Enhanced Thermoelectric Efficiency of Porous Silicene Nanoribbons

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There is a critical need to attain new sustainable materials for direct upgrade of waste heat to electrical energy via the thermoelectric effect. Here we demonstrate that the thermoelectric performance of silicene nanoribbons can be improved dramatically by introducing nanopores and tuning the Fermi energy. We predict that values of electronic thermoelectric figure of merit $ZT_e$ up to 160 are achievable, provided the Fermi energy is located approximately 100 meV above the charge neutrality point. Including the effect of phonons yields a value for the full figure of merit of $ZT = 3.5$. Furthermore the sign of the thermopower $S$ can be varied with achievable values as high as $S = \pm/\sim 500 \text{ } \mu \text{V/K}$. As a method of tuning the Fermi energy, we analyse the effect of doping the silicene with either a strong electron donor (TTF) or a strong electron acceptor (TCNQ) and demonstrate that adsorbed layers of the former increases $ZT_e$ to a value of 3.1, which is insensitive to temperature over the range 100 K – 400 K. This combination of a high, temperature insensitive $ZT_e$, and the ability to choose the sign of the thermopower identifies nanoporous silicene as an ideal thermoelectric material with the potential for unprecedented performance.

In the recent years, the challenge of removing heat from nanoelectronic devices\(^2\) and thermoelectrically converting waste heat into electricity has attracted huge scientific interest\(^2\), not only due to the questions posed for fundamental science, but also because thermoelectric energy conversion is an essential requirement for the next generation of nanoscale electronic, optoelectronic and photonic devices\(^5\). The efficiency of a thermoelectric device and material is determined by its thermoelectric figure of merit ($ZT$) defined as:

$$ZT = \frac{S^2GT}{\kappa}$$

(1)

where $S$ is the Seebeck coefficient (thermopower), $G$ is the electrical conductance, $T$ the temperature and $\kappa$ the thermal conductance given by $\kappa = \kappa_e + \kappa_p$, where $\kappa_e (\kappa_p)$ is the electronic (phononic) contribution to $\kappa$. Clearly $ZT$ could be enhanced by increasing the power factor ($S^2GT$) or decreasing the thermal conductance and therefore a high-performance thermoelectric material should possess a large Seebeck coefficient and electrical conductance and simultaneously a low thermal conductance. The search for new materials with enhanced thermal properties continues to intensify, because these factors are correlated and increasing $ZT$ to values greater than unity requires a delicate optimisation of several material properties.

One promising approach has been to reduce the contribution $\kappa_p$ of parasitic phonons by nanostructuring materials\(^4\). Although acoustic phonons are the main heat carriers in bulk crystals, nanostructures can exhibit significantly lower phonon thermal conductances $\kappa_p$, due to increased phonon boundary scattering, changes in the phonon density of states and modified phonon dispersion in low-dimensional materials\(^5\). The nanostructuring of materials is also a promising route to increasing the power factor, because it can lead to sharp features in the electronic density of states and the transmission coefficient $T(E)$ describing the propagation of electrons of energy $E$ through a device. It is well known that the thermopower $S$ is controlled by the asymmetry of $T(E)$ at the Fermi energy $E_F$ and therefore if $E_F$ is close to such an asymmetry, both $S$ and $ZT$ will be enhanced. Unfortunately, asymmetries, even if they occur, are not necessarily located near $E_F$ and therefore a method of tuning them is required. In a nanoscale device, one could of course consider introducing a third gate electrode to control such features, but in practice this costs energy and does not solve the problem of designing a new material.

The above considerations suggest that an effective strategy for enhancing thermoelectric properties should 1) start from a parent material with low intrinsic thermal conductance, 2) nanostructure the material to further reduce the thermal conductance, 3) implement additional nanostructuring to introduce sharp features in $T(E)$ and 4) chemically modify the material to move these sharp features towards the Fermi energy. In this paper our aim is to demonstrate that silicene, a new counterpart of graphene is an ideal material for implementing the four...
key elements of this strategy, because it is not only CMOS-compatible, but also it possesses a low intrinsic thermal conductance, which can be further reduced by nanostructuring the material to form nanoribbons.

