Tuning quantum electron and phonon transport in two-dimensional materials by strain engineering: a Green’s function based study†

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Novel two-dimensional (2D) materials show unusual physical properties which combined with strain engineering open up the possibility of new potential device applications in nanoelectronics. In particular, transport properties have been found to be very sensitive to applied strain. In the present work, using a density-functional based tight-binding (DFTB) method in combination with Green’s function (GF) approaches, we address the effect of strain engineering of the transport setup (contact–device(scattering)–contact regions) on the electron and phonon transport properties of two-dimensional materials, focusing on hexagonal boron-nitride (hBN), phosphorene, and MoS2 monolayers. Considering unstretched contact regions, we show that the electronic bandgap displays an anomalous behavior and the thermal conductance continuously decreases after increasing the strain level in the scattering region. However, when the whole system (contact and device regions) is homogeneously strained, the bandgap for hBN and MoS2 monolayers decreases, while for phosphorene it first increases and then tends to zero with larger strain levels. Additionally, the thermal conductance shows specific strain dependence for each of the studied 2D materials. These effects can be tuned by modifying the strain level in the stretched contact regions.

1 Introduction

A variety of fascinating phenomena in electron and thermal transport arise in materials when the length scales associated with their physical dimensions or intrinsic structure approach the nanoscale. Especially since the isolation and characterization of graphene,1 a broad variety of two-dimensional (2D) materials with similar honeycomb lattice structure have been synthesized;2 examples include hexagonal boron-nitride (hBN),3,4 phosphorene,5 silicene,6 as well as the family of transition-metal dichalcogenides (TMDs).7–9

Many of these 2D materials have high potential for nanoelectronics and energy applications.10,11 Therefore, it is of great interest to reveal how their physical properties can be tailored by varying various control parameters. This can include covalent or non-covalent chemistry,12,13 atomic doping,14 quantum confinement,15 and mechanical strain,16–18 among others. In particular, the influence of mechanical effects on the electrical and thermal conductivity in 2D materials has been addressed both experimentally8,19–24 and theoretically.25–38 In experiments, several straining techniques have been developed, but due to the challenge of manipulating nanoscale matter, only a few of them have already been proved to be feasible.16,18,39 For instance, Wang et al.,23 by employing in situ strained Raman spectroscopy, found that the influence of strain on the vibrational modes in few-layer black phosphorus is anisotropic. This effect was also recently observed by using a modified bending technique to apply uniaxial strain in ultrathin black phosphorus.40 A reduction of the band gap in single- and bilayer MoS2 has also been reported, induced by bending the flexible substrate in which they are supported24 and by considering cylindrical cavities.41 Strain-induced phonon softening has been observed in MoS224 and WS222 monolayers, which may alter their thermal behavior. However, more systematic experimental measurements of phonon transport properties in novel two-dimensional materials are still necessary.

From the modelling point of view, non-equilibrium molecular dynamics simulations have been widely used to study the influence of strain on the thermal conductivity of 2D materials,30,31,38

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revealing clear differences in their thermal response. While the thermal conductivity in silicene\(^{32}\) and hBN\(^{38}\) first increases with the tensile strain and then decreases, for other materials like graphene\(^{10}\) and MoS\(_2\)\(^{35}\) it decreases with increasing strain, similar to their bulk phase. It has also been shown, by employing first-principles calculations, that strain engineering can tune the electronic bandgap in nanomaterials such as few-layer phosphorene,\(^{25,26}\) MoS\(_2\) allotropes,\(^{19,42,43}\) hBN nanoribbons,\(^{28}\) and graphene/hBN hetero-bilayers.\(^{29}\) The thermal anisotropy in phosphorene has also been found to be strain dependent, increasing under uniaxial strain.\(^{27}\) Moreover, using non-equilibrium Green’s function techniques, it has been shown that tensile strain leads to a semiconducting-to-metal transition in single layer MoS\(_2\) for elongations of the order of 11\%,\(^{35}\) and to anomalous strain dependence of the thermal conductance in phosphorene.\(^{25}\)

