STUDY OF THE STRUCTURAL AND ELECTRONIC PROPERTIES OF SULFUR DOPING STANENE NANORIBBON: A CASE DFT

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Article Info

Abstract

Volume: 7 Issue: 2 Jun: 2025 Received: May. 28th, 2024 Accepted: Jun. 15th, 2025 Page No: 385-396 The structural and electronic properties of sulfur-doped armchair stanene nanoribbons (ASnNRs) have been investigated using Density Functional Theory (DFT). The diverse structural and electronic characteristics induced by the substitution of sulfur atoms were comprehensively analyzed through first-principles calculations, including formation energy, optimized structural parameters, projected density of states (PDOS), and spatial charge density distribution. Various doping configurations were considered by replacing Sn atoms with S at different concentrations and atomic positions, resulting in characteristic doping types such as single-atom doping (top-1S, valley-1S), two-atom doping (ortho, meta, para), and full 1:1 substitution with a 6Sn-6S structure. The results reveal significant changes in the bandgap, increasing slightly from 0.26eV in the pristine state to approximately 0.34eV in the meta configuration, moderately decreasing to 0.15eV in the 100% substitution case, and sharply decreasing in the other configurations. Moreover, most sulfur-doped configurations exhibit non-magnetic behavior similar to pristine ASnNRs, while strong magnetism emerges only in the fully substituted 100% case. These findings demonstrate that sulfur doping can fundamentally modify the electronic and magnetic properties of the material, highlighting its potential application in future spintronic devices.

Keywords: applied DFT, new device. S doped Sn, spintronic device

1. Introduction

In recent years, two-dimensional (2D) materials have garnered considerable interest from the scientific community due to their outstanding mechanical, physical, chemical, and optical characteristics (Abtew et al., 2014; Leenaerts et al., 2008; Wang et al., 2012). Among these materials, graphene has emerged as one of the most notable monolayer systems. Nevertheless, despite its remarkable properties, graphene faces certain limitations, including toxicity, the absence of an intrinsic bandgap, and incompatibility with existing silicon-based electronic technologies. To address these drawbacks, significant efforts have been made to discover alternative 2D materials with honeycomblike lattices composed of group-IV elements, such as silicene (Si) (Drummond et al., 2012; Hu et al., 2013, 2014), germanene (Ge) (Xia et al., 2014; Kaloni et al., 2014), and antimonene (Sb) (Kaloni et al., 2015; Aktürk et al., 2016).

Extensive research has been devoted to investigating the exceptional physical properties of these nanomaterials, particularly focusing on their tunable bandgaps and the effects of external factors on their structural and electronic behaviors (Le et al., 2019; Davoudiniya et al., 2019). Among these alternatives, stanene a group-IV 2D material structurally analogous to graphene, silicene, and germanene has emerged as a promising candidate. It exhibits distinctive characteristics, including ultra-high carrier mobility, a gapless electronic structure in its pristine state, and a Dirac-like linear dispersion near the Fermi level.

Owing to these advantages, the fabrication and investigation of atomically thin, group-IV honeycomb materials have become areas of significant interest. Over the past decades, various experimental methods have been developed to synthesize such materials (Bui et al., 2018; Yarmohammadi et al., 2018). Notably, silicene and germanene have been successfully synthesized via molecular beam epitaxy (MBE) techniques (Bui, Yarmohammadi, 2018; Phuong et al., 2018), while the recent successful epitaxial growth of a monolayer of tin atoms has laid the groundwork for advancing 2D stanene research (Hoi, Yarmohammadi, 2018).