Since silicon is the most common material used in the electronics industry, it is highly desirable to utilise silicon-compatible materials for thermoelectric energy conversion. Bulk silicon has a very low $ZT (<0.01)$ and therefore as a first step in a strategy for enhancing thermoelectric performance it is natural to focus on silicon, which is a recently-observed one-atom-thick crystalline form of silicon atoms arranged in a slightly buckled honeycomb lattice structure\(^6\)\(^-{12}\). Silicene nanoribbons have been synthesised on silver (111)\(^1\)\(^\text{13-15}\), gold (110)\(^1\)\(^6\), iridium (111)\(^2\) and the zirconium diboride (0001)\(^2\)\(^8\),\(^9\) substrates and are predicted to be stable on non-metallic substrates\(^3\)\(^0\). Calculations of thermoelectric properties of armchair and zigzag silicene nanoribbons with and without hydrogen-passivated edges suggest that this material may be attractive for thermoelectric devices\(^3\)\(^1\)\(^-{34}\), because the thermal conductivity of 2D silicene is predicted to be much smaller than bulk silicon and its counterpart graphene\(^3\)\(^5\), with only ~10% of the total phononic thermal conductivity being due to the out-of-plane acoustic phonons\(^3\)\(^6\),\(^3\)\(^7\). Both of these desirable features arise from the presence of small buckling, which breaks the reflection symmetry of the structure\(^3\)\(^8\),\(^3\)\(^9\).

Further reductions in the phonon contribution arise from additional nanostructuring. For example the thermal conductivity of a silicene nanosheet $\sigma_p^{\text{SiNS}} = (6-30)W/mK$\(^3\)\(^1\),\(^3\)\(^5\),\(^3\)\(^7\) reduces to $\sigma_p^{\text{ZSiNR}} = [0.16 - 1.4]W/mK$ in zigzag silicene nanoribbons\(^3\)\(^2\),\(^3\)\(^4\). This could be potentially even lower in porous silicene, since the lattice thermal conductivity is reduced in nanoporous semiconductors\(^5\)\(^8\) such as nanoporous Bi\(^4\)\(^9\), Ge\(^4\)\(^0\), graphene\(^4\)\(^1\),\(^4\)\(^2\), Bi\(_2\)Te\(_3\)\(^4\)\(^3\) and SiGe\(^4\)\(^5\). Moreover, it is been shown that placing nanopores in bulk silicon greatly reduces the thermal conductivity and enhances $ZT$ by the factor of two\(^4\)\(^6\).

Since the low phonon thermal conductance of silicene is well established and therefore elements 1) and 2) of the above strategy are satisfied, in this paper we focus steps 3) and 4) and demonstrate that they can be achieved by inserting nanopores into silicene nanoribbons, whose edges are terminated by hydrogen or oxygen and by introducing adsorbates to tune the position of features in $T(E)$ relative to $E_F$. In view of the low value of $\kappa_p$, we will focus primarily on the electron contribution in thermoelectric figure of merit $ZT_e$ (obtained by setting $\kappa_p = 0$ in equation 1) and show that for ribbons containing nanopores with hydrogen-passivated edges, $ZT_e$ could be enhanced to values as high as 160 at room temperature by creating sharp features in the $T(E)$ and controlling the Fermi energy or by

Figure 1 | Sketch of the molecular structure of the Silicene and its alloys. (a) silicene molecular structure, (b) a TTF (top) and TCNQ (bottom) doped silicene ribbon with two layers of dopant, (c) silicene monolayer ribbon with hydrogen terminated edges (ZSiNR-H), (d) silicene monolayer containing a nanopore (ZSiNR-P). All edges are terminated with hydrogen. (e) silicene monolayer ribbon with an oxygen terminated scattering region and hydrogen terminated electrodes (ZSiNR-HO), (f) silicene monolayer ribbon with oxygen terminated edges (ZSiNR-O), (g) as for (d), but with adsorbed Tetracyanoquinodimethane (TCNQ) and (h) as for (d), but with adsorbed Tetrathiafulvalene (TTF).
introducing adsorbates such as Tetrathiafulvalene (TTF) and Tetracyanoquinodimethane (TCNQ) onto the silicene surface. We will then show that by including the \( k_p \) of silicene nanoribbons, a high value of the full \( ZT \) of order 3.5 is achievable.

