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SUPPLEMENTARY INFORMATION

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

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1 Comparing with results for uniaxial strain

As it was mentioned in the main text, in this study, we have considered special periodic boundary conditions to be only focused on the strain influence in the contacts for quantum transport properties in two-dimensional materials. However, we have also compared our results with those obtained by considering the standard model for uniaxial strain, i.e., relaxing the cell parameters in the periodic direction (Y-axis, opposite to the transport direction) in order to get ride of extra forces.

We show the results of the strain dependence of bond lengths and their corresponding D parameter for hBN, phosphorene, and MoS_2 monolayer in Fig. S1 and Fig. S2, respectively. Electron transmission functions are also plotted in Fig. S3. The projected electronic density of states (EDOS) on individual atomic shells and its variation with the applied unixial strain are shown in Fig. S4. In Fig. S5, we compared the variation with the strain of the phonon transmission functions obtained by considering setup I, setup II, and unixial strain.

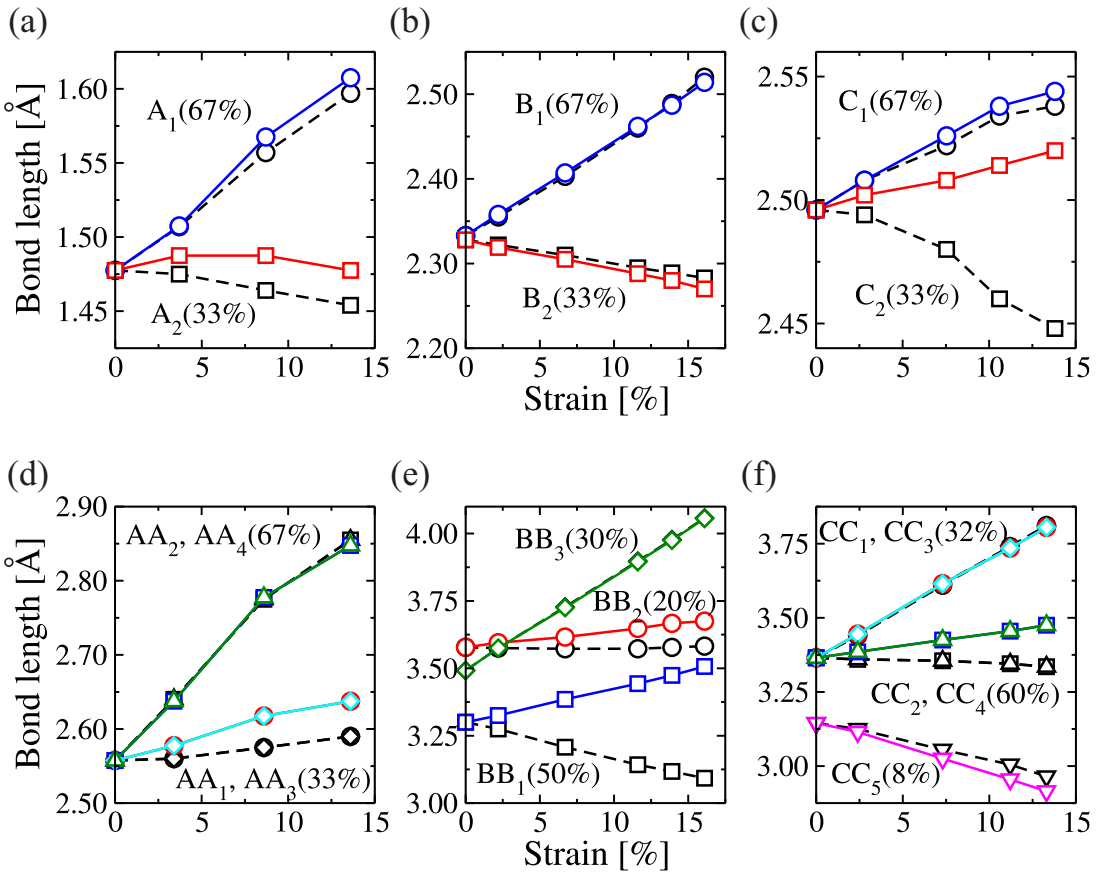

Figure S 1 Bond length at first and second neighbors as a function of the applied strain for (a, d) hexagonal boron-nitride, (b, e) phosphorene, and (c, f) MoS_2 monolayer, respectively. Here, the population of each bond has been analyzed by separating first and second neighbors and it is shown in all the graphs. We compare the results correspond to homogeneously strained materials by considering setup II (solid lines, different color) and the standard uniaxial strain (dashed lines, black color).