Stanene is regarded as a highly promising material for applications in areas such as photocatalysis, energy storage and conversion systems (Mirabbaszadeh et al., 2018), and nanoelectronic devices (Yarmohammadi, 2018). DFT calculations have confirmed that pristine stanene exhibits a zero bandgap when spin-orbit coupling (SOC) is neglected. However, the inclusion of SOC induces a bandgap of approximately 0.1eV, indicating its potential in optoelectronic technologies. Additionally, this bandgap can be further modulated to around 0.3eV through suitable functionalization strategies (Cao, 2015), rendering stanene an excellent platform for quantum spin Hall applications. Furthermore, theoretical predictions suggest that stanene could demonstrate topological superconductivity and superior thermoelectric performance compared to silicon (Pumera, 2011), underlining its potential for next-generation spintronic and quantum computing technologies.

Doping has proven to be an essential approach for tailoring the electronic and magnetic properties of graphene-like 2D materials. The incorporation of foreign atomic impurities can induce structural modifications in stanene and lead to desirable adjustments in its bandgap and electronic features (Pumera, 2014). Accordingly, doping stanene monolayers with various elements has been proposed as an effective method to extend its application prospects. Several approaches have been explored to tune stanene's electronic properties (Yang et al., 2013; Fiori et al., 2014), including functionalization techniques (Liu et al., 2015). For instance, Wang et al. demonstrated that constructing a van der Waals heterostructure comprising stanene and hexagonal boron nitride (h-BN) could significantly enhance the material's bandgap compared to its pristine form (Chen et al, 2016).

In a recent study, we examined the adsorption effects of alkali and alkaline earth metals such as Na, Mg, and Al on amchair stanene nanoribbons, revealing notable changes in their magnetic and optical properties, which indicate potential for a variety of technological applications (Meng et al., 2016). Moreover, other investigations have comprehensively analyzed the adsorption behavior, magnetic characteristics, and electronic structures of stanene-based nanomaterials and heterostructures (Xu et al., 2013; Liu et al., 2011).

Building upon these findings, the present work focuses on the substitutional doping of S atoms into ASnNRs to assess how these dopants affect the crystal structure and electronic

properties of stanene. Our study emphasizes the redistribution of charge density through orbital interactions among neighboring atoms and examines the material's optical behavior by analyzing its dielectric function and absorption coefficient. These results could offer valuable insights and underscore the potential of this novel material system for future electronic and photonic device applications.

2. Computational method

In this project, DFT calculations were performed using the Vienna Ab initio Simulation Package (VASP). The Perdew-Burke-Ernzerhof (PBE) functional within the generalized gradient approximation (GGA) framework was employed to evaluate the exchange-correlation energy arising from Coulomb interactions. Electron-ion interactions were described via the projector augmented-wave (PAW) method, with the electronic wave functions expanded in a plane-wave basis set using a cutoff energy of 500eV.

To sample the Brillouin zone, Monkhorst-Pack k-point grids were adopted, set to $12 \times 1 \times 1$ for structural optimization and $100 \times 1 \times 1$ for high-accuracy electronic structure calculations. Geometry optimizations were carried out until the Hellmann-Feynman force on each atom was less than 0.01 eV/Å, and the electronic self-consistent field (SCF) convergence threshold was set to 10^{-6}eV . These settings ensured reliable convergence for both structural and electronic properties in all calculations.

We calculate the adsorption energy after fusion using the following formula (1):

$$\Delta E = E_{System} - mE_S - E_{\text{Pristine}} + nE_{Sn} \tag{1}$$

Where E_{System} represents the formation energy of the entire system after substitution, E_S is the formation energy of one S doping atom, and E_{Sn} is the energy of one substrate atom, m is the number of doping atoms, n is the number of atoms remaining in the substrate, Epristin is the total initial substrate energy.

3. Results and discussion

3.1. Structure properties

In this study, a systematic investigation was carried out on substitutional doping of various elements including the metal S into the ASnNRs substrate. The primary objective was to examine how these dopants influence the structural, electronic, and magnetic properties of the material after doping. To achieve this, an ASnNR model consisting of 12 Sn atoms and 4H atoms was employed. The atomic arrangement of the pristine nanoribbon is presented in Fig. 1.



