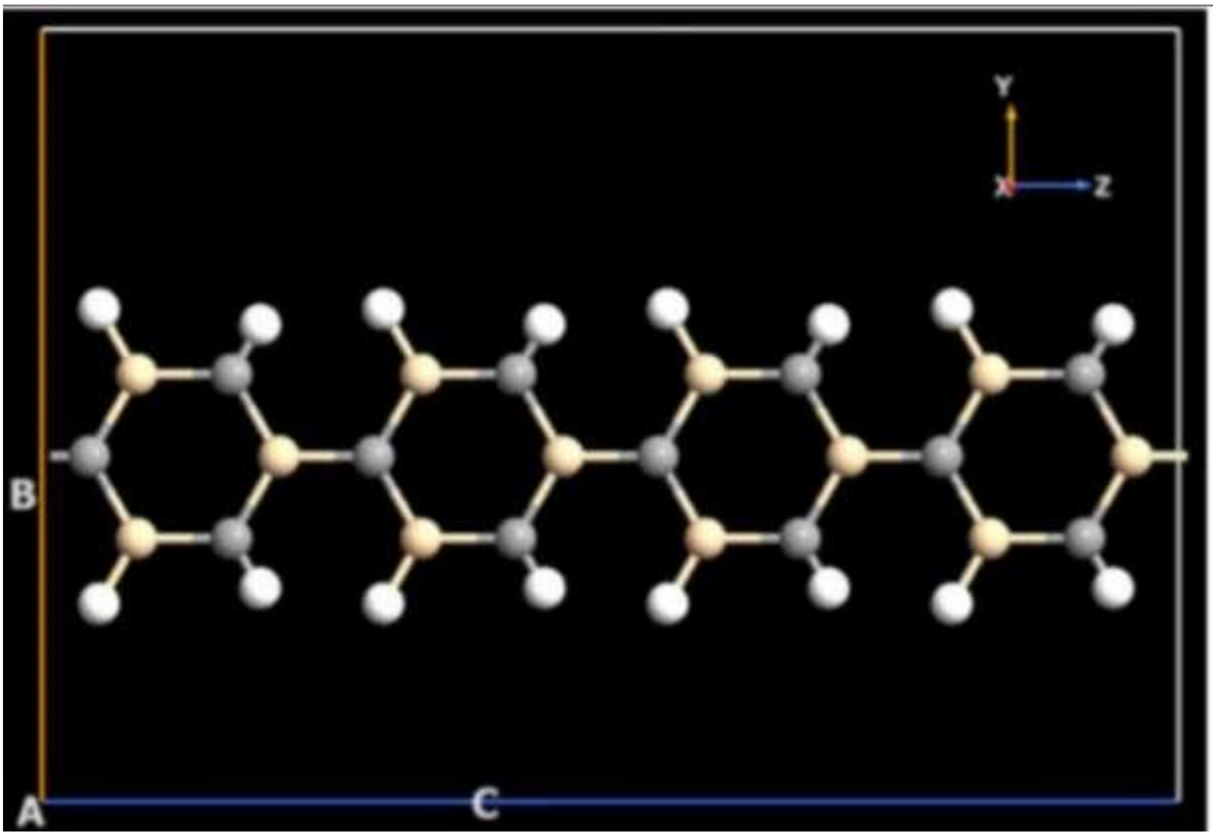


Fig 1. TOP And Side View of Geometric Structure of ZSiCNRs. [53]