**Results and Discussion**

We have calculated the electronic contribution to the thermal conductance, the Seebeck and Peltier coefficients and \( ZT_e \) for the structures shown in Figure 1c–h. The optimized lattice constant (\( a_0 \)) and buckling (\( d \)) of the silicene nanoribbon shown in Figure 1a are found to be 3.6 Å and 0.53 Å, respectively, similar to that reported elsewhere. The engineered silicene nanoribbons shown in Figure 1 include: a zigzag monolayer silicene nanoribbon with hydrogen terminated edges (ZSiNR-H, Figure 1c), a zigzag monolayer silicene nanoribbon containing a nanopore with all edges terminated by hydrogen (ZSiNR-P, Figure 1d), a zigzag monolayer silicene nanoribbon with...
ribbon with a central region containing oxygen terminated edges, connected to hydrogen-terminated leads (ZSiNR-HO, Figure 1e), and a zigzag monolayer silicene nanoribbon with oxygen terminated edges (ZSiNR-O, Figure 1f). The nanoribbons length and width in all cases are almost equal ($L < 6$ nm (scattering region $< 3.48$ nm), $W < 3$ nm) and the pore diameter is $< 1.3$ nm. We shall find that a key strategy for improving the thermoelectric performance of these structures involves tuning the Fermi energy ($E_F$). As an example of how this could be achieved, we investigated the effect of introducing adsorbates onto the surface of the ZSiNR-P hydrogen-terminated nanoribbon, as shown in Figures 1f and 1g. The latter show examples of such functionalised ribbons containing adsorbed TTF (a strong electron donor) and TCNQ (a strong electron acceptor), which form charge-transfer complexes with the silicene.

Silicene nanoribbons and nanopores. For the structures (c) to (f) of Figure 1, Figure 2 shows results for electrical conductance $G$, the electronic contribution of the thermal conductance $\kappa_e$, the thermopower $S$ and the Peltier coefficient $\Pi$ of the junction as a function of the temperature ($T$). All of these properties are obtained from the energy ($E$) dependence of the electron transmission coefficient $T(E)$, shown in Figure 2a.

Figure 2 shows that the silicene nanoribbons ZSiNR-H, ZSiNR-HO and ZSiNR-O possess high electronic thermal conductances and low thermopowers and consequently their figures of merit ($ZT_e$) are low. However, the results for the silicene monolayer nanoribbon containing a nanopore (ZSiNR-P) show that $ZT_e$ is significantly improved by placing a hole in the ribbon. This arises because the densities of states of all four structures possess sharp peaks around the Fermi energy $E_F$ due to band bending in the corner of the $k$-space in silicene band structure, which introduces a sharp feature (indicated by an arrow in Figure 2a) in $T(E)$ near $E_F$. Furthermore the $T(E)$ of ZSiNR-P possess the desirable feature that $T(E)$ is almost zero on either side of the peak. This feature is associated with edges states, which is why it is sensitive to the chemical nature of the edge terminations. These edge states are a well-known feature of nanoribbons with zigzag edges and lead to a significant improvement in the thermopower (Figure 2e) as well as a reduction in the thermal conductance (Figure 2d). Edge states have been predicted earlier theoretically and observed experimentally in graphene nanoribbons. By comparing ZSiNR-P with ZSiNR-H or by comparing ZSiNR-HO with either ZSiNR-P or ZSiNR-O, Figure 2 demonstrates the general trend that introducing scattering reduces both the electrical and thermal conductances and simultaneously increases the thermopower. Figure 2 also reveals the attractive property that ZSiNR-P possesses the highest room-temperature $ZT_e$ (of order 1.4) and that this high thermoelectric efficiency is preserved over a wide range of temperature from 100 K to 500 K.

To highlight the role of sharp features near $E_F$ in the transmission coefficients of Figure 2a, we investigate a simple model for which

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**Figure 4** | Room temperature thermal properties of the ZSiNR-H, ZSiNR-HO, ZSiNR-O and ZSiNR-P in different Fermi energies $E_F$.
(a) The variation of room-temperature values of $ZT_e$ (inset is $ZT$ on the logarithmic scale), (b) electronic thermal conductance $\kappa_e$ and (c) Seebeck coefficient $S$ as a function of $E_F$ for ZSiNR-H, ZSiNR-HO, ZSiNR-O and ZSiNR-P. The main part of fig. 4a shows $ZT_e$ for ZSiNR-P on a linear scale.

