Structural, Electronic, and Transport Properties of Silicane Nanoribbons

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Structural, electronic, and transport properties of silicane nanoribbons

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Silicane ribbons do not suffer from aromatic dependence of the band gap making them a more promising candidate for near-term nanoelectronic application compared to armchair graphene nanoribbons. The structural, electronic, and transport properties of free-standing sp$^3$-hybridized armchair- and zigzag-edge silicane nanoribbons have been investigated using ab initio and nonlocal empirical pseudopotential calculations. Under ambient conditions, two-dimensional silicane sheets will spontaneously break into stable one-dimensional ribbons similar to density functional theory studies of graphene ribbons. The calculated low-field electron mobility and ballistic conductance show a strong edge dependence, due to differences in the effective mass and momentum relaxation rates along the two transport directions. The mobility in zigzag-edge ribbons is found to be approximately twenty times higher than in armchair-edge ribbons.

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I. INTRODUCTION

Recent experiments have shown that it is possible to grow silicene strips (silicene nanoribbons) or silicene sheets—a Si monolayer with two-dimensional honeycomb lattice similar to graphene—on Ag(110)$^{1-3}$ and Ag(111)$^{4-6}$ substrates. This has attracted much attention because of the compatibility of these structures and processes with conventional Si-CMOS technology. Theoretical calculations have revealed that sp$^3$ hybridization in a low-buckled silicene structure, also known as silicane, is more stable and favorable than sp$^2$ hybridization, although both structures exhibit an opening of a band gap.$^{7-10}$ Also, it has been shown that the silicane is either a direct or indirect band gap semiconductor depending on the hybridized configurations (i.e., chair or boat like)$^{7,8,11}$ and the chairlike configuration is always energetically more stable than the boatlike configuration.$^{11}$ Silicane nanoribbons (SiNRs), the one-dimensional Si counterpart of graphene-NRs, can be classified as armchair-edge or zigzag-edge, depending on its edge structure (aSiNR and zSiNR, respectively).

Recent density functional theory (DFT) calculations have shown an aromatic dependence of the band gap with the number of atoms along the width of “edge-only” H-passivated aSiNR with a buckled configuration.$^{9,12,13}$ This aromatic dependence is also reported for armchair graphene-NRs and has often been attributed to the increase bond strength and strain in the edge atoms in the literature.$^{14}$ While strain plays a role, alone it does not explain the difference in the band gap scaling trends for the family of ribbons with 3N, 3N + 1, and 3N + 2 atoms since the edge strain would be equivalent across these three categories. Instead, the scaling trends stem from the spatial localization of the π electrons into Clar sextets$^{15}$ along the edges of sp$^2$-bonded materials that fix specific Kekulé patterns in the ribbons based on the number of atoms along the width. This behavior of graphene ribbons is comprehensively explained in the work of Wassmann et al.$^{16}$

To the author’s knowledge the electronic structure and band gap scaling in fully sp$^3$-hybridized SiNRs has not been studied and no literature exists about charge carrier transport properties in SiNRs. This is particularly important for nanoelectronics application since the aromatic dependence of the band gap is an undesired property negatively affecting the electronic transport properties.$^{17}$

In this study, we investigate the structural, electronic, and transport properties of sp$^3$-hybridized (chair-like) aSiNRs and zSiNRs. We employ the computationally efficient nonlocal empirical pseudopotentials (EPs) of Refs. 18 and 19, which have been shown to predict the electronic properties of bulk Si and of Si nanowires in agreement with experimental data and results of ab initio calculations. Calculated results from EPs for SiNRs are benchmarked to the results obtained using DFT as implemented in the Vienna ab initio simulation package (VASP)$^{20,21}$ with a plane-wave basis expansion and an energy cutoff of 450 eV. The electron-ion core interaction is represented by the projector augmented wave (PAW)$^{22}$ method and we have employed the Perdw-Burke-Ernzerhof (PBE) exchange correlation functional in the generalized gradient approximation (GGA).$^{23}$