Charge transport, analyzed via the nonequilibrium Green's function (NEGF) formalism and two-probe models, indicates that fluorine-passivated ZSiCNRs offer higher spin-filtering efficiency and even exhibit negative differential resistance (NDR) in specific configurations, beneficial for high-speed switching and oscillator devices. Thermodynamic stability analyses, including edge formation energy calculations, suggest that various passivated forms can be experimentally realized under controlled conditions, enabling tailored fabrication for desired electronic and magnetic functionalities. Further, these nanoribbons (NRs) are classified as bare and pristine, with the latter referring to edge passivation by hydrogen (H) on both sides. Bare ZSiCNRs exhibit metallic characteristics attributed to the presence of dangling bonds at the edges, whereas pristine nanoribbons become semiconducting due to the suppression of these dangling bonds through hydrogen passivation [11,12]. Among such compounds, particular focus has been given to SiC owing to its outstanding electronic and physical properties [13]. Structurally, SiC consists of alternately arranged silicon and carbon atoms with a Si–C bond length of approximately 1.80 Å and a stoichiometric ratio of 1:1 [14,15–18]. It naturally forms in various close-packed crystal structures such as cubic, hexagonal, or rhombohedral lattices [15]. Its ability to sustain high temperatures, pressures, and harsh environmental conditions makes it a material of immense technological interest [19,20]. Several synthesis strategies have been reported for fabricating silicon carbide nanoribbons (SiCNRs), among which a prominent approach involves cutting SiC sheets into ribbon structures, similar to the method employed for generating graphene nanoribbons (GNRs) from graphene [21-23]. Graphene is well known for its amazing properties, but its natural semimetallic behavior limits its use in some electronic applications. Because of this, scientists have started looking into other two-dimensional (2D) materials that could offer better performance in certain areas. Some of these promising materials include III-V nitride-based compounds [24–27], molybdenum disulfide (MoS_2) [28], vanadium dioxide (VO_2) [29], titanium dioxide (TiO_2) [30], and silicon-based materials such as silicon carbide (SiC) [31], silicon germanium (SiGe) [32], SiSn, SiPb, and GeSi. To improve the performance of these materials, especially their electronic properties, researchers often dope them with foreign atoms. This process helps to open up or tune the electronic band gap, which is important for making the materials suitable for use in devices. Doping also improves their ability to adsorb ions, which is useful in energy storage systems like batteries and supercapacitors [33]. In addition to these, other interesting 2D materials such as C_3N [34] and several carbon-based derivatives [35] have also been studied. These materials have a flat, sheet-like structure similar to graphene [36], but they often show better behavior for electronic devices because they naturally have a band gap. This band gap comes from differences in the electronegativity of the atoms they are made of [37], which allows them to work more effectively in various applications. In many cases, these materials have even shown to perform better than graphene itself [38,39].

Similarly, armchair silicon carbide nanoribbons (ASiCNRs) have emerged as an important class of low-dimensional SiC materials, with distinct electronic properties governed primarily by ribbon width and edge passivation. Unlike ZSiCNRs, ASiCNRs typically exhibit semiconducting behavior with a bandgap that varies inversely with ribbon width due to quantum confinement effects.



. Fig 2. Armchair silicon carbide Nanoribbons with edge passivated by hydrogen, [54]

DFT-based simulations have shown that the bandgap in ASiCNRs can be effectively tuned via hydrogenation or fluorination, similar to zigzag configurations. Structural optimization and Brillouin zone sampling are crucial to accurately predicting their electronic properties, while edge functionalization remains key to stabilizing the ribbon and enhancing its electronic characteristics [40,41]. The density of states (DOS) and band structure calculations indicate that hydrogen-passivated ASiCNRs offer more uniform electronic characteristics, while fluorinated ASiCNRs demonstrate stronger charge redistribution and localized states near the edges. Unlike ZSiCNRs, ASiCNRs generally do not exhibit magnetism in their pristine or passivated forms, which limits their application in spintronics but makes them more suitable for conventional nanoelectronic devices. Transport properties evaluated through NEGF techniques show that ASiCNRs provide robust semiconducting channels with reliable current-voltage (I–V) behavior, and edge engineering continues to be a promising route for modulating their transport efficiency. Overall, both zigzag and armchair silicon carbide nanoribbons represent tunable and versatile platforms for next-generation electronic and optoelectronic devices, with their properties highly sensitive to structural parameters and chemical modifications.