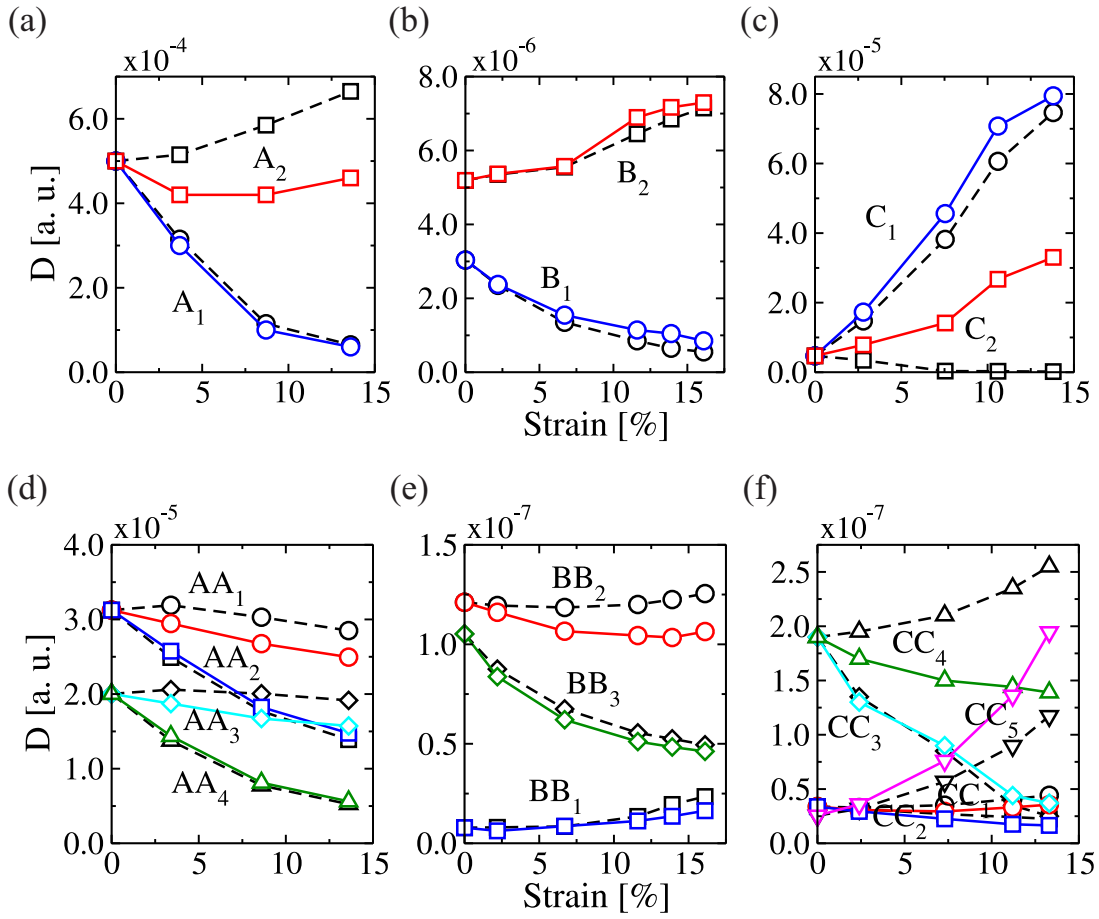

Figure S 2 *D* parameter as a function of the applied strain for (a, d) hexagonal boron-nitride, (b, e) phosphorene, and (c, f) MoS_2 monolayer, respectively. The population of the each bond is the same as presented in Fig. S1. In the graph (f), *D* values for CC_5 has been reduced by a factor of 20. We compare the results correspond to homogeneously strained materials by considering setup II (solid lines, different color) and the standard uniaxial strain (dashed lines, black color).