II. CRYSTAL STRUCTURE AND THERMODYNAMIC STABILITY

Figure 1 shows the atomic configuration of (a) an aSiNR and of (b) a zSiNR; all Si dangling bonds, including those at the top and bottom of the monolayer surface, are passivated by H atoms, creating the sp$^3$-hybridized bonding. The width of the SiNR is characterized by the number of Si-Si dimer lines or zigzag chains along the ribbon for the aSiNR or zSiNR, respectively, following the conventional notation for graphene-NRs.$^{14}$ The geometric relaxation is performed using the conjugate gradient (CG) algorithm within VASP in which the force-tolerance is set to 0.02 eV/A and a 1×1×8 Monkhorst-Pack k-point grid is used. The relaxed atomic geometry is then employed in EPs calculation by rescaling the bond length by the ratio of the relaxed to the unrelaxed geometry obtained from the DFT calculations. As shown in Fig. 2, the buckling height (denoted by Δy) is reduced from...
\[ \Delta y = 0.784 \text{ Å} \] (uniform when unrelaxed) to \[ \Delta y_1 = 0.724 \text{ Å} \] and \[ \Delta y_2 = 0.739 \text{ Å} \] (buckling heights of inner Si-Si atoms and edge Si-Si atoms, respectively, after the relaxation) while the Si-Si and Si-H bonding lengths are slightly increased for the 4-zSiNR. However, there is not a noticeable variation in the buckling heights after relaxation depending on the width and edge shape of the ribbons.

We also evaluate the relative thermodynamic stability of the SiNRs to the two dimensional (2D) silicane sheet by comparing the edge free energy using DFT as described in Ref. 24. The contribution to the hydrogen zero-point energy in the ribbons is negligible and for pressures below 100 atm the edge free energy can be calculated with the Helmholtz free energy. Assuming the gas phase H acts as a thermodynamic reservoir and is in chemical equilibrium with the silicane sheet, the edge free energy can be written as

\[ \gamma_{\text{edge}} = \frac{1}{2L} \left[ E_{\text{ribb}} - N_{\text{Si}} E_{\text{blk}} - \frac{(N_{\text{Si}} - N_{\text{H}})}{2} \mu_{\text{H}_2} \right], \]

where \( L \) is the length of the ribbon, \( E_{\text{ribb}} \) and \( E_{\text{blk}} \) are the total energies of the SiNR supercell and 2D silicane sheet, respectively, and \( N_{\text{Si}} \) and \( N_{\text{H}} \) are the number of Si and H atoms.

FIG. 2. (Color online) Atomic configuration of an (a) unrelaxed and a (b) relaxed 4-zSiNR for EPs and DFT calculations, respectively. Buckling heights are denoted by \( \Delta y \) for unrelaxed and \( \Delta y_1 \) (inner Si-Si atoms) and \( \Delta y_2 \) (edge Si-Si atoms) for relaxed geometry, respectively.

FIG. 3. Edge free-energy vs chemical potential for a 7-aSiNR and a 4-zSiNR referenced to the free energy of an infinite 2D silicane sheet (represented as dashed horizontal line at \( \gamma_{\text{edge}} = 0 \)). The top axes show the pressure, in bar, of H\(_2\) molecule corresponding to the chemical potential at \( T \) = 100, 300, and 600 K, following Refs. 25 and 37.
The chemical potential $\mu_H = \frac{1}{2}\mu_{H_2}$ at a given temperature $T$ and partial pressure $p$ of hydrogen is

$$
\mu_H(T, p) = \frac{1}{2} E_{H_2} + \mu_H(T, p^0) + \frac{k_B T}{2} \ln \left( \frac{p}{p^0} \right), \quad (2)
$$

where $E_{H_2}$ is the total energy of the isolated H$_2$ dimer and $p^0 = 1$ bar. The relative stability of the SiNRs can be determined by comparing the edge free energy $\gamma_{edge}$ as a function of $\mu_H$ as shown in Fig. 3, where the lowest energy corresponds to the most thermodynamically stable structure. We find that the overall stability of the SiNRs is essentially independent of the ribbon width for the structures simulated (widths of 0.58–1.92 nm for aSiNRs and 1.11–2.66 nm for zSiNRs) in which the stability changes by less than 0.1% as a function of ribbons width and Fig. 3 only shows the edge free energy for the 4-zSiNR and the 7-aSiNR. The ribbons are found to be more stable than the infinite silicane sheet (represented as a dashed horizontal line in Fig. 3) except at very low partial pressures of H and similar to graphene$^{25}$ and it is likely that the silicane sheet will spontaneously break into 1D ribbons under high H concentrations. In addition, contrary to graphene-NRs the aSiNRs are only slightly more thermodynamically favorable than zSiNRs. The difference in edge free energy between the aSiNRs and the zSiNRs is approximately 0.1 eV/Å under ambient conditions while in graphene-NRs the difference was calculated to be approximately four times greater.$^{25}$