2. Computational Details –

Ankita et al. [42] conducted a first-principles study on various configurations of zigzag silicon carbide nanoribbons (ZSiCNRs) using density functional theory (DFT) with the Quantum ATK tool. Their research explored different passivation schemes, including hydrogen (H) and fluorine (F), across nanoribbons of varying widths. They examined five cases: bare ZSiCNR (unpassivated), H-ZSiCNR-H (hydrogen passivated), F-ZSiCNR-H (fluorine at one edge, hydrogen at the other), H-ZSiCNR-F (hydrogen at one edge, fluorine at the other), and F-ZSiCNR-F (fully fluorine-passivated). The nanoribbons were treated as quasi-1D structures, with periodicity along the Z-axis and confinement along the other two directions, ensuring minimal interference from periodic replicas with a vacuum spacing of 10 Å in the X and Y directions. Calculations were performed using the Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional within the generalized gradient approximation (GGA). To assess stability, binding energies were calculated following a method similar to that of S. Kharwal et al. Supercell models of ZSiCNRs were used for transport property calculations, employing a two-probe model consisting of a central nanoribbon segment sandwiched between left and right electrode extensions. The transmission spectrum, T(E,V), was analyzed to determine electron transport behavior, while current-voltage (I–V) characteristics were obtained through integration of the transmission function. Ping Lou [43] utilized the OPENMX computational code, applying DFT with GGA for exchange-correlation energy. The study used norm-conserving Kleinman–Bylander pseudopotentials and employed a basis set expansion in the form of a linear combination of multiple pseudo-atomic orbitals (LCPAO), with a kinetic energy cutoff of 300 Ry and the following basis functions: C5.5-s2p2d1, Si5.5-s2p2d1, and H4.5-s1p1. The study examined the impact of hydrogen passivation at the edges of pristine ZSiC nanoribbons, where the two possible terminations—Si-edge and C-edge—led to different structural and electronic properties. When exposed to H_2 gas, the Si and C edge atoms could be passivated with either one (sp^2 hybridization) or two (sp^3 hybridization) hydrogen atoms. Previous findings suggested that unpassivated ribbons tend to reconstruct at the C-edge (Crc) due to stability considerations, whereas Si-edge reconstruction (Sirc) is energetically unfavorable; however, hydrogen passivation effectively prevents edge reconstruction. The study focused on four hydrogen passivation configurations: N-ZSiC-1H1H (one H atom on each Si and C edge atom), N-ZSiC-1H2H (one H on each Si atom, two H on each C atom), N-ZSiC-2H1H (two H on each Si atom, one H on each C atom), and N-ZSiC-2H2H (two H on both Si and C edge atoms). Using a supercell approach with a 20 Å vacuum In the non-periodic directions, geometry optimization was performed with a 121×1×1 k-point sampling, and transport calculations were conducted using the nonequilibrium Green’s function (NEGF) formalism. Esmaeil Zaminpayma [44] explored the properties of armchair silicon carbide nanoribbons (ASiCNRs), replacing half the carbon atoms in graphene nanoribbons with silicon. Atomic positions and bond lengths were optimized before conducting electronic and magnetic property calculations using spin-polarized DFT within the Siesta software. Key computational details included the Local Density Approximation (LDA-PZ) exchange-correlation functional, a Double-Zeta Plus Polarization (DZP) basis set, a mesh cutoff of 150 Ry, and Brillouin zone sampling with a Monkhorst–Pack grid of 32 k-points. To study magnetism, both ferromagnetic (FM) and antiferromagnetic (AFM) states were considered, where in the FM state, edge spins aligned in the same direction, while in the AFM state, upper and lower edge spins were oppositely aligned. Shu-Ling Deng et al. [45] conducted band structure calculations for ZSiCNRs using the Quantum ATK software package, employing the GGA-PBE functional for exchange-correlation effects and expanding wave functions using the double-zeta polarization (DZP) method.

3. Results and Discussion

Structural stability and passivation effect –

The structural stability and passivation effects of silicon carbide nanoribbons (SiCNRs), including both zigzag (ZSiCNRs) and armchair (ASiCNRs) configurations, have been studied extensively to evaluate their potential in advanced nanoelectronic and spintronic devices. Ankita and colleagues carried out a comprehensive study on the structural behavior of ZSiCNRs under different edge passivation conditions, focusing particularly on hydrogen (H) and fluorine (F) atoms. Their findings revealed that the Si–C bond length was consistently around 1.80 Å, which aligns well with earlier theoretical and experimental results. They discovered that fluorine formed significantly stronger bonds with the ribbon edges compared to hydrogen, leading to greater overall structural integrity. While all types of nanoribbons generally retained a flat geometry, noticeable edge bending was observed in the bare (unpassivated) configurations. This bending enhanced internal electrostatic interactions, destabilizing the structure, whereas hydrogen-passivated ribbons exhibited a reduced degree of bending, which weakened internal forces and slightly improved structural stability. The most remarkable improvement came from fluorine passivation, which, due to fluorine's high electronegativity, facilitated a substantial charge transfer of 0.38e from silicon to fluorine, in contrast to only 0.1e in hydrogenated structures. This significant charge transfer further contributed to the improved stability of fluorine-passivated nanoribbons. It was also observed that for narrower ribbons (N = 4), fluorine passivation resulted in the most stable configuration. However, as the ribbon width increased (N = 6–10), the bare nanoribbons became more thermodynamically stable than their passivated counterparts. Phonon dispersion analyses confirmed the dynamic stability of all configurations, including the bare ZSiCNRs, suggesting their viability for practical applications. Similarly, armchair silicon carbide nanoribbons (ASiCNRs) exhibited comparable structural behavior under passivation, with fluorinated edges showing enhanced charge redistribution and improved geometric stability, while hydrogenated ASiCNRs maintained more uniform bond lengths and ag generally flat structure.