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**Figure 5** | Thermoelectric properties of the intrinsic and doped ZSiNR-P with various dopant and concentrations.
(a) Transmission coefficient $T(E)$ (see SI for a magnified version of this figure), (b, c) electrical and thermal conductance ($G$, $\kappa$), (d, e) Peltier ($\Pi$) and Seebeck ($S$) coefficients and (f) figure of merit as a function of temperature. Results are shown for a monolayer silicene nanopore (ZSiNR-P) with a perfect zigzag silicene ribbon electrodes, a monolayer silicene nanopore with TCNQ functionalized zigzag silicene nanoribbon electrodes with low concentration of TCNQ (ZSiNR-P-TCNQ) and with higher concentration of TCNQ (ZSiNR-P-2×TCNQ), a monolayer silicene nanopore with TTF functionalized zigzag silicene ribbon electrodes with low concentration of TTF (ZSiNR-P-TTF) and with higher concentrations of TTF (ZSiNR-P-2×TTF and ZSiNR-P-4×TTF).
To estimate the $\kappa_p$ for the structure of figure 1d, we note that for a perfect zigzag silicene nanoribbon of width equal to the bridging sections of silicene above and below the pore of Figure 1d is predicted to have a phononic thermal conductance $\kappa_p$ of less than $6 \times 10^{-11}$ W/K. This value contrasts markedly with graphene, whose thermal conductance is predicted to be a factor of at least 50 times higher. As discussed in the introduction, boundary scattering by nanoropes can lead to a further order of magnitude reduction in $\kappa_p$ and therefore a value of $\kappa_p$ on the scale of $\sim 10^{-12}$ W/K would seem reasonable for the structure of Figure 1d. For the model $T(E)$ of Figure 3a, Figure 3f shows the full $ZT$ when the thermal conductance is dominated by phonons, with a high thermal conductance of $\kappa_p = 2 \times 10^{-11}$ W/K. This demonstrates that even in the most unfavourable scenario, the full $ZT$ could achieve a value as high as 3.5 for values of $\sigma$ and $E_F$ lying in the red region of Figure 4f (where $\sigma \sim E_F = 0.1$). The transmission coefficient of the silicene nanorope (ZSiNR-P) shown in Figure 2a could be approximately modelled by $b = 1, a = 0$ with the width of $\sigma = 0.025$ and a mean of $E_F = 0.015$ around the Fermi energy. The crossover of dotted lines in Figure 3e shows the model $ZT$, at room temperature, which is in good agreement with the value of $ZT$, obtained from the more accurate $T(E)$ shown in Figure 2f. By increasing $E_F$, Figure 3f suggests that values of the full figure of merit as high as $ZT = 3.5$ are possible. On the other hand (see SI) for the ZSiNR-O ($a = b = 5$) and ZSiNR-H ($a = 1, b = 3$), the presence of a non-zero background suppresses the achievable values of $ZT$. For this reason, we now focus on tuning the properties of the H-terminated nanorope and demonstrate that high values of $ZT_c$ can be achieved by doping the surface of the silicene.

**Adsorbate-functionalized silicene.** For the purpose of improving intrinsic material performance, a method of shifting $E_F$ by doping the silicene nanoribbon is needed. Since covalent bonding of dopants to the nanoribbons may adversely affect electronic properties, we now consider tuning the Fermi energy by adsorbing planar molecules which interact with the surface only through weak pi-pi interactions. The first adsorbed molecule we study is Tetracyanovalene (TCNO) which is a strong donor and the second is Tetracyanoquinodimethane (TCNQ), which is a strong acceptor.

In the presence of adsorbates, calculations were performed by relaxing the adsorbates to find their minimum-energy states on the surface of the silicene (see methods), which yielded an optimized distance between the silicene and TCNQ of 3.1 Å and 3.54 Å for TFT. For the lowest dopant concentrations, we place a monolayer or sub-monolayer of TFT or TCNQ on the surface of the electrodes of ZSiNR-P, as shown in Figures 1g and 1h, whereas for the highest concentration, two layers above and below the silicene are included, as shown in Figure 1b. Figure 5 shows that TFT on silicene simultaneously increases the Seebeck coefficient, decreases the thermal conductance and increases $ZT_c$, from an undoped value of 1.4 to 1.7, 1.85 and 3.1 with increasing concentration from 21% to 43% and 87%, where the concentration of adsorbate is defined as the ratio of the number of TFT atoms to the number of silicene nanoribbon atoms. The inset of Figure 6 shows the variation of $ZT_c$ with $E_F$ for different concentrations of TFT and reveals that an 87% coverage produces a Fermi energy shift of approximately 3 meV. The transmission just around the Fermi energy is shown in Figure S2b of SI.