Fig 1. Initial configuration of S doping in SnNRs.

After performing DFT-based calculations using the VASP package, structural, electronic, and magnetic parameters were obtained for the cases of S doping in Sn, the results for the S doping ASnNRs as detailed in Table 1 below:

	meta	ortho	para	top-1S	valley-1S	1:1	pristine
E _P (eV)	-41.31	-36.23	-49.88	-39.86	-39.86	-16.59	-45.45
E _X (eV)	-2.15	-3.60	-7.15	-0.95	-0.95	-7.67	х
$E_{X+P}(eV)$	-53.99	-53.87	-53.90	-51.98	-51.98	-29.57	х
$\Delta E (eV)$	-5.26	-7.02	1.56	-11.17	-11.17	-5.31	Х
Buckl (Å)	0.79	1.59	1.07	1.00	0.90	0.90	1.00
Sn-Sn (Å)	2.87	2.85	2.86	2.82	2.82	х	2.82
Sn-S (Å)	2.65	2.46	2.47	2.82	2.82	2.54	х
S-S (Å)	4.09	3.75	5.33	х	х	х	Х
Sn-S-Sn (°)	104.35	93.69	96.70	108.05	108.05	108.05	х
Sn-Sn-Sn (°)	101.70	104.47	112.89	108.05	108.05	108.05	108.05
Mag (µ)	0.00	0.00	0.00	0.05	0.05	2.02	0.00
Eg (eV)	0.34	0.02	0.02	0.09	0.09	0.15	0.26

TABLE 1. Calculated results for various configurations of Pb-doped ASnNRs.

The results reveal that doping S atoms into ASnNRs does not significantly alter the Sn–Sn bond lengths, while the Sn–S bonds are shorter, measuring approximately 2.54Å compared to the Sn–Sn bond length of 2.82Å. Among the doping configurations, the Meta site exhibits the smallest buckling height of 0.79Å, whereas the Ortho configuration shows the largest distortion of 1.59Å. In contrast, the other configurations including para, top-1S, valley-1S, and 1:1 substitution case maintain buckling values comparable to that of the pristine structure at around 1.0Å.

In terms of bond angles, the Sn–Sn–Sn angles in the top, valley, and 1:1 S-doped configurations remain stable compared to the pristine structure. However, in the para configuration, this angle decreases to 112.89° , and it further reduces to 101.70° in the ortho and meta configurations. Notably, the Sn–S–Sn bond angles exhibit significant variations, with values decreasing to 96.69° and 96.70° in the ortho and para cases, respectively, while maintaining a value of 104.35° in the meta configuration. In contrast, the Sn–S–Sn angles remain stable in the top-1S, valley-1S, and 100% substitution cases. These results indicate that 1:1 S-doped configuration preserves good structural stability, despite the considerable reduction in bond lengths.

3.2. Electrial properties

For the case of S atom doping in ASnNRs (see Fig. 3), the calculated results indicate that partial substitution at individual positions such as meta, ortho, para, top-1S, and valley-1S does not induce significant magnetic moments in the system, remaining essentially similar to the pristine nanoribbon, with negligible magnetic values. This can be attributed to the fact that isolated S atoms, with an electronic configuration of [Ne] 3s²3p⁴, possess a closed-shell structure that, when introduced at low concentrations, exhibits insufficient interaction with surrounding Sn atoms to disrupt the overall spin symmetry of the nanoribbon. Additionally, the electronic hybridization between S and Sn orbitals at low doping levels does not generate localized unpaired spins capable of producing a net magnetic moment.