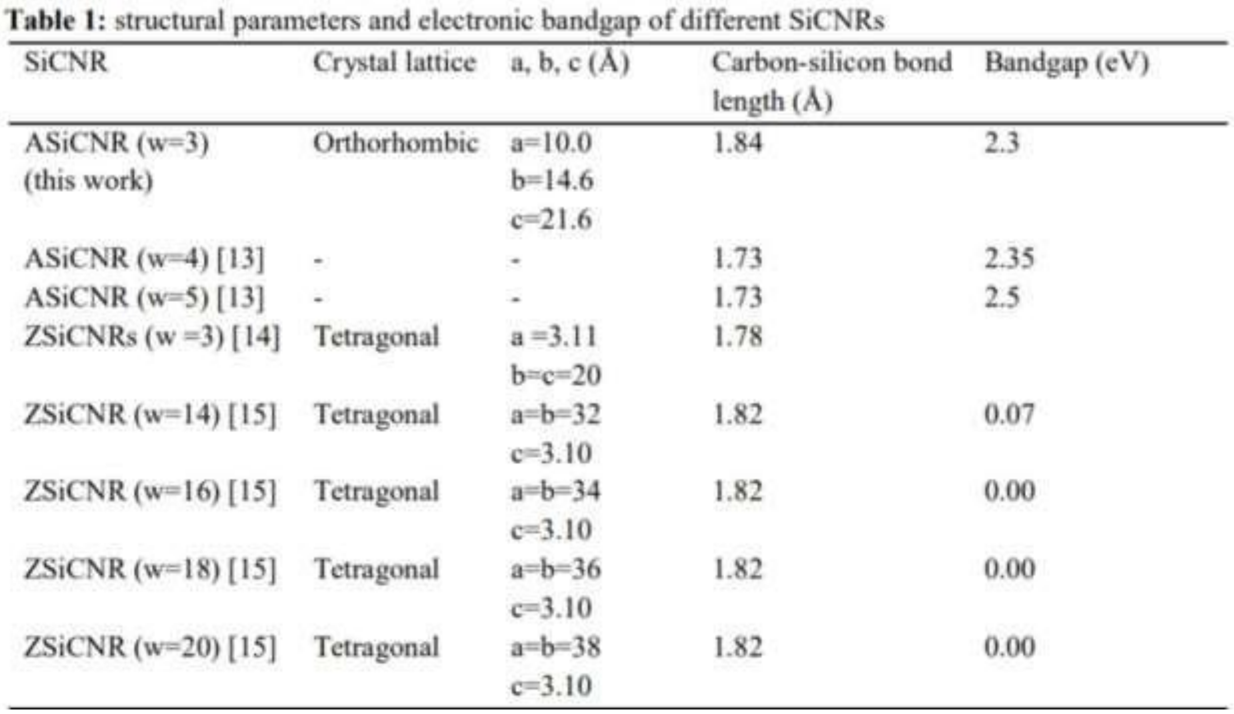


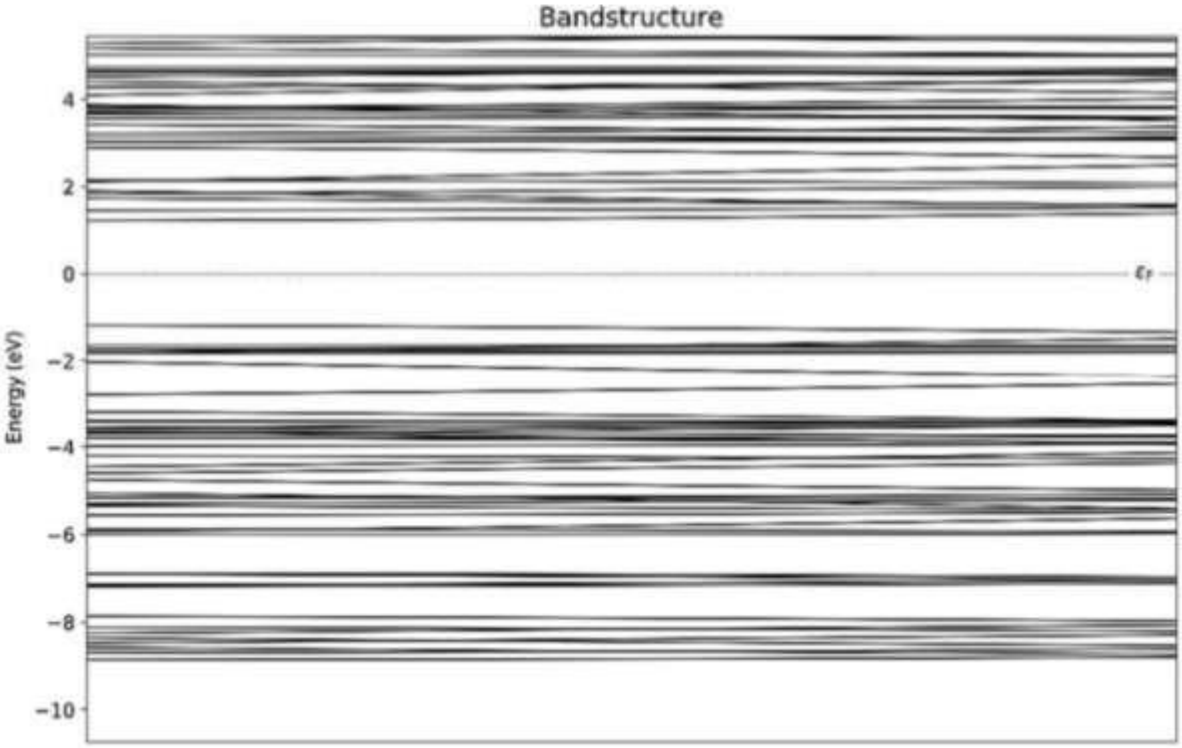
Table 1: structural parameters and electronic bandgap of different SiCNRs

