

Computational investigation of electronic, vibrational, and transport properties of silicon phosphide nanoribbons

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Two-dimensional (2D) silicon phosphide (SiP) has recently emerged as a promising semiconductor for electronic, optoelectronic, and thermoelectric applications due to its unique electronic and structural characteristics. One-dimensional (1D) nanoribbons (NRs) derived from 2D SiP offer a versatile and scalable platform for device miniaturization and performance enhancement in nanoelectronics. Motivated by their potential, we present a comprehensive first-principles investigation of the structural, electronic, dynamical, and electronic transport properties of SiP-NRs. Specifically, we focus on both bare and hydrogen-passivated armchair (A-NRs, HA-NRs) and zigzag (Z-NRs, HZ-NRs) configurations. Our results reveal that hydrogen passivation effectively suppresses edge reconstructions observed in bare SiP-NRs, thus dynamically stabilizing their structures. Analysis of electronic band structures demonstrates a clear width-dependent oscillatory behavior of the band gap in bare A-NRs, which diminishes significantly upon hydrogen termination. The width-scaled electronic conductance (G_e^{ws}) of HA-NRs exhibits a decreasing trend with increasing ribbon width, featuring distinct even-odd oscillations for n -type transport due to subband splitting effects. In contrast, HZ-NRs display notable deviations in p -type conductance from their 2D SiP counterpart, particularly at low temperatures (around 100 K), arising from residual localized edge states. However, with increasing width and temperature, transport behavior converges toward that of 2D SiP monolayers, indicating diminishing edge effects. Unlike their p -type counterparts, the n -type G_e values of the largest HA-NRs and HZ-NRs increase with the square root of temperature, similar to the n -type conductance trend observed in 2D SiP. This behavior is attributed to the evolution of the electronic transmission function ($\tau(E)$) from a steplike profile in narrow ribbons to an $E^{1/2}$ dependence in wider ribbons, analogous to the 2D counterpart. These findings highlight the significant influence of width and edge termination on the transport characteristics of SiP-NRs and underline their potential as fundamental building blocks for high-performance nanoelectronic and thermoelectric quasi-1D devices.

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I. INTRODUCTION

The successful isolation of graphene [1] and the subsequent discovery of its exceptional electronic, mechanical, and thermal properties [2,3] have spurred extensive research into two-dimensional (2D) materials. This breakthrough has led to the identification and synthesis of a diverse range of atomically thin materials, extending beyond carbon-based nanostructures to include ultrathin systems composed of group IV–V elements, transition-metal dichalcogenides, MXenes,

group III monochalcogenides, and their Janus derivatives [4,5]. These materials exhibit a variety of novel physical and chemical properties, including high carrier mobility, tunable band gaps, strong spin-orbit coupling, and exceptional mechanical flexibility, making them promising candidates for next-generation electronic, optoelectronic, and energy storage applications [6–8].

Among the various emerging 2D materials, silicon phosphide (SiP) monolayers [9], a member of the binary group IV–V monolayer family [10], have attracted considerable interest due to their multifunctional properties across different stoichiometric forms. Recent experimental advancements, including mechanical exfoliation and high-pressure melt growth methods, have enabled the successful fabrication of SiP monolayers, which theoretically exhibit a direct band gap of 2.64 eV [11–13]. Structurally, the synthesized SiP monolayer adopts an orthorhombic phase with space group $Cmc2_1$ (No. 36) and demonstrates semiconducting behavior [11,14].

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Furthermore, SiP monolayers exhibit exceptional thermal stability, high carrier mobility, strong optical absorption, and unique electronic transport properties, making them promising candidates for a variety of applications [9,12,14,15].

Building on these advancements, Huang *et al.* have systematically explored various stoichiometries of Si_xP_y ($y/x \geq 1$) monolayers using a structural search algorithm (calypso) combined with first-principles calculations to identify stable or metastable configurations of this promising compound [16]. Their study has revealed that a hexagonal SiP monolayer with a space group of $P\bar{6}m2$ is energetically favorable and structurally stable. Moreover, due to its low formation energy, the experimental realization of the $P\bar{6}m2$ phase through deposition and self-assembly has been regarded as achievable [17]. Beyond its structural stability, $P\bar{6}m2$ SiP exhibits a distinctive electronic band structure characterized by a Mexican hat-shaped valence band, which significantly enhances its thermoelectric efficiency [18]. Additionally, its Janus derivatives, formed by combining SiP with group V elements, exhibit Rashba spin splitting in the conduction band, highlighting their potential for spintronic applications [19]. Given the versatile properties of both stoichiometric forms of 2D SiP, this material has emerged as a highly promising candidate for applications in thermoelectrics, field-effect transistors (FETs), optoelectronic devices, and photocatalytic water splitting [13,18,20–24].

Beyond 2D materials, their quasi-one-dimensional (quasi-1D) counterparts, known as nanoribbons (NRs), have gained increasing attention due to their tunable electronic properties, which are highly dependent on width, lattice orientation, edge configuration, and passivation chemistry [25,26]. Among them, graphene nanoribbons (GNRs) have been extensively studied and employed in various applications, including GNR-based field-effect transistors, integrated circuits, graphene-based sensors, DNA sequencing, and energy storage devices [27–37]. Furthermore, the electronic transport properties of GNRs can be tailored through structural modifications, such as edge disorder, defect engineering, and chemical functionalization [38–42].

Beyond graphene, NRs derived from other 2D semiconductors have also been synthesized and theoretically investigated, demonstrating promising electronic properties at the nanoscale [43–49]. For instance, fabricated silicene nanoribbons have emerged as strong candidates for future nanoelectronic applications [50–56]. Similarly, the electronic and quantum transport properties of pristine and chemically terminated phosphorene nanoribbons (PNRs) have been explored using density-functional theory (DFT) combined with nonequilibrium Green's function formalism [57–59]. Notably, Shen *et al.* have reported that a dual-gate FET based on PNRs exhibits a high on/off ratio of 10^3 [60], further highlighting the potential of NRs in electronic applications.