In summary, we have developed a new strategy for improving the thermoelectric performance of silicene-based nanoribbons by investigating the effect of introducing nanoropes and varying their edge termination. We have demonstrated that the thermopower and electronic thermoelectric figure of merit $ZT_c$ can be improved by introducing nanoropes and tuning their Fermi energy. By shifting the Fermi energy by approximately 100 meV from the charge-neutrality point, we predict that huge values of $ZT_c$ up to 160 are possible and that the sign of the thermopower can be varied with achievable values as high as $S = \pm 500 \, \mu V/K$. As a method of...
tuning the Fermi energy, we analysed the effect of doping the silicene with either a strong electron donor (TTF) or a strong electron acceptor (TCNQ) and demonstrated that doping by the former tended to decrease the value of $ZT_\alpha$, because the Fermi energy shift was in an unfavourable direction. On the other hand, we found that doping with TTF increased the room-temperature value to $ZT_\alpha$ to 3.1 and that this value is insensitive to temperature over the range 100 K – 400 K. This combination of a high temperature-insensitive $ZT_\alpha$ and the fact that the low phonon thermal conductance renders $ZT_\alpha$ comparable with the full figure of merit $ZT$, identifies nanoporous silicene as an ideal thermoelectric material with the potential for unprecedented performance.

**Methods**

To find the optimized geometry and ground state Hamiltonian of the structures of interest, we employed the SIESTA\(^{1}\) implementation of Density Functional Theory (DFT) using the generalized gradient approximation (GGA) of the exchange and correlation functional with the Perdew-Burke-Ernzerhof parameterization (PBE)\(^{2}\) a double zeta polarized basis set, a real-space grid defined with a plane wave cut-off energy of 250 Ry and a maximum force tolerance of 40 meV/Ang. The calculation with VDW-DF exchange and correlation functional with BH parameterization was also carried out to check the GGA-PBE result in some cases. The BH is the same as DRSLL with some modification\(^{3}\). From the converged DFT calculation, the underlying mean-field Hamiltonian was combined with our transport code, GOLLUM\(^{4}\), which is an implementation of the non-equilibrium Green’s function (NEGF) method. This yields the transmission coefficient $T(E)$ for electrons of energy $E$ (passing from the source to the drain) via the relation

$$T(E) = \text{Trace} \left\{ \Gamma_L(E) G_0 G^\dagger_L(E) \Gamma_R(E) G^\dagger_R(E) \right\}$$

where $G_0$ is the electronic contribution of the thermal conductance $\kappa(T)$, the thermo-power $S(T)$ and the Peltier coefficient $\Pi(T)$ of the junction as a function of the temperature are given by