However, in the case of 1:1 substitution, where 1:1 of Sn atoms in the nanoribbon are replaced by S atoms, the system undergoes significant changes in both its electronic and magnetic properties. The dramatic increase in the total magnetic moment is likely due to the collective resonance effect of S–S interactions combined with substantial modifications in the electronic band structure, resulting in a redistribution of charge density and the formation of spin-polarized states near the Fermi level. In this fully substituted configuration, the complete removal of Sn atoms disrupts the original electronic environment of the nanoribbon, and the interactions among S atoms intensify spin splitting, giving rise to strong ferromagnetic behavior with a remarkably high total magnetic moment. This phenomenon highlights the critical role of dopant concentration and dopant–dopant interactions in determining the magnetic characteristics of doped 2D nanoribbon systems.

In the case of S doping at the Meta position in Sn nanoribbons, the calculated results indicate a noticeable increase in the bandgap, rising from 0.26eV in the pristine structure to 0.34eV. This bandgap widening can be attributed to several interrelated factors involving the atomic characteristics of sulfur and its interaction with the surrounding Sn lattice. Firstly, sulfur possesses a smaller atomic radius and higher electronegativity compared to tin, with values of approximately 100pm and 2.58, respectively, against 140pm and 1.96 for Sn. The replacement of a Sn atom by a S atom at the Meta position leads to localized structural distortion and a significant redistribution of charge density in the vicinity of the doping site.

Due to its higher electronegativity, the S atom tends to attract surrounding electrons more strongly, resulting in a local accumulation of charge density around itself and a corresponding depletion in adjacent Sn atoms. This localized charge polarization affects the electronic states near the Fermi level, specifically by slightly lowering the energy levels of the valence band maximum (VBM) and raising those of the conduction band minimum (CBM). Additionally, the distinct electronic configuration of sulfur (3s²3p⁴) forms more stable and lower-energy hybridized states when interacting with the 5s²5p² orbitals of Sn atoms.

At the Meta position, which lies within the central region of the nanoribbon where the bulk electronic states are most densely distributed, this doping-induced electronic rearrangement exerts a stronger influence on the overall band structure compared to doping at edge or corner positions. The hybridization of S–Sn bonds at this location not only perturbs the valence and conduction bands but also reduces the density of states near the Fermi level, contributing to a modest broadening of the bandgap. Consequently, the doping of S at the meta position effectively suppresses the overlap between the conduction and valence bands, leading to a bandgap increase of approximately 0.08eV relative to the pristine nanoribbon. This finding highlights the critical role of dopant position and electronegativity in modulating the electronic properties of 2D nanoribbon systems.

When substituting S atoms into SnNRs at specific positions such as ortho, para, top-1S, and valley-1S, the bandgap (Eg) exhibits a significant reduction from the pristine value of 0.26eV to nearly zero. This pronounced decrease can be attributed to the strong perturbation introduced by the S dopants at these particular sites, which substantially modifies the electronic structure of the nanoribbon. At these doping positions, the sulfur atoms, possessing a distinct electronegativity and a smaller atomic radius compared to Sn, alter the local electronic environment by creating impurity states within the bandgap region.

The substitution at as ortho, para, top-1S, and valley-1S cases directly affects the delocalized π -conjugated system along the nanoribbon edges, where the electronic density of states (DOS) is most sensitive. The strong electronic hybridization between the S 3p orbitals and the Sn 5p orbitals leads to the formation of new defect levels near the Fermi level, resulting in a narrowing of the bandgap. Moreover, the interaction strength and the symmetry-breaking effects induced by S dopants at these sites enhance the overlap of the conduction band minimum (CBM) and valence band maximum (VBM), causing the band edges to merge.

Unlike the Meta site, where the dopant is more embedded within the backbone of the nanoribbon and its influence is relatively localized, the as ortho, para, top-1S, and valley-1S cases are located in regions with higher charge density and stronger coupling to the nanoribbon's conductive channels. This difference in local electronic environment leads to more substantial charge redistribution and impurity level formation at these positions, accelerating the closure of the bandgap. Consequently, the bandgap is suppressed towards zero, indicating a transition from semiconducting to metallic-like behavior. This finding underscores the site-dependent nature of dopant-induced electronic modulation in SnNR-based nanostructures, where both the type and position of dopants critically dictate the resulting electronic properties.