Motivated by their potential as versatile building blocks for device miniaturization and enhanced performance in nanoelectronics, we present a comprehensive first-principles investigation into the structural, electronic, vibrational stability, and electronic transport properties of SiP-NRs. Specifically, we focus on armchair (A-NRs) and zigzag (Z-NRs) configurations derived from the highly symmetric hexagonal 2D SiP monolayer. Employing DFT calculations coupled with the

Landauer transport formalism, we systematically analyze both bare and hydrogen-passivated SiP-NRs. Structural reconstructions observed in bare SiP-NRs, resulting from unsaturated dangling bonds at the edges, are effectively suppressed by hydrogen passivation, yielding hydrogen-passivated armchair (HA-NRs) and zigzag (HZ-NRs) configurations with enhanced dynamical stability. Detailed analyses of electronic band structures, electronic transmission spectra, and conductance profiles highlight distinct width- and edge-dependent variations in their ballistic transport behavior. Our findings emphasize how edge passivation significantly modulates the electronic band gap, state localization, and consequently the electronic transport characteristics. These insights underline the potential of both bare and hydrogen-passivated SiP-NRs as promising candidates for next-generation nanoelectronic, thermoelectric, and quantum device applications.

II. METHODOLOGY

First-principles DFT calculations [61,62] were performed using the Vienna *Ab initio* Simulation Package (VASP) [63–66] to investigate the structural, electronic, and vibrational properties of SiP-NRs. The exchange-correlation potential was treated using the generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional [67]. Convergence tests were conducted to determine the optimal k -point sampling and energy cutoffs for each NR. The plane-wave basis set cutoff energy for projector-augmented wave [68] pseudopotentials was set to 520 eV, and the Brillouin zone (BZ) was sampled using a Γ -centered $16 \times 16 \times 1$ k mesh for the parent 2D SiP, with proportional scaling applied to SiP-NRs. To eliminate spurious interactions between adjacent NRs, a vacuum spacing of 30 Å was introduced along the nonperiodic directions. Structural optimizations were performed using convergence criteria of 10^{-5} eV for total energy and 10^{-2} eV/Å for atomic forces. Since the GGA-PBE formalism tends to underestimate electronic band gaps, the band structures of both bare and H-passivated SiP-NRs were further refined using the Heyd-Scuseria-Ernzerhof (HSE06) functional [69,70]. The HSE06 functional was constructed by mixing 25% of the exact Hartree-Fock exchange potential with 75% of PBE exchange and 100% of PBE correlation energy. To assess the dynamical stability of SiP-NRs, phonon spectra were computed using the small-displacement method, and the interatomic force constants were extracted using the phonopy package [71]. In addition to phonon calculations, *ab initio* molecular dynamics (AIMD) simulations were conducted to evaluate the thermal stability of these systems. The simulations were carried out in a microcanonical ensemble at constant temperatures of 300 and 600 K for a total duration of 6 ps, using a time step of 1 fs.

To evaluate transport coefficients, we adopted the Landauer-Büttiker formalism, which provides a unified framework for ballistic, diffusive, and even localized transport regimes [72,73]. Although originally developed for coherent quantum transport, it has been widely shown to yield results consistent with semiclassical approaches such as the Boltzmann transport equation in the appropriate limits [74].

In the Landauer-Büttiker formalism, conductance of the system is determined by the transmission function ($\tau(E)$) as

$$G = \frac{2e^2}{h} \int dE \tau(E) \left(-\frac{\partial f_{\text{FD}}(E, E_F, T)}{\partial E} \right), \quad (1)$$

where f_{FD} is the Fermi-Dirac distribution function, E_F is the Fermi level, and T is temperature. Transmission function encapsulates all the effects of the electronic structure and scattering processes.

In quasi-1D systems such as nanoribbons, ballistic transport typically dominates over diffusive transport at sub-micrometer length scales, due to reduced phase space for scattering. Quantum confinement restricts carriers to discrete energy modes, which govern conductance in this regime. Therefore, in the case of SiP-NRs, we assume the ballistic regime, justified by the condition that the device length remains shorter than the electron-phonon mean-free path and that long-range crystalline order is preserved throughout the system. Since the transmission probability equals unity, transmission function equals the number of available modes. Namely,

$$M(E) = \sum_{n, \mathbf{k}_\perp} \Theta(E - E_n(\mathbf{k}_\perp)), \quad (2)$$

where Θ is the unit step function, and the sum runs over transverse wave vectors $\mathbf{k}_\perp$ and band indices n .

In the ballistic regime, additional electronic states contribute to transport as temperature increases. This is due to the broadening of the Fermi-Dirac distribution function, and also because the electron-phonon mean-free path is much longer than the device length by design [75,76].

For SiP-NRs, transport direction was set along the z axis for both armchair and zigzag NRs. A $1 \times 1 \times 50 k$ -point mesh was used to ensure convergence. This approach is widely used in evaluating electronic and phononic transport in low-dimensional materials [77–79] and provides a reliable estimate of conductance in the ballistic regime.