$$G(T) = G_0 T_0$$

$$\kappa(T) = \frac{L_L L_R - L_j^2}{\hbar T_0}$$

$$S(T) = \frac{L_j}{e T_0}$$

$$\Pi(T) = T S(T)$$

The thermo-power $S(T)$ can be expressed as

$$S(T) = \frac{1}{T} \frac{d}{dT} \left( T \ln \frac{G(T)}{G_0} \right)$$

**References**

1. Naka, H. et al. Soft synthesis of single-crystal silicon monolayer sheets. Angew. Chem. Int. Ed. 45, 6303–6306 (2006).
2. Cahangirov, S., Topsakal, M., Aktürk, E., Şahin, H. & Ciraci, S. Two- and One-Dimensional Honeycomb Structures of Silicon and Germanium. Phys. Rev. Lett. 102, 236804 (2009).
3. Vogt, P. et al. Silicene: Compelling Experimental Evidence for Graphenelike Two-Dimensional Silicene. Phys. Rev. Lett. 108, 155501 (2012).
4. Kim, J., Fischetti, M. V. & Aboud, S. Structural, electronic, and transport properties of silicene nanoribbons. Phys. Rev. B. 86, 205323 (2012).
5. Kamal, C., Chakrabarti, A., Banerjee, A. & Deb, S. Silicon Beyond Mono-layers: Different Stacking Configurations And Their Properties. J. Phys.: Condens. Mat. 25, 085508 (2013).
6. Sadeghi, H., Bailey, S. & Lambert, C. J. Silicene-based DNA nucleobase sensing. Appl. Phys. Lett. 104, 103104 (2014).
7. Huang, S. T., Kang, W. & Yang, L. Electronic structure and quasiparticle bandgap of silicene structures. Appl. Phys. Lett. 102 (2013).
8. Sadeghi, H. Electrical Transport Model of Silicene as a Channel of Field Effect Transistor. J. Nanosci. Nanotechnol. 14, 4178–4184 (2014).
9. Jamgotchian, H. et al. Growth of silicene layers on Ag (111): unexpected effect of the substrate temperature. J. Phys.: Condens. Mat. 24, 172001 (2012).
10. Feng, B. et al. Evidence of Silicene in Honeycomb Structures of Silicon on Ag(111). Nano Lett. 12, 3507–3511 (2012).
11. Enriquez, H., Vizzini, S., Kara, A., Lalimi, B. & Oughaddou, H. Structure of nanosheets on silver surfaces. J. Phys.: Condens. Mat. 24, 314211 (2012).
12. Lalini, B. et al. Epitaxial growth of a silicon sheet. Appl. Phys. Lett. 97, 223109 (2010).
13. Auffray, B. et al. Graphene-like silicon nanoribbons on Ag(110): A possible formation of silicene. Appl. Phys. Lett. 96, 183102 (2010).
14. Chen, L. et al. Evidence for Dirac Fermions in a Honeycomb Lattice Based on Silicon. Phys. Rev. Lett. 109, 056804 (2012).
15. Padova, P. D. et al. Evidence of Dirac fermions in multilayer silicene. Appl. Phys. Lett. 102, 163106 (2013).
16. Bolle, A. et al. Enhancing the Oxidation of Silicon with Non-Reactive Encapsulation. Adv. Funct. Mater. 23, 4340–4344 (2013).
17. Feng, B. et al. Observation of Dirac cone warping and chirality effects in silicene. Acc. Chem. Res. 49, 9049–9054 (2013).
18. Chen, L., Feng, B. & Wu, K. Observation of a possible superconducting gap in silicene on Ag(111) surface. Appl. Phys. Lett. 102, 081602 (2013).
19. Avila, J. et al. Presence of gapped silicene-derived band in the prototypical $(3	imes3)$ silicene phase on Ag(111) surfaces. J. Phys.: Condens. Mat. 25, 262001 (2013).
20. Chen, L., Feng, B. & Wu, K. Observation of superconductivity in silicene. arXiv:1301.1431 (2013).
21. Lin, C.-L. et al. Structure of silicene grown on Ag(111). Appl. Phys. Express. 5, 045802 (2012).
22. Tchalal, M. R. et al. Formation of one-dimensional self-assembled silicon nanoribbons on Au (110)–(2×1). Appl. Phys. Lett. 102, 083107 (2013).
23. Meng, L. et al. Buckled Silicene Formation on Ir(111). Nano Lett. 13, 685–690 (2013).
24. Fleurence, A. et al. Experimental Evidence for Epitaxial Silicene on Diboride Thin Films. Phys. Rev. Lett. 108, 245501 (2012).
25. Friedlein, R., Fleurence, A., Sadowski, J. T. & Yamada-Takamura, Y. Tuning of silicene-substrate interactions with potassium adsorption. Appl. Phys. Lett. 102, 221603 (2013).
26. Kokott, S., Pfirgau, P., Matthies, L. & Rechtsteiner, F. Nonmetallic substrates for growth of silicene: an ab initio prediction. J. Phys.: Condens. Mat. 26, 185002 (2014).
27. Zhang, X. et al. Thermal conductivity of silicene calculated using an optimized Stillinger-Weber potential. Phys. Rev. B. 89, 054310 (2014).
28. Pan, L. et al. Thermoelectric properties of armchair and zigzag silicene nanoribbons. Phys. Chem. Chem. Phys. 14, 13588–13593 (2012).