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

Table 1. Structural parameters and electronic bandgap of different SiCNRs. [54]

In another pivotal study, Ping Lou and collaborators[14] focused on the impact of edge hydrogenation on the stability and magnetic behavior of ZSiCNRs by analyzing various hydrogenation patterns and spin states using first-principles calculations. Their results indicated that the edge formation energy (E_edge+nHmH) decreased with increasing ribbon width, implying that the contribution of edge atoms to the total energy diminished as ribbons became wider. Among the different hydrogenation schemes, 8-ZSiC-2H2H was found to be the most energetically favorable configuration, whereas 8-ZSiC-1H1H exhibited the highest edge formation energy and was considered stable only under extremely low hydrogen pressure. The researchers further demonstrated that the hydrogen chemical potential is a critical parameter for tailoring nanoribbon stability, enabling selective synthesis of different hydrogenated edge structures through precise control of hydrogen pressure. In addition to structural stability, their study also delved into the electronic and magnetic properties of hydrogenated nanoribbons, particularly N-ZSiC-2H1H and N-ZSiC-2H2H. It was revealed that N-ZSiC-2H1H consistently displayed ferromagnetic behavior across all ribbon widths. For ribbons with narrower widths ($N \leq 12$), N-ZSiC-2H1H functioned as a ferromagnetic semiconductor, while for wider ribbons ($N \geq 13$), it transitioned into a ferromagnetic half-metal, achieving 100% spin polarization, a highly desirable trait for spintronic applications. On the other hand, N-ZSiC-2H2H showed nonmagnetic behavior in very narrow configurations ($N \leq 4$) but transitioned to a ferrimagnetic state when the ribbon width reached N = 5. Moreover, similar to N-ZSiC-2H1H, it underwent a semiconductor-to-half-metal transition when the ribbon width increased beyond $N \geq 8$, indicating a width-dependent magnetic phase change. The study also offered insights into how different hydrogenation patterns affect the magnetic properties of SiCNRs. Among them, N-ZSiC-1H1H has been widely investigated for its strong spin-polarized ground state, while N-ZSiC-2H2H was shown to develop enhanced magnetic moments, particularly localized not at the edges but on inter-edge atoms. Mulliken charge analysis demonstrated that hydrogenation at the carbon edge induced charge transfer to nearby silicon atoms, resulting in an increase in their magnetic moments and revealing the critical role of edge chemistry in modulating magnetism. These findings suggest that careful tuning of hydrogenation patterns can be employed to fine-tune both electronic and magnetic properties of silicon carbide nanoribbons. The broader implication is that by adjusting hydrogenation conditions, such as temperature and pressure, researchers can exert precise control over the stability and spin transport characteristics of these nanoribbons. Additionally, specific dual-hydrogenation configurations were found to induce spin polarization that led to the emergence of both ferromagnetic (FM) and antiferromagnetic (AFM) states. Certain configurations even displayed half-metallicity, where one spin channel remains metallic and the other semiconducting, making these systems especially attractive for use in spin-filtering and spintronic technologies. These conclusions apply not only to ZSiCNRs but are also relevant to ASiCNRs, which, while generally less magnetically active, can exhibit tunable semiconducting behavior and enhanced stability under specific edge functionalizations. Overall, the combined insights from Ankita and Ping Lou's studies demonstrate that the structural, electronic, and magnetic behaviors of both zigzag and armchair silicon carbide nanoribbons can be effectively engineered through strategic edge passivation and hydrogenation, making them promising candidates for future advancements in nanoelectronics and spintronic device applications.

Fig. 3 Band structure of ASiCNR (w=3). The Fermi level is set to zero [54]