III. RESULTS AND DISCUSSION

A. Structural and electronic properties

SiP-NRs were derived from a highly symmetric 2D SiP monolayer by cleaving along the armchair and zigzag directions, as illustrated in Fig. S1 of the Supplemental Material (SM) [80]. The 2D SiP monolayer considered in this study crystallizes in the $P\bar{6}m2$ space group with a lattice constant of 3.53 Å. The resulting SiP-NRs are labeled as armchair (A-NR- n) and zigzag (Z-NR- n), where n (ranging from 4 to 13) denotes the number of Si-P dimer lines in A-NRs and zigzag chains in Z-NRs along the width direction, as shown in Fig. 1. After structural optimization, bare A-NRs and Z-NRs exhibit edge reconstructions due to the presence of dangling bonds at the edges, as depicted in Figs. 1(a) and 1(b). Such edge reconstructions are well documented in the literature and are known to induce structural distortions and localized electronic states, significantly affecting the electronic and transport properties of NRs. To suppress these edge-induced reconstructions, hydrogen passivation was applied to the outermost Si and P atoms, which effectively

eliminates structural instabilities and leads to dynamically stable hydrogen-passivated SiP-NRs (HA-NRs and HZ-NRs), as depicted in Figs. 1(c) and 1(d). This approach has been widely adopted to stabilize NRs, prevent undesired electronic midgap states, and recover the intrinsic band structure of the material [81,82]. Additionally, to examine the possibility of magnetic ordering and the influence of atomic parity, we performed comprehensive spin-polarized calculations on both zigzag and armchair SiP-NRs, with and without hydrogen passivation, over a range of ribbon widths, including both even and odd numbers of Si atoms. In all cases, the systems consistently converge to a nonmagnetic ground state with zero total magnetic moment. While certain Si-P-based quasi-1D systems have been reported to exhibit magnetic behavior under specific configurations [83], our findings indicate that SiP-NRs remain nonmagnetic, irrespective of ribbon orientation, width, or edge termination.

The electronic band structures of A-NR-9, Z-NR-9, HA-NR-9, and HZ-NR-9 are shown in Figs. 2(a)–2(d), as computed using both the PBE and HSE06 exchange-correlation functionals. Additionally, the variation of the band gap with ribbon width for all investigated SiP-NRs is presented in Figs. 2(e)–2(h). Previous studies have demonstrated that 2D SiP exhibits semiconducting character with a PBE (HSE06) band gap of 1.52 eV (2.22 eV) [18]. The distinctive valence-band topology of 2D SiP, characterized by a Mexican hat-like dispersion, makes it particularly promising for high-performance ballistic transport applications. Similar to the 2D parent structure, both bare A-NRs and Z-NRs remain indirect band-gap semiconductors, as confirmed by HSE06 calculations. However, the band gap of A-NRs exhibits a strong width-dependent oscillatory behavior, whereas in Z-NRs with widths $n > 5$, the band gap remains nearly constant. For A-NRs, the amplitude of oscillations diminishes with increasing width beyond $n > 8$, and the trend suggests that the oscillations vanish for $n > 13$. Similar oscillatory trends in band gap as a function of width have been observed in GNRs [84,85], as well as in other group IV–V NRs, such as GeP₃ nanoribbons and zigzag hydrogenated antimonene nanoribbons [86,87].

The band-gap values of both A-NRs and Z-NRs are expected to approach those of their 2D SiP counterparts as their width increases. However, this trend is disrupted in bare NRs due to pronounced edge effects. The presence of unsaturated dangling bonds at the edges introduces localized states, which in turn lead to the emergence of additional conduction- (CB) and valence bands (VB) near the Fermi level, as observed in both A-NRs and Z-NRs.

To further examine the role of edge states, we analyzed the band-decomposed charge densities of selected bands in the HA-NRs and HZ-NRs, as shown in Fig. S2 of the SM [80]. These charge-density distributions reveal that the majority of the charge is localized at the edge atoms and rapidly decays toward the central Si and P atoms. In A-NRs, structural reconstructions at both edges simultaneously contribute to the two lowest CBs and the uppermost VB, as illustrated in Fig. S2(a) and S2(e) of the SM [80]. In contrast, for Z-NRs, only one edge contributes to the two topmost VBs and the lowest CB, due to its asymmetric reconstructed motifs, as depicted in Figs. S2(b) and S2(f).