III. ELECTRONIC BAND STRUCTURE

The electronic band structure of both aSiNRs and zSiNRs using EPs and DFT with unrelaxed as well as fully relaxed geometry are shown in Fig. 4. Notice that the geometry relaxation slightly raises the energy of the conduction bands relative to the valence-band maximum (VBM), increasing the band gap in both the EPs and the DFT results. As expected

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**FIG. 4.** (Color online) Electronic band structure of a 4-zSiNR and 7-aSiNR using EPs [(a) and (c)] and DFT [(b) and (d)] with unrelaxed (dotted lines) and fully relaxed (solid lines) geometry. The top of the valence band is arbitrarily set to zero. The insets show in detail the conduction band structure near the CBM, which is set to zero.
from our previous study on the transferability of the EPs to Si nanowires,\textsuperscript{18} the band structure obtained using EPs shows very similar characteristics to the DFT results, in both cases exhibiting a direct band gap at $\Gamma$ in zSiNRs and an indirect gap near the edge of Brillouin zone (BZ) in aSiNRs, as shown here for the particular case of a 4-zSiNR and a 7-aSiNR. However, the values of the band gap obtained using DFT are more than 1 eV smaller than the EPs. The geometry relaxation is not responsible for this difference because even for an unrelaxed atomic configuration the DFT result still remains significantly smaller than the EPs. The geometry relaxation is not responsible for this difference because even for an unrelaxed atomic configuration the DFT result still remains significantly smaller than the EPs gap, as shown in Fig. 4 where the band structure for the relaxed and unrelaxed geometries are represented by solid and dotted lines, respectively. Thus the smaller band gap from DFT can be attributed to the well-known "band gap underestimation problem" of DFT-GGA.\textsuperscript{26–28} It should also be noticed that the energy dispersion obtained using EPs is "denser" than the DFT result in the conduction bands [as magnified in insets in which the conduction band minima (CBM) are set to zero] for both zSiNR and aSiNR, a consequence of the different approximations on which EPs and DFT are based.

As mentioned above, it is interesting to study the possible aromatic dependence of the band gap in SiNRs considering that it is absent in the case of graphene-NRs with $sp^3$ hybridization, as this bonding configuration removes the resonant states (Clar structures).\textsuperscript{15,29} The width dependence of the band gap and effective mass ($m^*$) at the CBM for both aSiNRs and zSiNRs is shown in Fig. 5, where the band gap and the mass obtained from EPs and DFT are represented as solid and open symbols, respectively. The gap ($\Delta E_g$, shown in Fig. 5(a)) is the difference between the calculated band gap of the SiNRs and the gap of bulk Si (1.16 eV for EPs and 0.626 eV for DFT). Unlike what is found for armchair graphene-NRs\textsuperscript{14,30} and "edge-only" H-passivated aSiNRs,\textsuperscript{9,12,13} aSiNRs and zSiNRs do not show the aromatic dependence of the band gap in either the EPs or DFT calculations. Instead, the band gap decreases nonlinearly as the ribbon width increases due only to the quantum confinement effects similarly to what has been reported for graphene-NRs.\textsuperscript{29} This lack of aromatic dependence of the band gap in aSiNR and zSiNR is the result of the $sp^3$ bonding which ensures fourfold coordination for all Si atoms and therefore is not affected by the Clar resonances which control the band structure in the $sp^2$ bonding of the armchair graphene-NR. Also, we notice that the band gaps of the zSiNRs show a smaller variation than the aSiNRs implying better controllability of the band gap in the sub-three-nanometer regime. This situation is somewhat different from what has been found for graphene-NRs, case in which the gap exhibits the same quantitative trend regardless of the edge shape.\textsuperscript{29} As already mentioned, the band gap is direct for zSiNRs but indirect for aSiNRs for all calculated widths. As expected from the band gaps, the electron effective masses at CBM

![FIG. 5.](https://example.com/fig5.png)

**FIG. 5.** (Color online) (a) Difference between the calculated band gap for ribbons and the band gap for bulk Si, $\Delta E_g$, shown as a function of ribbon width for aSiNRs and zSiNRs. The band gaps from EPs and DFT are represented by solid and open symbols, respectively. The electron effective mass (in unit of the free electron mass, $m_0$) at the CBM along the $+k_z$ is shown as a function ribbon width in (b) for aSiNRs and in (c) for zSiNRs. Solid (open) symbols identify EPs (DFT) results.