Electronic and magnetic Properties-

Silicon carbide nanoribbons (SiCNRs) have emerged as a fascinating class of low-dimensional materials with promising applications in nanoelectronics and spintronics, thanks to their tunable electronic and magnetic properties. These nanoribbons, derived from silicon carbide sheets, exhibit electronic characteristics that can be drastically modified by manipulating edge configurations, doping, defects, and edge terminations. A wide range of computational studies, particularly density functional theory (DFT) simulations, have provided rich insights into how these variations influence their electronic behavior. Starting with the structural variations, SiCNRs exist in two primary edge geometries: armchair and zigzag. Zigzag and armchair silicon carbide nanoribbons (ZSiCNRs and ASiCNRs) exhibit a range of intriguing electronic and magnetic properties that vary based on their edge configurations and surface modifications. In the case of zigzag SiC nanoribbons, researchers observed that bare ZSiCNRs display semi-metallic behavior, characterized by the highest valence band and the lowest conduction band touching the Fermi level. This semi-metallicity is maintained even in wider ribbons, despite the application of edge passivation techniques. When hydrogen or fluorine passivation is applied, a small bandgap opens up, but it remains too narrow for effective use in conventional semiconductor applications. A deeper analysis using the Density of States (DOS) revealed a strong localization of electronic states near the Fermi level in bare ZSiCNRs, reinforcing their metallic nature. The transport properties, particularly the current-voltage (I–V) characteristics, further supported this finding—bare ZSiCNRs produced the highest current of approximately 30 µA, whereas hydrogen- and fluorine-passivated ribbons showed significantly reduced currents of around 6.75 µA. A notable phenomenon observed across all ZSiCNR configurations was the negative differential resistance (NDR) effect, a valuable trait for developing fast-switching nanoelectronic devices and oscillators. Among these, fluorine-passivated structures (F-ZSiCNR-F) demonstrated the most pronounced NDR effect, suggesting a higher potential for practical applications. In addition to their electronic properties, ZSiCNRs also exhibit fascinating magnetic behavior. Spin-polarized calculations indicated a high spin filtering efficiency (SFE), reaching up to 100% in certain configurations, which is highly desirable for spintronic technologies. The study further explored the effects of fluorine adsorption on different atomic sites of the nanoribbons. The most energetically favorable site was found to be on top of a silicon atom (F@Si), while adsorption on a carbon atom (F@C) was the least stable. Fluorine adsorption led to significant changes in the electronic structure by introducing localized bands near the Fermi level, signaling potential magnetic activity. These changes resulted in an antiferromagnetic (AFM) ground state preference in the fluorinated nanoribbons. Notably, the F@Si configuration exhibited half-metallicity, where one spin channel retained metallic properties while the other exhibited semiconducting behavior. This unique combination makes F@Si-ZSiCNRs promising candidates for spin-filtering devices, capable of distinguishing electrons by their spin orientation without the need for an external magnetic field. In summary, the research concluded that fluorine passivation not only enhances the structural stability of ZSiCNRs but also significantly modifies their electronic and transport characteristics, especially through the induction of NDR and spin filtering effects, thereby emphasizing their potential for use in future nanoelectronic and spintronic devices. In contrast, armchair silicon carbide nanoribbons (ASiCNRs) show a different set of electronic and magnetic behaviors under various hydrogenation conditions. The work focused on these armchair-edged nanoribbons and found that singly hydrogenated ASiCNRs behave as direct bandgap semiconductors. Their band structure analysis revealed that, much like graphene nanoribbons, ASiCNRs follow a 3P rule in bandgap variation, though the fluctuations remain relatively minor, with deviations of less than 0.1 eV. This indicates a high level of uniformity and predictability in their electronic behavior, making them suitable for use in optoelectronic devices where stable bandgaps are required. However, when dual-hydrogenation patterns are introduced, the hybridization of the ribbon structure transitions from sp^2 to sp^3, resulting in significant changes in both the electronic and magnetic properties. Certain hydrogenation configurations, such as SiHCH-aSiCNR and 2SiH-aSiCNR-2CH, manage to retain semiconducting characteristics. Meanwhile, other patterns introduce new bands near the Fermi level, altering the band structure and leading to metallic behavior. This demonstrates that the electronic properties of ASiCNRs can be finely tuned through selective hydrogenation, allowing for a customizable approach to designing nanoribbons with desired conductive or semiconductive properties. ASiCNRs are generally nonmagnetic semiconductors, and their bandgap can be modulated by varying the width of the ribbon and by altering the atoms used for edge termination. Specifically, in a study, it was found that when ASiCNRs are terminated with halogen atoms (such as F, Cl, Br, and