In the case of alternating 1:1 substitution between S and Sn atoms in ASnNR lattice, the bandgap decreases moderately from 0.26eV to approximately 0.15eV, which is notably less than the significant bandgap reduction observed in other isolated doping configurations. This moderate narrowing of the bandgap can be attributed to the periodic and ordered arrangement of S atoms within ASnNR structure. In this 1:1 configuration, the substitution introduces a more uniform potential modulation throughout the nanoribbon, preserving a relatively balanced electronic structure and preventing the formation of highly localized impurity states near the Fermi level.

The alternating substitution pattern maintains a certain degree of lattice periodicity and symmetry, which helps to stabilize the overall electronic band structure. Unlike random or isolated doping at edge or asymmetric positions which induces strong local perturbations, breaks the system's symmetry, and introduces mid-gap defect states the ordered 1:1 arrangement of S atoms distributes the perturbation evenly. This even distribution weakens the impact of dopant-induced states near the conduction and valence band edges, resulting in a smoother modification of the electronic bands rather than abrupt defect state formation.

Additionally, the similar electronegativity of sulfur (2.58) relative to tin (1.96) helps to limit drastic charge transfer effects between adjacent atoms in the periodic array, thereby minimizing charge localization and the emergence of impurity bands within the bandgap. Consequently, the conduction band minimum (CBM) and valence band maximum (VBM) shift closer together but do not overlap as dramatically as in the isolated dopant cases, leading to a moderate reduction of the bandgap to 0.15eV.

This behavior highlights the role of dopant distribution and lattice symmetry in controlling the electronic properties of doped nanoribbons. It suggests that periodic, alternating doping patterns can be an effective strategy to fine-tune the electronic structure of 2D nanomaterials while preserving desirable semiconducting characteristics, in contrast to random or edge-focused doping schemes that risk transforming the material into a metallic state.



Fig. 2. The structure (a) PDOS, (b) BAND, and (c) DOS of pristine ASnNRs

Based on Fig 2a, 2b, the PDOS and band structure are plotted over the energy range from -8eV to 4eV. In the pristine configuration, the electronic states primarily consist of Sn (s, p, d) orbitals. Among these, the Sn(s) states are distributed throughout the entire region from the valence band maximum to the conduction band minimum, with strong contributions observed between -8eV and -4.3eV, and weaker contributions from -2.6eV to 4eV. Meanwhile, the Sn(p) orbitals are broadly distributed but exhibit dominant contributions from -3eV to 4eV, especially around the Fermi level. In contrast, the Sn(d) orbitals contribute weakly and play an insignificant role in the formation of the bandgap (Eg) in Sn nanoribbons. As shown in Fig. 2c, the DOS structure of ASnNRs exhibits strong states in the energy range from -1eV to -2eV, with a peak intensity of approximately 11 states/eV. The unit cell, along with the spin-up and spin-down components, displays complete symmetry, indicating that this material possesses no magnetic properties, as also presented in Table 1.



(b)



Fig 3. The PDOS of six cases S doped SnNRs

Based on Fig. 3, the PDOS structures of the systems doped with S (s, p) orbitals reveal a notable hybridization between the Sn(p) and S(p) orbitals, clearly observable across the configurations. In the meta configuration (see Fig. 3a), there is a predominant contribution of the S(p) orbitals around the Fermi level, extending from the valence band maximum to the conduction band minimum. However, these energy states remain relatively weak and primarily act as electron acceptor levels, leading to an increase in the bandgap (Eg) in this case to 0.34eV. In contrast, the ortho, para, top-1S, and valley-1S configurations generally exhibit a stronger contribution of the S(p) orbitals. At these higher local concentrations, the significant contribution of electrons to this energy region considerably alters the band structure, causing a substantial reduction in the bandgap, driving it towards nearly 0eV. As a result, the doped materials in these configurations exhibit metallic-like behavior. In the case of 1:1 S substitution (see Fig. 3f), a significant hybridization and orbital overlap occur between the S(s) orbitals and predominantly the Sn(p) orbitals, as the S atoms successively interact with the surrounding Sn atoms in a configuration distinct from the other doping cases. This enhanced electronic exchange results in an increased density of conduction electrons, consequently reducing the band gap energy to 0.15eV compared to the initial 0.26eV value of the pristine structure.