There is, however, an issue that has not yet been considered in previous theoretical studies: the modelling of the effect of strain on the transport setup (contact-device(scattering)–contact regions) and its impact on charge (and phonon) transport. In this study, we provide a better understanding of how different ways of applying a strain do impact on the electronic and thermal response of three selected 2D materials: hBN, phosphorene, and MoS\(_2\) monolayers (see Fig. 1). For this, we combine a density functional tight-binding (DFTB) approach\(^{44}\) with Green’s function techniques\(^{45,46}\) to achieve both a realistic description of the electronic, structural, and vibrational properties of the materials and their quantum electrical and thermal response. Based on the partitioning scheme shown in Fig. 1(b), we have considered three possible theoretical setups, which may mimic different experimental ones: (I) the device region is strained while the contact regions are not, (II) both the device and contact regions have the same strain level (i.e., homogeneously strained system), and (III) the contact regions are stretched or compressed with respect to the device region. Here, the applied strain is defined as \(s[\%] = (L_s - L_0) \times 100/L_0,\) where \(L_s\) and \(L_0\) are the lattice constants of strained and unstrained monolayers (in the \(x\)-direction). Our results demonstrate that by engineering the strain level in the transport setup, several transport scenarios can be obtained, which can provide routes to optimizing the electrical and thermal response of these materials with potential implications e.g. for their thermoelectric behavior.

2 Computational methods

We compute the electron and phonon transport properties of the studied nanostructures using the Landauer approach, i.e. neglecting inelastic scattering effects. As a result, electron and phonon transport channels are treated independently and the key quantity to be computed is the corresponding transmission function for electrons \(\tau_{el}(E)\) and phonons \(\tau_{ph}(\omega)\).\(^{13,45–48}\) The common partitioning scheme for both electrons and phonons is used based on the division of the system into three regions, left and right contacts, and a device (scattering) region (see Fig. 1(b)). Here, we remark that the strain level in the contact regions will be modified depending on the transport setup under consideration, as explained before. Moreover, both the contact and the device regions are composed of the same material, so that we can directly focus on strain effects. All the calculations were performed using periodic boundary conditions in the \(y\)-direction, i.e. perpendicular to the transport direction. For each material, we have considered the same box length along the \(y\)-direction for all strain levels in the \(x\)-direction, which produces an extra force in the periodic direction after increasing the strain. The electron transmission coefficient \(\tau_{el}(E)\) is calculated as

\[
\tau_{el}(E) = \text{Trace}(G^rT_{el}G^aT_{el}),
\]

where

![Fig. 1](image-url) (a) Atomistic view of the studied two-dimensional materials: hexagonal boron-nitride, phosphorene, and molybdenum disulfide (MoS\(_2\)) monolayers. (b) Schematic representation of the partition scheme for transport calculation using the Green’s function technique. We also show the transport setups under consideration. For all the 2D materials, electron and phonon transport is along the zigzag direction (\(X\)-axis).
where the retarded Green’s function $G^r$ is obtained from the Hamiltonian $H$ and overlap $S$ matrices of the central region, $G^r = (ES - H - \Sigma^r_1 - \Sigma^r_2)^{-1}$, and the broadening function $I_{LR} = \frac{i}{2(\Sigma^r_1 - \Sigma^r_2)}$ with $\Sigma^r_1$ being the electrode self-energies. The electronic linear conductance is then immediately obtained as $G = (2\pi^2)/(h^2)\Gamma_E (E = E_F)$, with $E_F$ denoting the Fermi energy of the system considered as a variable.

The phonon transmission coefficient $\kappa_{ph}(\omega)$ is calculated using a similar expression as in eqn (1) by performing the substitution $H \rightarrow K$ and $ES \rightarrow \omega I$, where $I$ is a unit matrix and $K$ is the dynamical matrix.\textsuperscript{34,46,49} The thermal conductance is then computed as

$$\kappa_{ph} = \frac{1}{2\pi k_B T} \int_0^\infty (\hbar \omega)^2 \left(\frac{\epsilon^{\hbar \omega/k_B T}}{(\hbar \omega/k_B T - 1)}\right)^2 \kappa_{ph}(\omega) d\omega.$$ 