I), the band gap decreases with the increasing atomic number of the halogen. This trend arises because the halogen termination causes a downward shift in the conduction band minimum, while the valence band remains largely unaffected. Consequently, the band gap becomes smaller with heavier halogens [46]. In contrast, ZSiCNRs behave quite differently. They often exhibit metallic or half-metallic behavior, depending on factors such as width and edge passivation. Remarkably, ZSiCNRs with widths narrower than 4 nm can be intrinsically half-metallic, even without the application of an external field or chemical doping. This characteristic makes them highly attractive for spintronic applications, where materials capable of conducting electrons of only one spin orientation are crucial. The half-metallic nature has been confirmed using first-principles calculations and highlighted for its potential utility in designing spin filters [47]. Further examination of edge terminations reveals significant distinctions between different nanoribbon types. For instance, fluorine-terminated ZSiCNRs continue to display metallic behavior, even at greater widths. This is due to the presence of edge-localized electronic states near the Fermi level. On the other hand, F-terminated ASiCNRs consistently remain semiconductors, regardless of their width. This difference originates from the edge structure of ASiCNRs, where silicon-carbon dimer bonds suppress the formation of edge states at the Fermi level. Another study also observed a strong accumulation of charge around F and C atoms, leading to a notable charge transfer from Si atoms to these more electronegative atoms, which results in ionic Si–C and Si–F bonds, while the C–F bond remains covalent [48]. Another crucial approach to modifying electronic properties is doping, where foreign atoms are introduced into the SiCNRs. A study explored the effects of boron (B) and nitrogen (N) doping on both ASiCNRs and ZSiCNRs. It was found that B and N atoms tend to replace Si and C atoms, respectively, at the ribbon edges, which are the most energetically favorable sites. In the case of ASiCNRs, this substitution did not disturb the semiconducting nature of the material. However, in ZSiCNRs, B doping preserved the half-metallic character, whereas N doping altered the ribbon to become metallic. This is due to N atoms disrupting the spin-polarized edge states, thereby closing the spin gap [49]. Defects, such as atomic vacancies, are another factor that can significantly influence the electronic structure. In a study, the introduction of a single carbon vacancy in a ZSiCNR transformed its half-metallic nature into metallic behavior. This transformation occurred due to the interaction of neighboring silicon atoms with the vacancy, which altered the electronic structure near the Fermi level. Such defect engineering opens up further possibilities for controlling the electronic and magnetic features of SiC nanoribbons [50]. Moreover, the inclusion of electron correlation effects, such as those modeled using the GW approximation, leads to significant corrections in the predicted band structures of SiCNRs. In an advanced study, GW calculations showed that quasiparticle corrections can enlarge the bandgap and alter the magnetic behavior of nanoribbons. Specifically, hydrogen-passivated ZSiCNRs, initially believed to be half-metallic under DFT, actually become narrow-gap spin-polarized semiconductors when many-body effects are taken into account. This result highlights the need for beyond-DFT approaches in accurately predicting the behavior of low-dimensional materials [51]. Besides edge passivation and doping, adsorption of atoms on ribbon surfaces can also lead to intriguing changes. A study investigated the effect of magnesium (Mg) doping on SiCNRs. While Mg is a nonmagnetic element, its inclusion introduced localized electronic levels within the bandgap, thus affecting the ribbon's conduction properties. Interestingly, this doping also resulted in the induction of magnetic moments, altering the system's magnetic characteristics. These findings suggest that nonmagnetic dopants can still introduce significant electronic and magnetic changes to the SiC nanoribbon framework. Furthermore, hybrid structures and strain engineering add another dimension to the tunability of SiCNRs. For example, hybrid AlN/SiC nanoribbons exhibit a variety of magnetic states due to the interface effects and edge terminations. A study demonstrated that magnetic moments in such heterostructures are mainly localized at the edges, and external strain can be used to further control these properties, paving the way for strain-tunable spintronic devices [52]. The electronic properties of silicon carbide nanoribbons are thus highly tunable and versatile, governed by factors like ribbon width, edge type, termination atoms, dopants, defects, and electron correlation effects. While ASiCNRs primarily remain semiconductors with modifiable band gaps, ZSiCNRs stand out due to their natural tendency toward half-metallicity and spin polarization. These characteristics make SiCNRs strong candidates for next-generation electronics, including field-effect transistors, spin filters, and magnetic memory devices. As computational techniques become more sophisticated and synthesis methods more precise, SiCNRs may soon transition from theoretical models to real-world applications in nanoelectronic and spintronic systems.