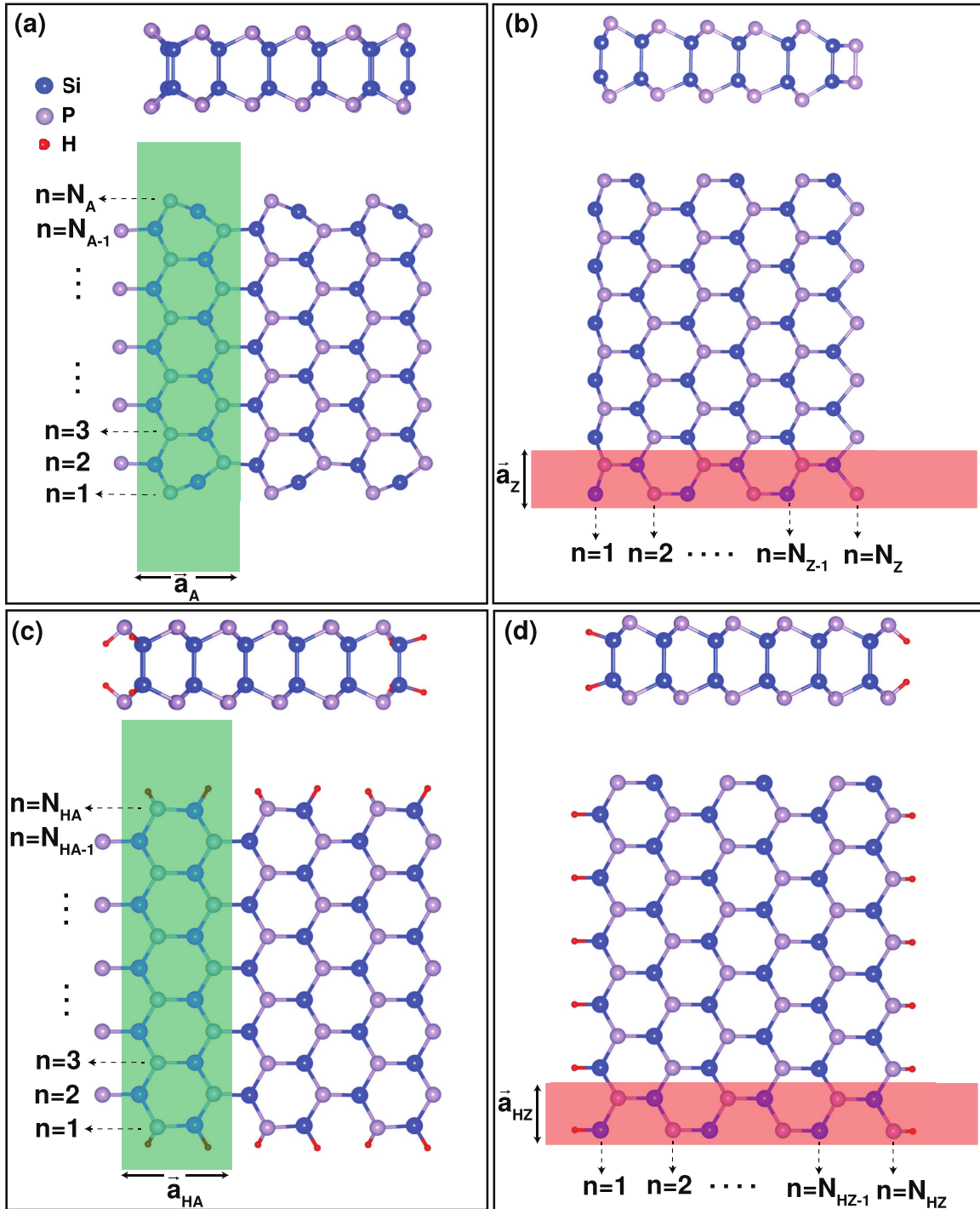


FIG. 1. Side and top views of the optimized geometries of SiP-NRs: (a) bare armchair (A-NR- n), (b) bare zigzag (Z-NR- n), (c) hydrogen-passivated armchair (HA-NR- n), and (d) hydrogen-passivated zigzag (HZ-NR- n) configurations. The parameter n denotes the number of Si-P dimer lines in armchair nanoribbons and the number of zigzag chains in zigzag nanoribbons along the width direction.

Upon hydrogen passivation, the charge-density distributions shift toward NR center, except for the VB of HZ-NRs, where localized edge states persist, as shown in Figs. S2(g) and S2(h) of the SM [80]. The band-gap values of hydrogen-passivated NRs are significantly larger than those of bare NRs, and gradually converge toward the band gap of 2D SiP as the width increases. These results confirm that narrower NRs exhibit larger band gaps due to quantum confinement effects.

Additionally, the oscillatory band-gap behavior seen in A-NRs is almost entirely suppressed in HA-NRs. The electronic band structures of HA-NRs and HZ-NRs for $4 \leq n \leq 13$ are provided in Fig. S3 and S4 [80]. Interestingly, the electronic band structures reveal that in HA-NRs with even-numbered n , the two lowest CBs become degenerate, whereas for odd-numbered n , they split at the Z high-symmetry point. This feature could play a crucial role in determining the electronic

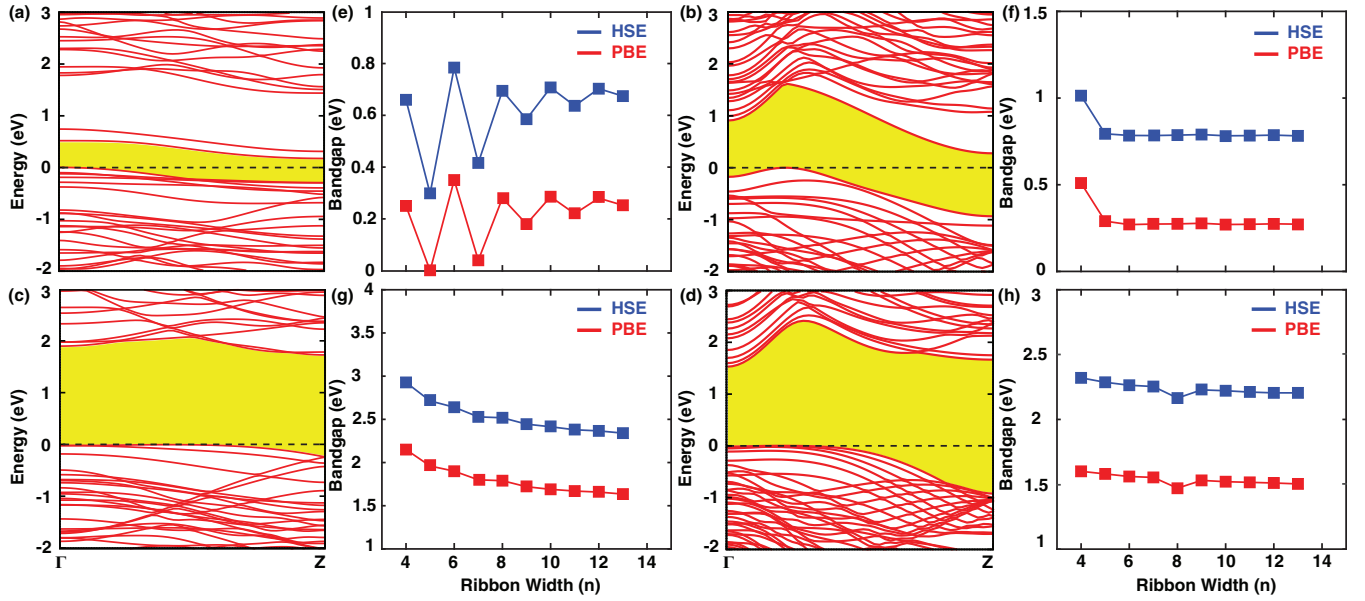


FIG. 2. Electronic band structures and band-gap variations with ribbon width for (a), (e) A-NR-9; (b), (f) Z-NR-9; (c), (g) HA-NR-9; and (d), (h) HZ-NR-9. The electronic band structures of all investigated HA-NRs and HZ-NRs are provided in Figs. S3 and S4 of the SM [80].

transport properties of HA-NRs, as illustrated in Fig. S3 of the SM [80].