Here, $k_B$ and $\hbar$ are the Boltzmann and the Planck constants, respectively. This expression is obtained by a linear expansion in the applied temperature difference $\Delta T$ of the quantity $N_u(T + \Delta T) - N_u(T)$, where $N_u$ is the Bose–Einstein distribution. The thickness of the monolayers is taken to be 3.3 Å for hBN, 5.24 Å for phosphorene, and 6.09 Å for MoS$_2$. To gain additional insight into the influence of strain on the thermal transport properties, we have also defined the quantity

$$D_{i-j} = \text{Trace}[K_{ij}(K^T)_{ij}].$$

Here, the indices $ij$ denote neighboring atoms in the corresponding structure. The real number $D_{i-j}$ is obtained by using the $3 \times 3$ sub-matrix $K_{ij}$ associated with the force constants of atoms $i$ and $j$. $D_{i-j}$ thus gives information on the bond strength for each atomic pair $i-j$. In order to have a better understanding of the transport setups defined in this work, we compare our results with those corresponding to the standard model of uniaxial strain, i.e. not fixing the box length along the periodic direction ($y$-axis), which removes the imposed extra force.

In this work, both the electronic Hamiltonian matrix and the interatomic force constants are obtained using the DFTB method as implemented in the DFTB+ software package.\textsuperscript{14} The DFTB method is based on density-functional based parametrization of a general tight-binding Hamiltonian. Hereby, the system eigenstates are expanded into a minimal valence basis set of linear combination of atomic orbitals (LCAO), which are determined from self-consistent atomic LDA calculations. Additionally, the effective Kohn–Sham potential is approximated as a superposition of localized potentials of neutral atoms.\textsuperscript{50} This method has been already successfully applied for studying the physical properties of two-dimensional materials and has been found to provide a good quantitative agreement with experimental data and other higher-level theoretical methods.\textsuperscript{13,48,51–54} Here, all the crystal structures have been optimized by using the conjugate gradient method with a force-threshold criterion of $10^{-4}$ Hartree per Bohr radius.

### 3 Results and discussion

#### 3.1 Structural properties

Since the structural changes in the materials upon applying a strain are strongly correlated with modifications of the molecular orbital overlap and vibrational spectrum, and hence with the electron and thermal transport properties, we first address the strain dependence of the nearest-neighbor (first and second) bonds (see Fig. 2). The bond lengths for the unstrained systems found after energy minimization are as follows: hBN: $A_1 = A_2 = 1.48 \text{ Å}$, P: $B_1 = 2.334 \text{ Å}$, $B_2 = 2.328 \text{ Å}$, and MoS$_2$: $C_1 = C_2 = 2.50 \text{ Å}$. These values are close to those obtained from full DFT calculations.\textsuperscript{25,55,56} In Fig. 2, it can be seen that bonds along the transport direction are strongly influenced by the applied strain with the exception of $C_1$ due to the more compact structure of the MoS$_2$ monolayer. Concerning the $A_2$, $B_2$, and $C_2$ bonds, we have found that their behavior under an applied strain depends on the number of atomic layers. Thus, the $A_2$ bond slightly increases in magnitude, but after 6% of strain it starts to decrease again. In contrast, for the other 2D materials composed of more than one atomic layer, the influence of strain on the bonds is quite different: the $B_2$ and $C_2$ bonds monotonically decrease and increase, respectively. This effect mainly occurs for periodic boundary conditions.

![Fig. 2](image-url) Bond lengths at first and second neighbors as a function of the applied strain for (a and d) hexagonal boron-nitride, (b and e) phosphorene, and (c and f) MoS$_2$ monolayers, respectively. Here, the population of each bond has been analyzed by separating first and second neighbors and it is shown in all the graphs. These results correspond to homogeneously strained materials, setup II.
(extra force) and the corresponding reduction of the interlayer distance after stretching the material. It disappears, though, by applying standard uniaxial strain, as shown in the ESL.\textsuperscript{†}

Moreover, when the bond analysis goes to second neighbors (see Fig. 2(d)–(f)), the B–B (AA\textsubscript{1,2}), N–N (AA), and Mo–Mo (CC\textsubscript{1,2}) bonds generate planar isosceles triangles whose size uniformly increases with the strain. In addition, because of the number of atomic layers, P–P and S–S bonds also display an extra bond between atoms located at different layers, which slightly increases for P–P (BB\textsubscript{2}) bonds and decreases for S–S (CC\textsubscript{5}) bonds upon increasing the strain. In summary, we see that bond lengths in phosphorene and MoS\textsubscript{2} monolayers display non-monotonous strain dependence, while those for hBN are uniformly stretched.