29. Zberekci, K., Wierzbicki, M., Barna, J. & Swirko, R. Thermoelectric effects in silicene nanoribbons. Phys. Rev. B. 88, 115404 (2013).
30. Yang, K., Cahangirov, S., Cantareno, A., Rubio, A. & D’Agosta, R. Thermoelectric properties of atomically thin silicene and germanene nanomaterials. Phys. Rev. B. 89, 125403 (2014).
31. Xie, H., Hu, M. & Bao, H. Thermal conductivity of silicene from first-principles. Appl. Phys. Lett. 104, 131906 (2014).
32. Gu, X. & Yang, R. First-Principles Prediction of Phononic Thermal Conductivity of Silicene: a Comparison with Graphene. arXiv preprint arXiv:1406.2874 (2014).
33. Bickelhaupt, K. et al. Thermal conductivity of silicene nanosheets and the effect of isotopic doping. J. Phys.: D Appl. Phys. 47, 165301 (2014).
34. Mingo, N. & Brodini, D. A. Thermoelectric power factor of nanoporous semiconductors. J. Appl. Phys. 101, 014322 (2007).
35. Song, D. W. et al. Thermal conductivity of nanoporous bismuth thin films. Appl. Phys. Lett. 84, 1883–1885 (2004).
36. Lee, J.-H. & Grossman, J. C. Thermoelectric properties of nanoporous Ge. Appl. Phys. Lett. 95, 013106 (2009).
37. Hu, J., Ruan, X. & Chen, Y. P. Thermal Conductivity and Thermal Rectification in Graphene Nanoribbons: A Molecular Dynamics Study. Nano Lett. 9, 2730–2735 (2009).
42. Chang, P.-H. & Nikolic, B. K. Edge currents and nanopore arrays in zigzag and chiral graphene nanoribbons as a route toward high-ZT thermoelectrics. Phys. Rev. B. 86 (2012).
43. Mortazavi, B., Potschke, M. & Cuniberti, G. Multiscale modeling of thermal conductivity of polycrystalline graphene sheets. Nanoscale 6, 3344–3352 (2014).
44. Zhang, Y., Xu, G., Han, F., Wang, Z. & Ge, C. Preparation and Thermoelectric Properties of Nanoporous Bi2Te3-Based Alloys. J. Electron. Mater. 39, 1741–1745 (2010).
45. Lee, H. et al. Effects of nanoscale porosity on thermoelectric properties of SiGe. J. Appl. Phys. 107, 094308 (2010).
46. Lee, J.-H., Galli, G. A. & Grossman, J. C. Nanoporous Si as an Efficient Thermoelectric Material. Nano Lett. 8, 3750–3754 (2008).
47. Ding, Y. & Ni, J. Electronic structures of silicon nanoribbons. Appl. Phys. Lett. 95, 083115 (2009).
48. Song, Y. L., Zhang, Y., Zhang, J. M. & Lu, D. B. Effects of the edge shape and the width on the structural and electronic properties of silicene nanoribbons. Appl. Surf. Sci. 256, 6313–6317 (2010).
49. Ding, Y. & Wang, Y. Electronic structures of zigzag silicene nanoribbons with asymmetric sp2−sp3 edges. Appl. Phys. Lett. 102, 143115 (2013).
50. Ezawa, M. & Nagaosa, N. Interference of Topologically Protected Edge States in Silicene Nanoribbons. Phys. Rev. B 88, 121401(R) (2013).
51. Nakada, K., Fujita, M., Dresselhaus, G. & Dresselhaus, M. S. Edge state in graphene ribbons: Nanometer size effect and edge shape dependence. Phys. Rev. B. 54, 17954–17961 (1996).
52. Kobayashi, Y., Fukui, K.-t., Enoki, T., Kusakabe, K. & Kaburagi, Y. Observation of zigzag and armchair edges of graphite using scanning tunneling microscopy and spectroscopy. Phys. Rev. B. 71, 193406 (2005).
53. Núñez, Y. et al. Scanning tunneling microscopy and spectroscopy of the electronic local density of states of graphite surfaces near monoatomic step edges. Phys. Rev. B. 73, 085421 (2006).
54. Lahiri, J., Lin, Y., Bozkurt, P., Olevnik, I. I. & Batzill, M. An extended defect in graphene as a metallic wire. Nat. Nano. 5, 326–329 (2010).
55. Anderson, P., Lee, P. & Saitoh, M. Remarks on giant conductivity in TTF-TCNQ. Solid State Commun. 13, 595–598 (1973).
56. Soler, J. M. et al. The SIESTA method for ab initio order-N materials simulation. J. Phys.: Condens. Mat. 14, 2745 (2002).
57. Perdew, J. P., Burke, K. & Ernzerhof, M. Generalized Gradient Approximation Made Simple. Phys. Rev. Lett. 77, 3865–3868 (1996).
58. Berland, K. & Hyldgaard, P. Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. Phys. Rev. B. 89, 035412 (2014).
59. Ferrer, J. et al. GOLLUM: a next-generation simulation tool for electron, thermal and spin transport. New J Phys 16, 093029 (2014).

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H.S. and S.S. have performed the calculations. H.S. and C.J.L. conceived the idea and wrote the paper.

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