Based on the results presented in Fig. 4, the electronic band structures are consistent with the projected density of states (PDOS) shown in Fig. 3 for the respective cases. In particular, regarding the total density of states (DOS), the most prominent DOS intensity is observed in the case of 1:1 sulfur doping, with a peak value reaching up to 11 states/eV within the energy range from -1eV to -2eV around the unit cell, while other configurations exhibit relatively lower DOS values within this energy region.

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Moreover, the spin-up and spin-down configurations for both the pristine and various doped cases remain balanced, confirming the non-magnetic nature of these systems. In contrast, the 100% S-doped configuration (see Fig. 4f) exhibits a noticeable imbalance between the spin-up and spin-down DOS, resulting in strong magnetism as indicated in Table 1.

Where ρ_{System} represents the formation energy of the entire system after substitution, ρ_S is the formation energy of one doping atom, and ρ_{Sn} is the energy of one substrate atom, m is the number of doping atoms, n is the number of atoms remaining in the substrate, $E_{pristin}$ is the total initial substrate energy, see (2) equation:

$$\Delta \rho = \rho_{System} - \rho_{Pristine} + n\rho_{Sn} - m\rho_{S}$$
(2)

		Orbitals				
Positions	Charg density	S	р	d		
		(e/Å ³)	(e/Å ³)	(e/Å ³)		
pristine	Х	15.51	15.25	0.63		
meta		-6.33	-3.45	-0.40		
ortho		18.59	18.88	1.12		
para	٨٥	18.50	18.70	1.10		
top-1S	Δρ	18.90	18.46	0.94		
valley-1S		18.90	18.46	0.94		
100% S		16.11	14.25	1.82		

TABLE 2. Result calculation charge density of S doped SnNRs

By applying Equation (2), we calculated the results of doping in the configurations considered, as presented in Table 2. The analysis shows the charge density values for the Sn (s, p, d) orbitals in the pristine structure and after doping in six different cases, with $\Delta \rho$ representing the charge density difference resulting from the redistribution of electron density due to the hybridization and exchange interactions between the host and dopant atoms. The results indicate a decrease in charge density for all three orbitals in the meta configuration, which correlates well with the observed increase in band gap width previously reported in Table 1. In contrast, the case of 100% S substitution shows a slight increase in charge density compared to the pristine structure, suggesting a modest reduction in band gap, as discussed earlier. Conversely, the ortho, para, top-1C, and valley-1C configurations exhibit a significant increase in charge density, which is consistent with the substantial narrowing of the band gap, also detailed in Table 1.

4. Conclusion

Through a systematic investigation of atomic doping by substituting sulfur (S) atoms for tin (Sn) atoms in stanene nanoribbons (SnNRs) under various configurations, the obtained results reveal significant modifications in both the structural and physical properties of the material system. The incorporation of different dopant atoms into the structure produces distinct effects on the overall stability, structural characteristics, electronic properties, and magnetic behavior of the nanoribbons.

By controlling the type, concentration, and spatial distribution of dopant atoms, it is entirely feasible to design materials with tailored electronic and magnetic properties, suitable for specific applications. These findings open up significant potential for the development of next-generation functional devices, particularly in the fields of spintronics, nanoelectronics, and advanced sensor technologies, where the precise control of electronic band structures and magnetism at the nanoscale plays a crucial role.

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