![FIG. 6.](https://example.com/fig6.png)

**FIG. 6.** (Color online) 1D ballistic conductance (in unit of the quantum conductance $G_0 = 2e^2/h$) for a 4-zSiNR in (a) and a 7-aSiNR in (b) with the conduction band edge $E_{CBM}$ set to zero. The ballistic conductance calculated using EPs (DFT) is represented by solid (dotted) lines.
obtained using EPs are larger than those calculated using DFT for both aSiNRs and zSiNRs, while the masses for the aSiNR are larger than for the zSiNRs as shown in Figs. 5(b) and 5(c). Therefore we can expect an enhanced electron mobility in zSiNRs. However, the electron effective mass in aSiNRs does not simply increase proportionally to their band gap with increasing width as it happens in zSiNRs. The sudden jump of the mass (calculated using EPs) for the 7-aSiNR (w = 1.152 nm) is due to the very flat dispersion near the X point as a crossing occurs between the first and the second subband, as show in the inset of Fig. 4(c).

IV. BALLISTIC CONDUCTANCE AND ELECTRON MOBILITY

To assess the electronic transport properties along the (axial) z direction—which is equivalent to the [112] and [101] for aSiNR and zSiNR, respectively, as shown in Fig. 1—we calculate the ballistic conductances in SiNRs following Ref. 18 and the phonon-limited low-field electron mobility using the Kubo-Greenwood formula. We take into account electron-phonon scattering using the deformation potentials of bulk Si, thus ignoring phonon confinement, which is expected to enhance the overlap integral between the electron and the confined-phonon wave functions.31 Also, line-edge roughness scattering is neglected, so that our goal is simply to provide an upper bound for the electron mobility. Figure 6 shows the calculated ballistic conductances in units of the quantum conductance $G_0 = 2e^2/h$ for the 4-zSiNR (w = 1.108 nm) and the 7-aSiNR (w = 1.152 nm) using both EPs and DFT. The ballistic conductance is larger in the 4-zSiNR than in the 7-aSiNR due to the fewer Landauer channels present in the 7-aSiNR, as seen in Fig. 4, leading us once more to expect better transport properties in zSiNRs. The one-dimensional (1D) low-field electron mobility along the z direction is given by

$$\mu_{zz} = \frac{1}{n_l} \sum_\alpha n^{(\alpha)} \mu^{(\alpha)}_{zz},$$

where $\alpha$ is an index labeling the conduction subbands. The quantities $n_l$ and $n^{(\alpha)}$ represent the electron line density and the non-self-consistent electron density in subband $\alpha$, respectively.

![FIG. 7. (Color online) (a) Total electron-phonon momentum relaxation rate accounting for the acoustic and optical emission and absorption processes and (b) density-of-states for a 7-zSiNR (solid lines) and an 11-aSiNR (dashed lines) at the electron line density $n_l = 5 \times 10^5 \text{ cm}^{-1}$ and at $T = 300 \text{ K}$. The conduction band minimum $E_{CBM}$ is set to zero.](image)

![FIG. 8. (Color online) Phonon-limited electron mobility (a) as a function of the line density $n_l$ for 7-zSiNR (square) and 11-aSiNR (circle) at $T = 300 \text{ K}$ and (b) as a function of ribbon width for zSiNRs (square) and aSiNRs (circle) at an electron line density $n_l = 5 \times 10^5 \text{ cm}^{-1}$ and $T = 300 \text{ K}$.](image)
The mobility tensor $\mu^{(\alpha)}_{zz}$ is given by

$$\mu^{(\alpha)}_{zz} = \frac{2e}{\hbar n^{(\alpha)}} \sum_{k_z} v^{(\alpha)}(k_z) \tau^{(\alpha)}_{tot,z}(k_z) \frac{\partial f_0[E^{(\alpha)}(k_z)]}{\partial k_z}.$$  

where $v^{(\alpha)}(k_z) = (1/\hbar) dE^{(\alpha)}(k_z)/dk_z$ and $f_0[E^{(\alpha)}(k_z)]$ are group velocity and the electron distribution function at equilibrium (Fermi–Dirac), respectively. The total momentum relaxation rate $1/\tau^{(\alpha)}_{tot,z}(k_z)$ is given by

$$\frac{1}{\tau^{(\alpha)}_{tot,z}(k_z)} = \frac{1}{\tau^{(\alpha)}_{ac,c}(k_z)} + \frac{1}{\tau^{(\alpha)}_{op,(ab),z}(k_z)} + \frac{1}{\tau^{(\alpha)}_{op,em,c}(k_z)},$$