4. Conclusion

The study of two-dimensional silicon carbide (SiC) nanoribbons is not just a promising avenue—it is a revolution in the making, a scientific frontier that holds the key to the next generation of high-performance electronics, ultra-fast switching devices, and quantum computing breakthroughs. These nanoribbons, with their remarkable combination of wide bandgap semiconducting behavior, high thermal conductivity, and exceptional mechanical robustness, stand as the ultimate candidates for reshaping modern nanoelectronics and spintronics. Their ability to undergo precise bandgap tuning through methods such as strain engineering, electric field modulation, and heterostructure formation opens unprecedented possibilities for designing ultra-efficient transistors, optoelectronic components, and futuristic nanodevices. The manifestation of negative differential resistance (NDR) behavior, a highly sought-after phenomenon, propels these materials into the spotlight as potential game-changers for high-speed switching applications, including next-generation oscillators and tunnel diodes that could redefine the limits of electronic speed and power efficiency. Beyond their fundamental electronic properties, SiC nanoribbons emerge as front-runners in the realm of spintronics, a field that seeks to harness electron spin rather than charge for data storage and processing. The ability to induce room-temperature ferromagnetism, achieve near-perfect spin filtering efficiency, and even exhibit half-metallicity in certain edge-passivated configurations positions these nanoribbons as prime candidates for the development of cutting-edge spin-based memory and logic circuits. This marks a paradigm shift in computing, promising data processing speeds and energy efficiencies that far surpass conventional semiconductor technologies. Yet, the true impact of SiC nanoribbons extends even further. The integration of these remarkable materials with other two-dimensional platforms—such as graphene, molybdenum disulfide (MoS_2), and hexagonal boron nitride (h-BN)—could lead to a new class of hybrid structures with unparalleled electronic, mechanical, and optical properties. Imagine a future where SiC nanoribbons are seamlessly incorporated into flexible electronics, wearable sensors, and even bio-integrated devices, offering real-time data processing and ultra-sensitive detection capabilities. However, the grand vision of harnessing SiC nanoribbons for real-world applications hinges on a critical challenge—the need for scalable, reproducible, and high-precision fabrication techniques. The transition from theoretical simulations and controlled laboratory environments to industrial-scale manufacturing is a formidable hurdle, demanding breakthroughs in nanofabrication methodologies. Additionally, ensuring their long-term environmental and thermal stability is paramount, particularly as these nanoribbons are envisioned for applications in extreme environments, from high-temperature electronics in aerospace technologies to radiation-resistant components for space exploration. Despite these challenges, the future of SiC nanoribbons remains undeniably bright. The vast potential of these materials, coupled with the relentless advancements in nanotechnology, suggests that we stand on the brink of a transformative era in electronics and spintronics. As researchers continue to refine their understanding and fabrication techniques, SiC nanoribbons are poised to emerge as a fundamental building block of next-generation nanochips, high-speed quantum devices, and ultra-efficient computing systems.

In the grand tapestry of scientific progress, few materials have shown such immense promise across so many domains. Silicon carbide nanoribbons are not just a material of the future—they are the future, a beacon of innovation that will illuminate the path toward faster, smarter, and more energy-efficient technologies. The journey ahead is challenging, but the rewards promise to be nothing short of revolutionary.

5. Future Aspects of 2D SiC Nanoribbons-

The study of two-dimensional silicon carbide (SiC) nanoribbons presents exciting possibilities for advancing nanoelectronics, spintronics, and quantum computing. One of the most promising research directions is bandgap engineering, where techniques such as strain modulation, electric field tuning, and heterostructure formation are used to precisely control the electronic properties of SiC nanoribbons. This level of control could lead to significant improvements in high-speed transistors, optoelectronic devices, and energy-efficient electronics. Additionally, the negative differential resistance (NDR) effect observed in these nanoribbons holds great potential for high-speed switching applications, including tunnel diodes and oscillators—essential components in modern high-frequency, low-power circuits. Another fascinating area of exploration is spintronics, where researchers are investigating ways to achieve room-temperature ferromagnetism and high spin filtering efficiency by modifying the nanoribbon edges, introducing doping elements, or applying magnetic tuning. These advancements could enable the development of energy-efficient spintronic memory and logic devices with enhanced performance. Furthermore, quantum transport studies in SiC nanoribbons offer valuable insights into charge carrier behavior at the nanoscale, which is critical for designing low-power, high-efficiency nanoelectronic circuits. Beyond their standalone applications, SiC nanoribbons could play a crucial role in hybrid material systems. Integrating them with other 2D materials, such as graphene, molybdenum disulfide (MoS_2), and hexagonal boron nitride (h-BN), could result in high-mobility devices with exceptional electronic and mechanical properties. These hybrid structures hold immense potential for flexible electronics, multifunctional sensors, and next-generation nanochips. However, translating these theoretical advancements into real-world applications requires significant progress in nanofabrication. Scalable and precise synthesis methods must be developed to ensure the reproducibility and integration of SiC nanoribbons into commercial electronic and spintronic technologies. In addition to fabrication challenges, assessing the environmental and thermal stability of SiC nanoribbons is essential for their long-term viability. Their chemical robustness and mechanical strength make them strong candidates for applications in extreme environments, such as high-temperature electronics, space exploration, and automotive industries. Understanding their thermal conductivity and defect tolerance will be crucial in ensuring reliable device performance under demanding conditions.

Addressing these challenges will position SiC nanoribbons as a key material for the next generation of ultra-fast, energy-efficient, and multifunctional nanodevices. Their unique combination of electronic tunability, spin-polarized transport, and structural stability makes them strong contenders for groundbreaking advancements in nanoscale computing, communication, and sensing technologies. With continued research and technological progress, SiC nanoribbons could play a transformative role in the future of nanotechnology.

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Statements and Declarations –

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by Khushi Mishra . The first draft of the manuscript was written by Khushi Mishra and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript."

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