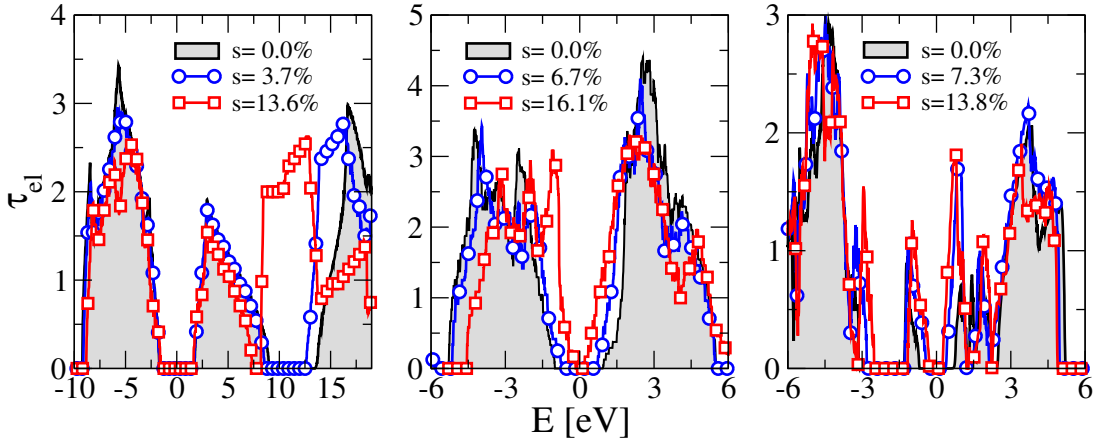

Figure S 3 Variation of the electronic transmission function with the uniaxial strain for hexagonal boron-nitride (left panel), phosphorene (center panel), and MoS_2 monolayer (right panel).

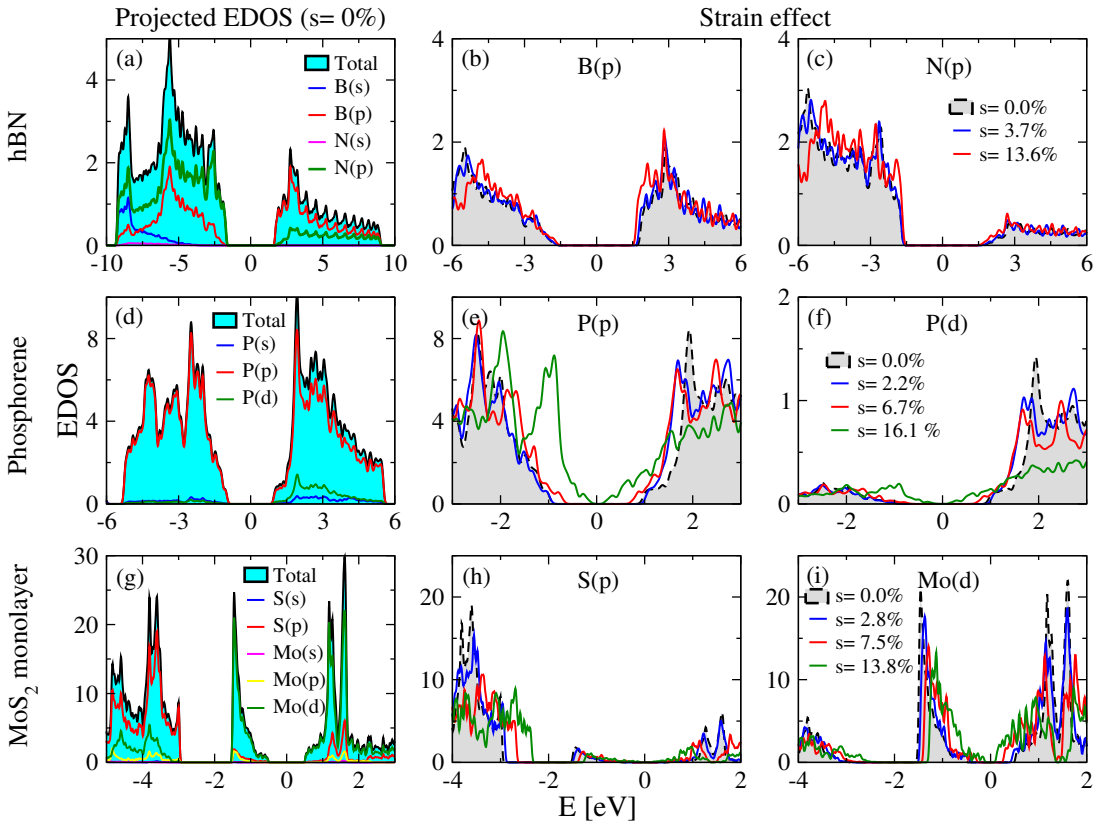

Figure S 4 Projected electronic density of states (EDOS) on individual atomic shells for unstrained (a) hBN, (d) phosphorene, and (g) MoS_2 monolayer. Contributions to the EDOS of the most relevant orbitals for the electron transport properties at different strain levels for hBN ((b) and (c)), phosphorene ((e) and (f)), and MoS_2 monolayer ((h) and (i)). These results correspond to homogeneously strained materials by considering the standard uniaxial strain.