FIG. 9. (Color online) (a) Conduction band structure (from $\Gamma$ to $X$, solid lines) and corresponding density of states (overlaid dashed lines) calculated using EPs for zSiNRs with width ranging from a 5-zSiNR to an 8-zSiNR. The second subbands at $\Gamma$ are identified by arrows. Fermi levels at a line density $n_l = 5 \times 10^5$ cm$^{-1}$ and $T = 300$ K are represented as a horizontal solid lines. (b) Electron occupation factor $f_0 \times (1 - f_0)$ at $\Gamma$ for the first (square) and second (circle) subbands as a function of width. (c) Phonon-limited momentum relaxation rate at $\Gamma$ for the first (square) and second (circle) subbands as a function of width. (d) Subband mobility for the first (square) and second (circle) subbands and their summation (open triangle) as a function of width. Keeping in mind that the total phonon-limited electron mobility is mainly controlled by the two lowest-energy subbands, a decrease of the Fermi level with increasing width results in a relatively lower occupation of the first subband, as shown in frame (b). This overshadows the reduced electron-phonon scattering, as shown in (c), which is dominated by a smaller overlap integral. Thus the mobility in the first subband decreases with increasing ribbon width. On the other hand, the energy of the second subband is reduced with increasing ribbon width, as indicated as arrows in (a) due to reduced confinement, resulting in increased subband occupation [shown in (b)] as well as in a reduced overlap integral and scattering rate [shown in (c)]. Thus the mobility in the second subband increases as the ribbon is widened from the 5-zSiNR to the 7-zSiNR. But moving to the 8-zSiNR, what we label “second” subband now replaces the “first” subband due to the band crossing, so that the trend reverses. Note that a degradation of the mobility with reduced confinement has been also discussed in Ref. 38 and this has been attributed to a reduced subband occupation.
where $\tau_{\text{ac}}^{(a)}(k_z), \tau_{\text{op}}^{(a)}(k_z), \text{and } \tau_{\text{op}}^{(a)}(k_z)$ are the momentum relaxation times due to scattering between electrons and bulk acoustic and optical (absorption and emission) phonons, respectively. The momentum relaxation rates, assuming elastic, and isotropic scattering and using equipartition approximation, can be written as

$$\frac{1}{\tau_{\text{ac(op),z}}^{(a)}(k_z)} = \frac{2\pi}{\hbar} |V_{\text{ac(op)}}|^2 \sum_{k_z'} F_{k_z,k_z'} \times \delta[E^{(a)}(k_z) - E^{(a)}(k_z')] ,$$

where $|V_{\text{ac(op)}}|^2 = (\Delta^2 k_B T)/(2\rho v_f^2)$ is the matrix element for scattering with acoustic phonons expressed in terms of a momentum-independent acoustic phonon deformation potential $\Delta_{\text{ac}} = 5.8$ eV, of the crystal mass density $\rho = 2.33 \times 10^{-3}$ kg/cm$^3$, and of the sound velocity $v_f = 9.20 \times 10^5$ cm/s for bulk Si.\textsuperscript{32-34} Similarly, for optical phonons, the matrix element is expressed as

$$|V_{\text{op}}|^2 = \left(\frac{D K_{\text{op}}^2}{2\rho w_{\text{op}}} \right) \left\{ \begin{array}{ll}
n_{\text{op}} & \text{(absorption)} \\
n_{\text{op}} + 1 & \text{(emission)} \end{array} \right. ,$$

where $(D K_{\text{op}}^2)$ is the optical deformation potential,\textsuperscript{32} $\hbar w_{\text{op}} = 61.12 \times 10^{-3}$ eV is the energy of the optical phonons,\textsuperscript{33} assumed to be dispersionless, and $n_{\text{op}} = 1/(e^{|\hbar w_{\text{op}}|/k_B T} - 1)$ is the phonon occupation number. The overlap integral $F_{k_z,k_z'}$ is calculated considering only $N$ processes (i.e., $G_z = 0$):

$$F_{k_z,k_z'} = \int d \vec{R} \left| \frac{\kappa^{(a)}_{k_z}(\vec{R})}{|\kappa^{(a)}_{k_z}(\vec{R})|} \right|^2 \left| \frac{\kappa^{(a)}_{k_z'}(\vec{R})}{|\kappa^{(a)}_{k_z'}(\vec{R})|} \right|^2 ,$$