### 3.2 Electron and phonon behavior

We now address quantum electron and phonon transport within the different setups described in the introduction and summarize the results in Fig. 3 and 4. Unstrained systems display a bandgap \( E_{\text{gap}} \) close to that reported by performing full DFT calculations:

\[
E_{\text{gap}}(\text{hBN}) = 3.44 \text{ eV},
\]

\[
E_{\text{gap}}(\text{phosphorene}) = 1.94 \text{ eV},
\]

\[
E_{\text{gap}}(\text{MoS}_2) = 1.36 \text{ eV}.
\]

The strain dependence of the bandgap is illustrated in Fig. 4, where the corresponding \( E_{\text{gap}} \) values for each applied strain were drawn from the corresponding transmission spectrum (transport gap). For hBN we found that the interface between contact and device regions strongly influences the electronic bands for energies larger than 10.0 eV but not for bands near the Fermi level (see Fig. 3(a)). As a consequence, the bandgap remains almost constant when unstretched contact regions are considered (setup I) and slightly reduces for stretched ones (setup II), e.g. up to 3.12 eV at 13.6% of strain. Qi \textit{et al.}\textsuperscript{28} have also observed this slight change of the bandgap for hBN by analyzing the influence of uniaxial strain on its electronic band structure computed at the DFT level. Moreover, we find a shift towards the Fermi level in the transmission peaks corresponding to energies \( E > 10.0 \text{ eV} \). This result clearly differs from that obtained for setup I, where the transmission channels for those energies are suppressed after increasing strain.

Unlike hBN, for phosphorene the applied strain mainly affects transmission channels around the Fermi level (see Fig. 3(b)). For setup I, these channels are suppressed with increasing strain and, hence, the electronic bandgap increases, whereas, when considering setup II, a small increase in the bandgap for weak strain is found, \( E_{\text{gap}} = 2.16 \text{ eV} \) at 2.2% of strain. Further increasing the strain reduces again the gap to values of 0.95 eV at 16.1% of strain. A similar effect has been theoretically reported for strained phosphorene.\textsuperscript{26,59,60} In the case of MoS\textsubscript{2} monolayer, we have obtained a reduction of the bandgap for the two setups. However, for setup I, \( E_{\text{gap}} \) becomes constant after 7.5% of strain, while for setup II the band edges move towards the Fermi level and the bandgap is almost suppressed at 13.8% of strain (\( E_{\text{gap}} \approx 0.02 \text{ eV} \)) leading to a semiconductor-to-metal transition.\textsuperscript{56} It is worth mentioning that this transition was also theoretically reported to happen after 11% of strain in single-layer MoS\textsubscript{2} and WS\textsubscript{2} by applying isotropic tensile strain.\textsuperscript{35} Similar to phosphorene, as a result of having a homogeneously

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**Fig. 3** Electron transmission function for (a) hexagonal boron-nitride, (b) phosphorene, and (c) MoS\textsubscript{2} monolayers at different strain levels. We have overlapped the results for setup I (○ – red lines) and setup II (solid blue lines). Each graph has its corresponding strain value.

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**Fig. 4** Strain dependence of the electronic bandgap in two-dimensional materials considering setup I (○ – blue lines) and setup II (□ – red lines) for transport calculation. For comparison, we also plot the results for the standard uniaxial strain (○ – dashed lines).
strained system (contact and device regions), we have new transport channels with high transmission probability around the Fermi level.