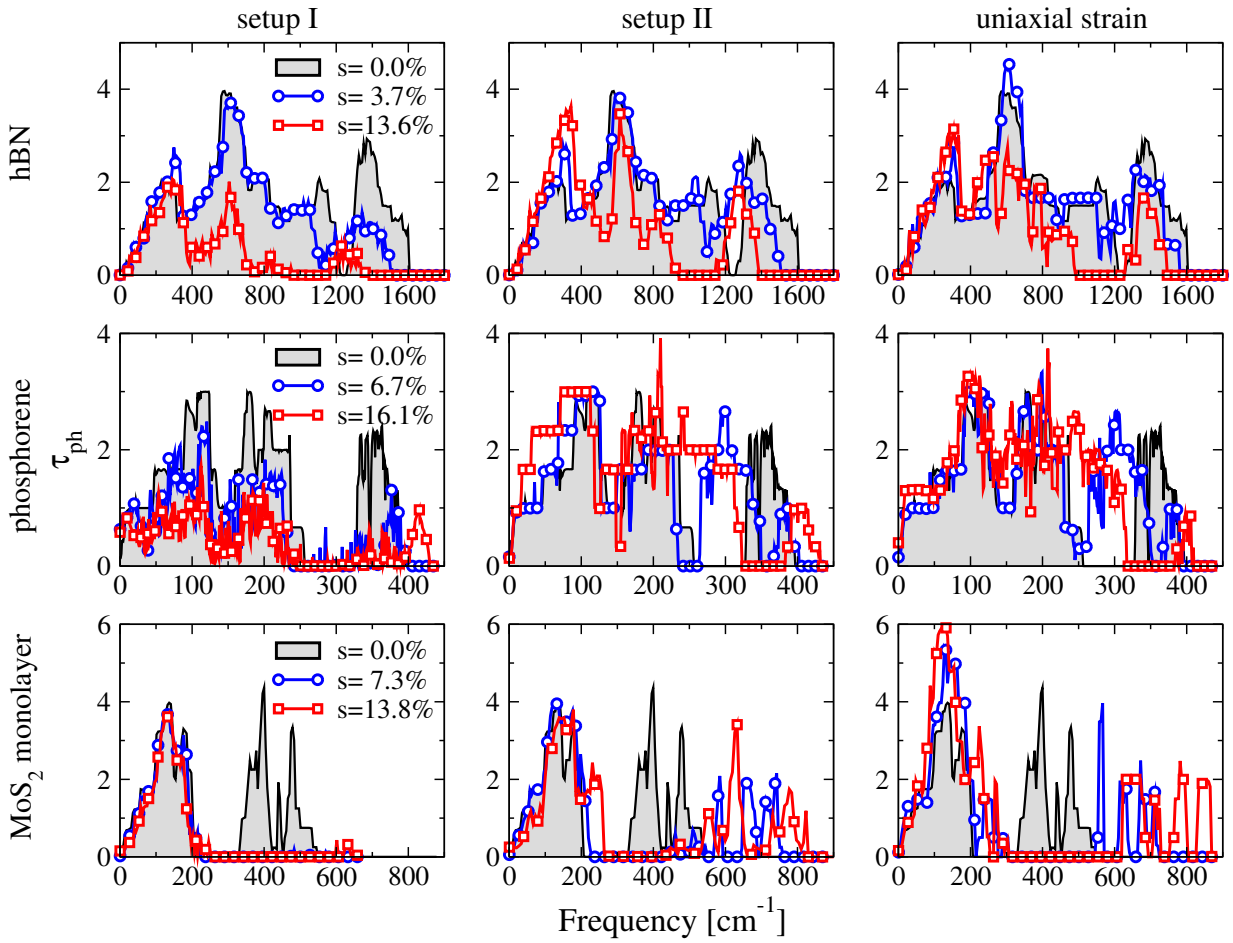

Figure S 5 Phonon transmission function for hexagonal boron-nitride, phosphorene, and MoS_2 monolayer by considering setup I, setup II, and the standard model for uniaxial strain.