Further insights into the electronic structure of SiP-NRs are provided by the density of states (DOS) analysis, as shown in Fig. 3. In A-NR-9, the valence-band maximum (VBM) is dominated by P atoms, whereas the conduction-band minimum (CBM) involves contributions from both P and Si atoms. For Z-NR-9, the DOS peaks at the VB and CB edges are primarily associated with Si atoms, whereas both Si and P

atoms contribute to the CB edge. Upon hydrogen passivation, distinct DOS peaks appear at the VB edge of HA-NR-9 and HZ-NR-9, corresponding to the van Hove singularities in the DOS of 2D SiP.

B. Dynamical stability

Following the analysis of the electronic properties of SiP-NRs with armchair and zigzag edges, we next assess their

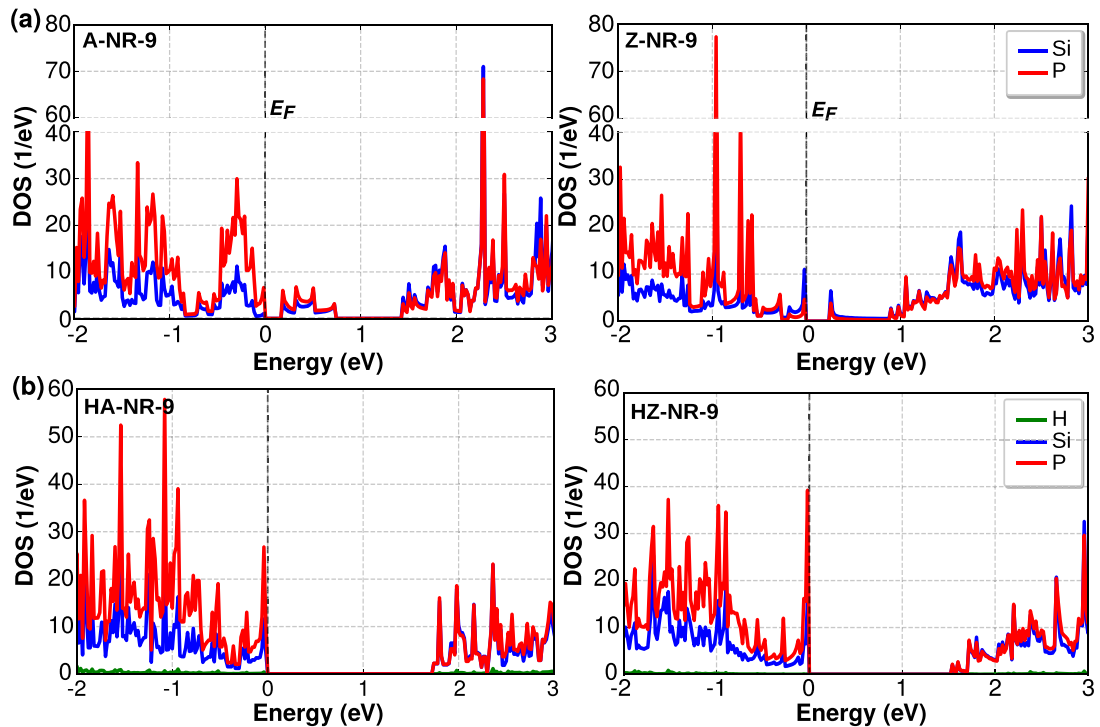


FIG. 3. Element-resolved density of states of (DOS) for (a) A-NR-9 and Z-NR-9, and (b) HA-NR-9 and HZ-NR-9.

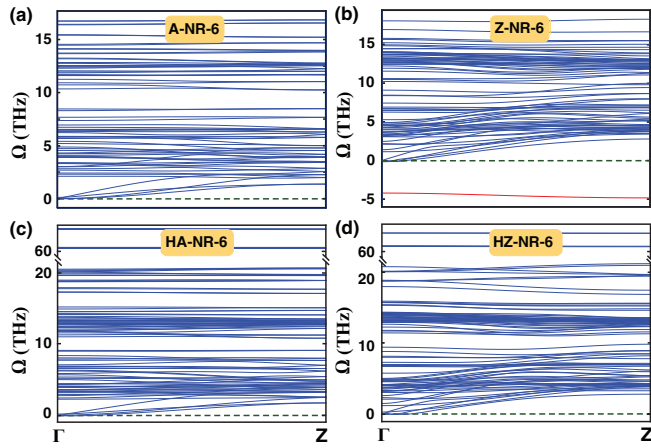


FIG. 4. Phonon dispersion spectra of bare (a) A-NR-6, (b) Z-NR-6, and hydrogen-passivated (c) HA-NR-6, (d) HZ-NR-6. The imaginary mode indicating dynamical instability in Z-NR-6 is shown in red.

dynamical stability through phonon dispersion calculations. As a reference, the phonon spectrum of 2D SiP was previously computed for a unit cell containing four atoms, yielding 12 phonon modes, all of with real frequencies throughout the BZ, confirming the dynamical stability of the 2D phase [18].

For each SiP-NR structure, we calculated the full phonon spectrum, which consists of $3N$ branches, where N is the number of atoms in the unit cell. For the considered width range ($n = 4$ to 13), this corresponds to 48 phonon modes at $n = 4$ (16 atoms) and to 216 modes at $n = 13$ (72 atoms). Similar to their 2D counterpart, all SiP-NRs exhibit three fundamental acoustic branches: longitudinal acoustic (LA), transverse acoustic (TA), and out-of-plane acoustic (ZA) branches. In addition, an extra twisting mode (TW) appears, which is characteristic of quasi-1D systems such as nanoribbons and nanotubes. This TW mode corresponds to a torsional oscillation of the ribbon around its central axis and propagates along the ribbon's length [88–91].

The phonon analysis reveals that A-NRs are dynamically stable for $n \geq 6$, even without hydrogen passivation [Fig. 4(a)]. In contrast, Z-NRs exhibit imaginary-frequency phonon branches, indicating dynamical instability. This is illustrated in Fig. 4(b) for the case of Z-NR-6, where the unstable phonon mode is highlighted in red.