In order to investigate the nature of the behavior of the bandgap in these two-dimensional materials, we compute the projected electronic density of states (PDOS) on individual atomic shells. In Fig. 5, we show the results by considering setup II. Here, one can see that the valence band edge of hBN is mostly composed of p-orbitals of nitrogen, while the conduction band edge is composed of p-orbitals of boron. s-Orbitals lie farther down in energy and do not play a relevant role in electron transport. Moreover, we have found that the population of states on the band edges increases with the strain and, hence, the bandgap slowly decreases. In phosphorene, the p-orbitals are also mediating electron transport. Their contributions dominate both valence and conduction bands, after increasing the strain (see Fig. 5(e) and (f)). However, unlike hBN, for a low strain level of 2.2%, PDOS on the band edges rearranges yielding a small increase in the bandgap, as shown in Fig. 4. In the MoS2 monolayer, the molybdenum d-states show the highest peaks on the electronic DOS around the Fermi level whilst the corresponding sulfur p-orbitals are predominant for energies E < −2.0 eV. In Fig. 5(i), we see that these peaks broaden and move towards the Fermi level under the influence of the strain, i.e., the bandgap is reduced. For setup I, the transport properties are dominated by the electronic properties of the contact region from where electrons are coming. Thus, it is expected that the bandgap remains unchanged regardless of the strain values, as it was found for the hBN monolayer. Nevertheless, because of the extra atomic layers in phosphorene and MoS2 that generate a different interface, some changes in the bandgap have been obtained. Despite having differences in the strain dependence in some bond lengths, we found that the electronic bandgap for homogeneously strained materials (setup II) shows a similar behavior as a function of the applied strain by considering the standard model of uniaxial strain (see ESI†). There are, however, quantitative differences due to the extra force along the y-direction produced by imposing periodic boundary conditions. In fact, besides modulating the electronic bandgap, it is also possible to control the electron transmission in these materials by imposing additional conditions during the transport measurement (e.g. biaxial strain).

The thermal transport properties also depend on the transport setup (see Fig. 6). Here, to have a better comparison with other works, we have considered a length of 100 nm to convert thermal conductance units [in units of W K−1] into thermal conductivity [in units of W m K−1]. Among the three studied two-dimensional materials, the hBN monolayer displays the highest thermal conductance kph at 300 K (∼310 W m K−1), followed by phosphorene (∼90 W m K−1). These values are close to those reported in
other experimental and theoretical works.9,27,34,38,61,62 On the other hand, regarding the bond strength, measured by the $D_{ij}$ parameter introduced in eqn (3), phosphorene shows the weakest bonds and hBN the strongest ones (see Fig. 7), a result related to their difference in Young’s modulus.63 Based on the strain dependence of bond lengths in the hBN monolayer (see Fig. 2(a) and (d)), it is expected that with the exception of the A$_2$ bond, the strength of the first and second neighbor bonds will decrease after increasing the strain (see Fig. 7(a) and (d)). Hence, the components of the dynamical matrix associated to these bonds (the strongest ones) become smaller and, then, the thermal conductance continuously decreases with increased applied strain, as can be seen in Fig. 6(a). This reduction of $\kappa_{ph}$ is higher for setup I because of the presence of an additional interface resistance between contact and device regions, which strongly blocks phonon transfer at higher frequencies, > 800 cm$^{-1}$ (see ESI†). It is worth noting that by considering setup II, the behavior of $\kappa_{ph}$ at room temperature (300 K) is in agreement with that reported by Zhu and Ertekin38 using non-equilibrium molecular dynamics and Boltzmann transport equation methods. This effect has been also observed in other one-atom thick layers by performing a self-consistent study of the linearized Boltzmann–Peierls equation for phonon transport.27

In the case of phosphorene and MoS$_2$ monolayers the influence of the strain is qualitatively different due to the presence of additional transport channels related to high frequency out-of-plane modes, which have their origin in the additional atomic layers (see ESI†). The thermal conductance in phosphorene monotonously decreases (setup I) and increases (setup II) with the strain (see Fig. 6). An increase in strain reduces the interlayer distance and, hence, the strength of the B$_2$ bonds increases, becoming higher than that of the B$_1$ bond (see Fig. 7(b)). As a result of this, the transmission probability increases at low frequencies (see ESI†) and so does the thermal transport. Z.-Y. Ong et al.,34 using NEGF-DFT techniques, also showed this effect in phosphorene at smaller uniaxial strain levels. For the MoS$_2$ monolayer, we found that despite the relatively small change of C$_1$ and C$_2$ bonds ($\sim 10^{-2}$ Å), the $D$ parameter considerably increases with the strain (see Fig. 7(c)). This sensitivity to the strain level is more pronounced for C$_1$ and CC$_5$ bonds (related to the S–S interlayer bond) which increase their initial $D$ value 8 times at 13.8% of strain as shown in Fig. 7(c) and (f), being the strongest bonds among the first and second neighbors. Therefore, the range of transmitting frequencies and the vibrational band gap increase and, after $\sim 7.3\%$ of strain, new transmission peaks emerge at the edge of the acoustic branch. Thus, the thermal conductance decreases for low strain levels and then it increases reaching values close to the initial values at zero strain independently of the temperature, as displayed in Fig. 6(c). We note that in the case of unstrained contact regions, the thermal conductance decreases with increasing strain level because of the continuous suppression of high frequency transmission channels.