2 In-plane and out-of-plane mode contribution to $\tau_{ph}(\omega)$

The mathematical definition of the dynamical matrix is,

$$\mathbf{K} = \{K_{i,j}\} = \frac{1}{\sqrt{M_i M_j}} \begin{cases} -\dfrac{\partial^2 U}{\partial u_i \partial u_j} & \text{if} \quad i \neq j \\ -\sum_{q \neq j} \dfrac{\partial^2 U}{\partial u_j \partial u_q} & \text{if} \quad i = j \end{cases}, \tag{1}$$

where u_i and u_j refer to any two atomic vibrational degree of freedom (i.e., displacements). U represents the total interactomic potential. M_i and M_j are atomic masses associated with the atoms i and j, respectively. Thus, the tensor of the dynamical matrix corresponding to atoms i and j can be calculated according the following expression,

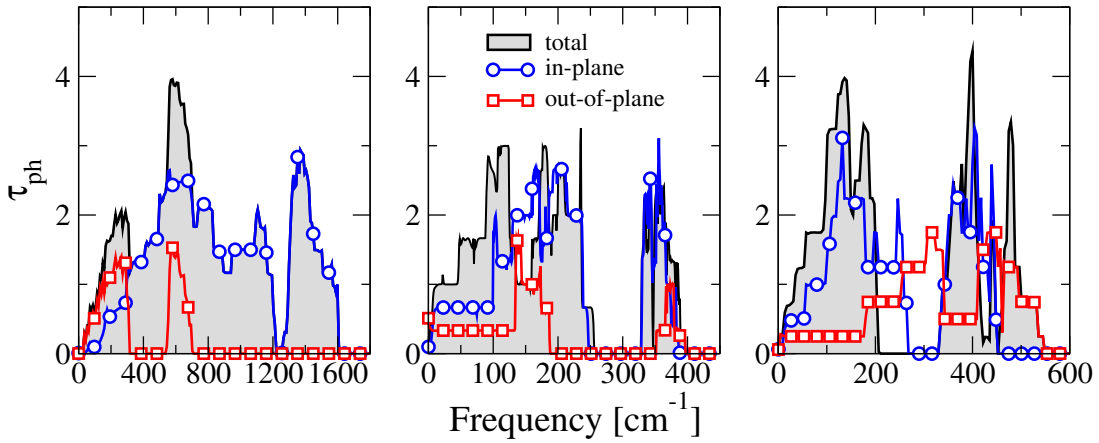

Figure S 6 Contribution of in-plane and out-of-plane vibrational modes to the phonon transmission function for hexagonal boron-nitride (left panel), phosphorene (center panel), and MoS_2 monolayer (right panel).

$$K_{i,j} = \frac{1}{\sqrt{M_i M_j}} \begin{vmatrix} \frac{\partial^2 U}{\partial u_{x,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{x,i} \partial u_{y,j}} & \frac{\partial^2 U}{\partial u_{x,i} \partial u_{z,j}} \\ \frac{\partial^2 U}{\partial u_{y,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{y,i} \partial u_{y,j}} & \frac{\partial^2 U}{\partial u_{y,i} \partial u_{z,j}} \\ \frac{\partial^2 U}{\partial u_{z,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{z,i} \partial u_{y,j}} & \frac{\partial^2 U}{\partial u_{z,i} \partial u_{z,j}} \end{vmatrix}. \tag{2}$$

To know the contribution of in-plane and out-of-plane modes to the phonon transmission function, $\tau_{ph}(\omega)$, we have considered the following changes in the definition of the tensor $K_{i,j}$:

- For in-plane modes, the tensor $K_{i,j}$ associated to the atoms i and j is redefined as,

$$K_{i,j} = \frac{1}{\sqrt{M_i M_j}} \begin{vmatrix} \frac{\partial^2 U}{\partial u_{x,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{x,i} \partial u_{y,j}} & 0 \\ \frac{\partial^2 U}{\partial u_{y,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{y,i} \partial u_{y,j}} & 0 \\ 0 & 0 & 0 \end{vmatrix}. \tag{3}$$

- For out-of-plane modes, the tensor $K_{i,j}$ associated to the atoms i and j is redefined as,

$$K_{i,j} = \frac{1}{\sqrt{M_i M_j}} \begin{vmatrix} 0 & 0 & \frac{\partial^2 U}{\partial u_{x,i} \partial u_{z,j}} \\ 0 & 0 & \frac{\partial^2 U}{\partial u_{y,i} \partial u_{z,j}} \\ \frac{\partial^2 U}{\partial u_{z,i} \partial u_{x,j}} & \frac{\partial^2 U}{\partial u_{z,i} \partial u_{y,j}} & \frac{\partial^2 U}{\partial u_{z,i} \partial u_{z,j}} \end{vmatrix}. \tag{4}$$

Then, those contributions were computed for hBN, phosphorene, and MoS_2 monolayer by employing Green's function technique and the results are shown in Fig. S6.