To eliminate the instability in Z-NRs, we introduced hydrogen passivation at the edges. This straightforward strategy successfully removes the imaginary phonon branches and restores dynamical stability for $n > 6$, as demonstrated for HZ-NR-6 in Fig. 4(d). Each added hydrogen atom introduces additional Si-H and P-H vibrational modes, which become more pronounced with increasing ribbon width. Upon hydrogen passivation, the maximum phonon frequency increases from 16.75 to 69 THz for HA-NR-6 and from 18 to 69 THz for HZ-NR-6.

In the case of A-NR-6, we observe that the ZA and TW modes become degenerate at the Z high-symmetry point, a typical feature of wide quasi-1D systems. Moreover, the TA mode exhibits a quadratic dispersion ($\propto q^2$) in the long-wavelength limit [$q \rightarrow 0$], similar to the ZA mode, due to

the reduced distinction between in-plane and out-of-plane vibrations in NRs [92]. For HA-NRs, the LA and TA modes tend to converge toward the lower optical branches, consistent with previous studies on other 1D materials [93–95]. Additionally, as ribbon width increases, the degeneracy between ZA and TW modes becomes more pronounced, resembling the phonon behavior of 2D SiP monolayer [96].

Finally, the thermal stability of SiP-NRs was further confirmed by AIMD simulations, which were performed for both bare and hydrogen-passivated configurations in armchair and zigzag orientations at 300 and 600 K. The obtained results for $n=6$ are presented in Figs. S7–S10 [80].

C. Electronic transport properties

To assess the potential of SiP-NRs for nanoelectronic device applications, it is essential to explore their electronic transport properties under zero-bias conditions. This section presents a comprehensive analysis of the transport characteristics of HA-NRs and HZ-NRs.

To enable an unbiased comparison between HA-NRs and HZ-NRs, the electronic transmission spectra were normalized by ribbon width to eliminate size-dependent effects. The resulting width-scaled (ws) transmission spectra ($\tau^{\text{ws}}(E)$) are shown in Fig. S3 and Fig. S4 [80]. Furthermore, to gain deeper understanding of the effect of width on transport behavior, unscaled electrical conductance (G_e) was calculated for H-NRs with widths ranging from $n=4$ to $n=13$, as shown in Fig. S5 and Fig. S6 [80]. These unscaled trends help to elucidate the origin of size-dependent features in the width-scaled electronic conductance (G_e^{ws}). It is also worth noting that the conductance values were evaluated at chemical potentials (μ) corresponding to the energy where $\tau(E)$ drops to zero.

1. Transport characteristics of HA-NRs

We begin by analyzing the electronic transport properties of HA-NRs. The $\tau^{\text{ws}}(E)$ exhibits a characteristic steplike profile reflecting the quantized nature of subbands in quasi-1D systems. Additionally, the temperature dependence of G_e^{ws} was computed for HA-NRs at various temperatures. Representative transmission and conductance results for HA-NR-6 and HZ-NR-6 are illustrated in Figs. 5(a) and 5(b). The following analysis focuses on both p -type and n -type transport characteristics as functions of width and temperature.

Figures 6(a) and 6(c) present the p -type G_e^{ws} of HA-NRs for even- and odd-numbered n , respectively. A pronounced decrease in G_e^{ws} is observed as the ribbon width increases from $n = 4$ to $n = 7$, particularly at temperatures below 500 K. This decline arises from the nearly constant $\tau(E)^{\text{ws}}$ near the VBM, despite the increase in width.

At elevated temperatures, the Fermi window function ($\partial f(E)/\partial E$) broadens, allowing additional conducting channels to contribute to transport. Consequently, G_e^{ws} exhibits enhanced thermal robustness. For instance, at 800 K, the p -type G_e^{ws} of odd- n HA-NRs remains nearly constant, which can be attributed to the linear increase in unscaled G_e with ribbon width (see Fig. S5(c) of the SM [80]). Moreover, the unscaled p -type G_e of HA-NRs is found to be nearly independent of temperature. This behavior originates from the quartic dispersion near the VB edge of the 2D

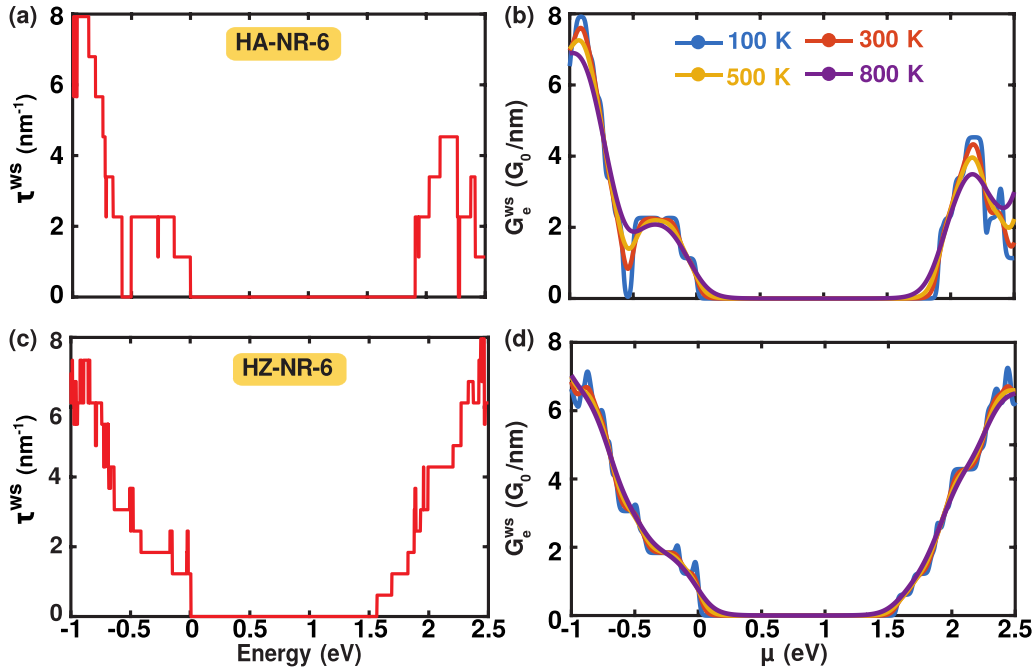


FIG. 5. Width-scaled electronic transmission spectrum ($\tau_e^{ws}(E)$) for (a) HA-NR-6 and (c) HZ-NR-6, and corresponding width-scaled electronic conductance (G_e^{ws}) for (b) HA-NR-6 and (d) HZ-NR-6 as a function of chemical potential (μ) from 100 to 800 K.