In-plane and out-of-plane mode contributions to the thermal conductance have also been computed to gain further insight into
the phonon transport properties (see Fig. 8). We have found that mostly in-plane modes are responsible for thermal transport in homogeneously strained hBN and phosphorene monolayers (setup II). However, in-plane mode contribution to $\kappa_{\text{ph}}$ is, as expected, strongly affected by imposing an extra interface between contact and device regions (setup I). Consequently, the total thermal conductance will be reduced as shown in Fig. 6. For MoS$_2$ (see the right panel in Fig. 8), the situation is different: the contributions of in-plane and out-of-plane modes to $\kappa_{\text{ph}}$ are quite similar due to the large overlap in their associated frequencies (see Fig. S6 in the ESI†). In fact, in homogeneous strained MoS$_2$ systems, both contributions monotonically increase up to a strain level of $\sim 9.0\%$ and then they start to decrease. As a consequence, the total $\kappa_{\text{ph}}$ changes its trend and slightly increases. This effect is strong at high temperatures. Similar to the electron transport properties, the strain dependence of the thermal conductance, considering setup II, for hexagonal boron-nitride and phosphorene is similar to that obtained by employing the standard model for uniaxial strain (see dashed lines in Fig. 6 and 8). However, for the MoS$_2$ monolayer, we found that, besides the effect on the transmission function observed with setup II, by applying uniaxial strains we obtain an increase of the transmission probability at low frequencies and, hence, $\kappa_{\text{ph}}$ will only increase. By imposing the extra force in the periodic direction ($y$-direction), we block transport channels corresponding to low frequencies which strongly influence the conduction through out-of-plane modes, as can be seen in Fig. 8.

Finally, we have considered a third transport setup that may be realized in specific experiments, where the contact regions are slightly stretched or compressed with respect to the strained device region (setup III, see Fig. 9(a)). The difference between strain levels is controlled by the variable $\Delta s[\%] = (L_{\text{cont}} - L_{\text{dev}}) \times 100/L_{\text{dev}}$. In Fig. 9, we show that, independently of the material, the electron transmission function is altered by engineering the strain in the contact regions. However, for hBN this effect is stronger for $E > 10.0$ eV, as expected from the previous discussion. We have also found that the bandgap of these two-dimensional materials increases for $\Delta s < 0$ and decreases for $\Delta s > 0$. This is related to the strain dependence of the electronic bandgap shown in Fig. 4. Thermal transport properties are more sensitive than electron properties to slight changes of the strain level in the contact regions. We thus find that the thermal conductance is reduced at any value of $\Delta s$, independent of whether the contact regions are stretched or compressed. This effect is a result of the extra interface between contact and device regions which introduces an additional scattering mechanism.

4 Conclusions

In conclusion, we have performed a GF-DFTB study of the effect of strain engineering of the transport setup (contact–device(scattering)–contact regions) on the quantum electron and phonon transport properties of hBN, phosphorene, and MoS$_2$ monolayers. We clearly demonstrated that the transport setup plays an important role in the control of the electronic bandgap (transmission channels) and the thermal conductance of the systems. Moreover, its influence becomes more dominant when materials with a larger number of atomic layers are considered; thus, both the electronic bandgap and thermal conductance of phosphorene increase by using unstretched and strained contact regions. Our results for homogeneously strained systems (setup II), with the exception of $\kappa_{\text{ph}}$ for the MoS$_2$ monolayer, are only quantitatively different from those corresponding to the standard model of uniaxial strain. Thus, strain engineering of the transport setup opens up the possibility of controlling transport properties by suggesting specific configurations to the experiments. It remains an open issue how the applied strain would affect the transport properties of heterostructures built of 2D materials, where the contact regions are more difficult to create. Our results clearly demonstrate that strain engineering can be efficiently exploited as an additional physical variable to control the electrical and thermal response of various 2D nanostructures.

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