in which $n_s = n_x = 51$ define a uniform two-dimensional mesh and the 2D wave function $\kappa^{(a)}_{k_z}(\vec{R})$ is given by

$$\kappa^{(a)}_{k_z}(\vec{R}) = \frac{1}{A^{1/2}} \sum_{a=0}^{A} \vec{G}_{i}^{(a)} \left( e^{i G_i^{(a)} \vec{R}} \right) ,$$

where the $\vec{G}_i$ and $\vec{R}$ represent in-plane reciprocal and direct lattice vectors, respectively, and $A$ is the normalization area on the 2D plane (i.e., $x$-$y$ plane of the unit cell in Fig. 1).

We evaluate the electron mobility using the eigenergies and Bloch functions calculated from the EPs with the relaxed geometry at 151 $k$ points along the 1D BZ and 15 conduction subbands which are sufficient for an accurate evaluation of the mobility.

Figure 7 shows (a) the total momentum relaxation rates and (b) the density of states at a given line density and at $T = 300$ K for the 7-zSiNR ($w = 1.995$ nm) and 11-aSiNR ($w = 1.920$ nm). The momentum relaxation rate for the 7-zSiNR is almost one order of magnitude smaller than for the 11-aSiNR near the conduction band edge, because of the smaller density of states. This is true for all ribbon widths so we expect a much higher electron mobility in zSiNRs than in aSiNRs. In Fig. 8, we show the calculated electron mobility in the 7-zSiNR and 11-aSiNR as a function of (a) electron line-density and (b) ribbon width. Note in Fig. 8(a) that the electron mobility saturates at a lower line density ($n_l < 10^6$ cm$^{-1}$ vs $n_l < 10^7$ cm$^{-1}$) and at a value about 25 times higher in the 7-zSiNR ($\sim 500$ cm$^2$/Vs vs $\sim 20$ cm$^2$/Vs) than in the 11-aSiNR.

A dramatically higher electron mobility is seen for the 7-zSiNR and can be ascribed to (1) the smaller band gap resulting in a smaller effective mass as shown in Fig. 5 and therefore a higher group velocity along a given axial crystallographic direction and (2) to a lower momentum relaxation rate due to the smaller density of states, as discussed above. Figure 8(b) shows the variation of the electron mobility with ribbon width. The main observation is that, contrary to expectations based on a simpler effective-mass model or what is seen in Si nanowires,\textsuperscript{31,35,36} the mobility does not show a monotonic decrease with decreasing width but varies somewhat abruptly. This is the result of several effects: for a given electron line-density the Fermi level changes nonmonotonically as a result of the changing band structure; as (sub)bands cross with varying ribbon width, the (transport) effective mass, and so the electron group velocity, and the occupation of the subbands also change nonmonotonically. Finally, also as a result of the (sub)band crossing, the overlap integrals, Eq. (8), change in a similar nonmonotonous fashion. The result of the complicated interplay among these various competing effects is shown in detail in Fig. 9(a). In this figure, we show the subband structures, density of states and Fermi level (relative to the CBM at a given electron line-density) for a varying ribbon width corresponding to 5- to 8-zSiNRs. The caption provides as qualitative explanation for the nonmonotonic behavior we have just mentioned.

V. CONCLUSIONS

In conclusion, we have investigated the structural, electronic, and transport properties of free-standing $sp^3$-hybridized (chair-like) aSiNRs and zSiNRs. DFT calculations show that $sp^3$-hybridized SiNRs (with either armchair or zigzag edges) in a buckled configuration are thermodynamically more stable than a silicane sheet under ambient conditions. The electronic band structure calculated using EPs is very similar to what is obtained using DFT for both zSiNRs and aSiNRs, with the expected exception of the value of the band gap. Both EPs and DFT predict a direct and an indirect gap for zSiNRs and aSiNRs, respectively, and the band gap shows no aromaticity with ribbon width for either the aSiNRs or the zSiNRs, result which has significant consequences on the electronic transport properties of these structures. Finally, we show a strong edge-shape dependence of the ballistic conductance and low-field electron mobility, both much larger in zSiNRs than in aSiNRs. Most notably, the phonon-limited mobility in zSiNRs is more than 20 times higher than in aSiNRs. As a result, also considering their compatibility with conventional Si-CMOS technology and the lack of aromaticity of their band gap compared to planar $sp^2$ bonding structures, zSiNRs are extremely interesting candidates for nanoelectronics applications.

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