SiP counterpart, which yields a high and relatively uniform DOS. As a result, the p -type G_e^{ws} values remain closely grouped across all investigated temperatures, ranging from 0.72 to 0.76 G_0/nm .

For HA-NRs with even-numbered n , the CBM in narrower ribbons is located slightly away from the Γ point, in contrast to odd-numbered ribbons where the CBM lies directly at the Γ point (see Fig. S3 [80]). This shift in even- n cases increases the number of accessible subbands contributing to transport, thereby enhancing the n -type conductance. As a result, a pronounced even-odd oscillation emerges in the G_e^{ws} for $4 \leq n \leq 13$, as shown in the inset of Fig. 6. The gradual reduction in oscillation amplitude with increasing ribbon

width is attributed to the diminishing influence of quantization effects and the eventual convergence of subband structures, which reduces the disparity in the number of contributing channels between even- and odd- n NRs.

As shown in Figs. 6(b) and 6(d), the n -type G_e^{ws} displays a clear decreasing trend with increasing width for both even- and odd-numbered HA-NRs across all temperatures. For even-numbered n , G_e^{ws} drops sharply from approximately 2 to 0.5 G_0/nm , whereas for odd-numbered n , the decrease is more gradual, converging toward a similar value. Ultimately, as the ribbon width increases, the conductance values for both even and odd n converge to $\sim 0.5 G_0/\text{nm}$, reflecting the diminishing influence of subband structure and quantum confinement effects.

In contrast to the relatively temperature-invariant behavior of G_e^{ws} at the VB edge, the n -type conductance values at the CB edge exhibit a clear temperature dependence, as illustrated in Fig. 6(d). Specifically, n -type G_e^{ws} spans a broader range, from 0.27 to 0.52 G_0/nm , as temperature increases. This sensitivity primarily arises from the energy-dependent variation of $\tau_e^{ws}(E)$, near the CB edge. As the width of HA-NRs increases, $\tau_e^{ws}(E)$ transitions from a discrete, steplike profile to an $E^{1/2}$ dependence, resembling its 2D counterpart [78]. As a result, the n -type G_e^{ws} is expected to scale approximately with $T^{1/2}$, reflecting the increasing number of thermally accessible conduction channels at elevated temperatures.

In summary, for the widest NR (HA-NR-13), the p -type G_e^{ws} consistently exceeds the corresponding n -type values across the investigated temperature range. Notably, the n -type G_e^{ws} can be enhanced by a factor of 4 by employing the narrowest ribbon configuration ($n = 4$), highlighting the significant role of quantum confinement in optimizing transport performance, as illustrated in Fig. 6(b).

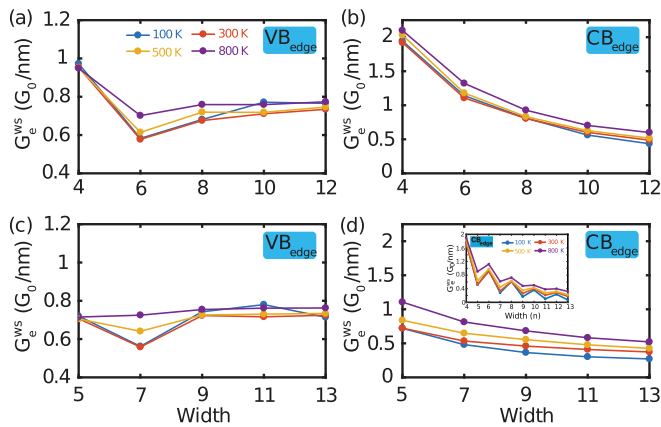


FIG. 6. G_e^{ws} profile of HA-NRs as a function of width for temperatures ranging from 100 to 800 K: (a) even-numbered n at the VB edge, (b) even-numbered n at the CB edge, (c) odd-numbered n at the VB edge, and (d) odd-numbered n at the CB edge. The inset highlights the even-odd oscillation in the n -type G_e^{ws} of HA-NRs.

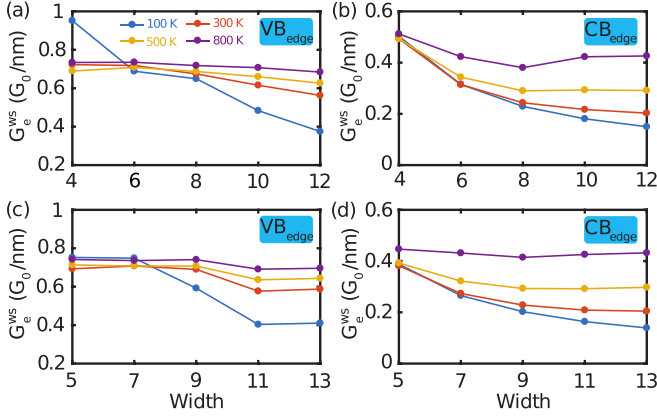


FIG. 7. G_e^{ws} profile of HZ-NRs as a function of ribbon width for temperatures ranging from 100 to 800 K: (a) even-numbered n at the VB edge, (b) even-numbered n at the CB edge, (c) odd-numbered n at the VB edge, and (d) odd-numbered n at the CB edge.

2. Transport characteristics of HZ-NRs

At 100 K, HZ-NR-4 exhibits a higher G_e^{ws} than at other temperatures, owing to a sharp decline in $\tau(E)$ within a narrow energy range. Since the unscaled G_e values increase linearly with width, the variations in p -type G_e^{ws} remain minimal up to HZ-NR-9 for temperatures above 100 K. However, a significant reduction in G_e is observed between HZ-NR-8 to HZ-NR-12 at 100 K, as illustrated in Figs. 7(a) and 7(c). For HZ-NR-13, the p -type G_e^{ws} ranges from 0.59 to 0.70 G_0/nm for temperatures from 300 to 800 K. In contrast, at 100 K, p -type G_e^{ws} exhibits a substantial deviation compared to its higher-temperature values. This discrepancy is attributed to localized edge states, which suppress $\tau^{\text{ws}}(E)$ at the VB edge, as depicted in Fig. S2(h) of the SM [80]. The difference in $\tau^{\text{ws}}(E)$ between HA-NRs and HZ-NRs has a more pronounced impact on G_e^{ws} at low temperatures. At elevated temperatures, deeper valence bands contribute more significantly to electronic transport, leading to the p -type G_e of HZ-NR-13 to closely align with that of HA-NR-13.

For HZ-NRs with both even- and odd-numbered widths, the n -type G_e^{ws} exhibits a decreasing trend across all temperatures below 800 K, as shown in Figs. 7(b) and 7(d). However, at 800 K, the n -type G_e^{ws} of HZ-NRs with odd-numbered n remains nearly constant. Furthermore, the n -type G_e^{ws} of HZ-NR-13 follows a trend similar to that of HA-NR-13, demonstrating a broader convergence range.

For comparison, the G_e^{ws} values of the widest nanoribbons, HA-NR-13 and HZ-NR-13, along with their parent 2D SiP, are presented as a function of temperature at the VB and CB edges in Figs. 8(a) and 8(b), respectively. The p -type G_e^{ws} values of HA-NR-13 closely match those of 2D SiP across all temperatures. In contrast, the p -type G_e^{ws} values of HZ-NR-13 deviate significantly from the 2D counterpart below 300 K, which can be attributed to the presence of localized charges on one edge of the HZ-NR, as shown in Fig. S2(h) [80]. As temperature increases and more subbands contribute to transport, the p -type G_e^{ws} of HZ-NR-13 gradually converges toward that of the HA-NR-13 and 2D SiP.

At the CB edge, n -type G_e^{ws} values of HA-NR-13, HZ-NR-13, and 2D SiP exhibit an almost linear dependence on

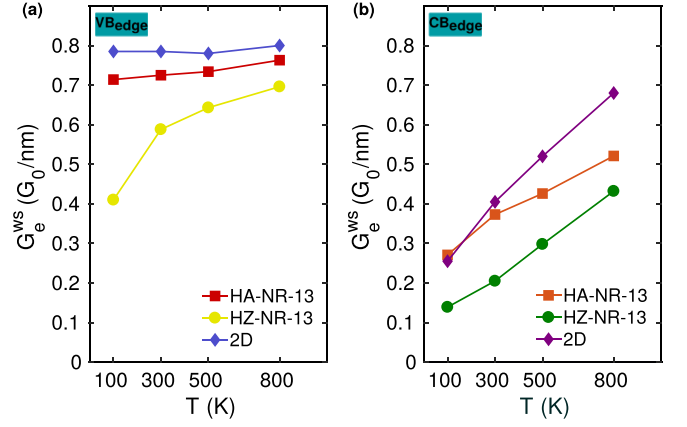


FIG. 8. Width-scaled electronic conductance G_e^{ws} of the widest SiP-NRs compared to their 2D SiP counterpart as a function of temperature at the (a) VB edge and (b) CB edge.

temperature up to 300 K. The slight deviations in the n -type G_e^{ws} values of NRs from those of 2D SiP can be attributed to subbands near the CB edge not scaling uniformly with ribbon width.

IV. CONCLUSION

Motivated by the peculiar electronic band structures and intriguing properties of group IV–V monolayers, we investigated the structural, electronic, dynamical stability, and transport properties of SiP nanoribbons (SiP-NRs) using a combination of density-functional theory (DFT) and the Landauer formalism. Our findings reveal that bare armchair SiP nanoribbons (A-NRs) exhibit dynamical stability when their width reaches $n=6$, whereas bare zigzag SiP nanoribbons (Z-NRs) remain dynamically unstable. Hydrogen passivation of the NR edges not only ensures the dynamical stability but also eliminates the edge reconstructions. Our calculations further demonstrate that A-NRs exhibit a strong even-odd oscillatory behavior in their electronic structure at narrow widths, which gradually diminishes as the ribbon width increases. This oscillation nearly vanishes upon hydrogen passivation, while the band gap approaches that of 2D SiP with increasing width. The n -type width-scaled electronic conductance (G_e^{ws}) of HA-NRs follows a descending trend with even-odd oscillations, whereas the p -type G_e^{ws} values exhibit a nearly constant trend, closely resembling the 2D SiP case. However, in HZ-NRs, the presence of residual edge states significantly affects p -type electronic conductance (G_e), leading to notable deviations from the 2D counterpart, particularly at 100 K. On the other hand, the n -type G_e values of the widest HA-NRs and HZ-NRs exhibit an almost square root of temperature dependence, similar to that of 2D SiP. This behavior is attributed to changes in the energy dependence of electronic transmission function ($\tau(E)$), which evolves from a steplike profile in narrow ribbons to an $E^{1/2}$ dependence in wider ribbons, consistent with the 2D limit.

With their scalability, tunable width, and edge-dependent properties, SiP-NRs offer a versatile platform for advancing device miniaturization and enhancing performance in nano-electronics, energy conversion, and quantum technologies,

making them promising candidates for next-generation applications.

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DATA AVAILABILITY

The data supporting this study's findings are available within the article.

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