Supporting Information for A Thermal Switch for Coherent Phonons Based on a Molecular Junction

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Thermal conductances of the molecular junction with armchair contacts

In Figure 1(a) and Figure 2 we plot the phonon transmission and the electrical conductance of (E)-stilbene and (Z)-stilbene sandwiched between two armchair GNR contacts. Similarly to what discussed in the main article in the case of zigzag contacts, Figures 1(b,c) display the transmission between individual phonon channels in the left and right contact, where black indicates full reflection and light yellow/light red indicates full transmission.

Thermoelectric figure of merit

The thermoelectric figure of merit can be calculated as,

$$ZT = \frac{S^2 G^e T}{G^{ph} + \kappa^e}, \tag{1}$$

where S is the Seebeck coefficient, G^e is the electronic conductance, T is the temperature, and G^{ph} and κ^e are the thermal conductance due to phonons and electrons, respectively. G^e and G^{ph} are calculated as indicated in Eqs. (1) and (2) of the manuscript, whereas S and κ^e are calculated from the electron transmission function (Eq. (3) of the manuscript) as follows,[1,2]

$$S(\mu) = \frac{1}{e\,T}\frac{L_1(\mu)}{L_0(\mu)}, \tag{2}$$

$$\kappa^e(\mu) = \frac{1}{T}\left\{L_2(\mu) - \frac{L_1(\mu)^2}{L_0(\mu)}\right\}, \tag{3}$$

where the functions $L_m(\mu)$ are defined as,

$$L_m(\mu) = \frac{2}{h}\int_{-\infty}^{\infty} \mathcal{T}(E)(E-\mu)^m \left(-\frac{\partial f_0(E,\mu)}{\partial E}\right) dE. \tag{4}$$

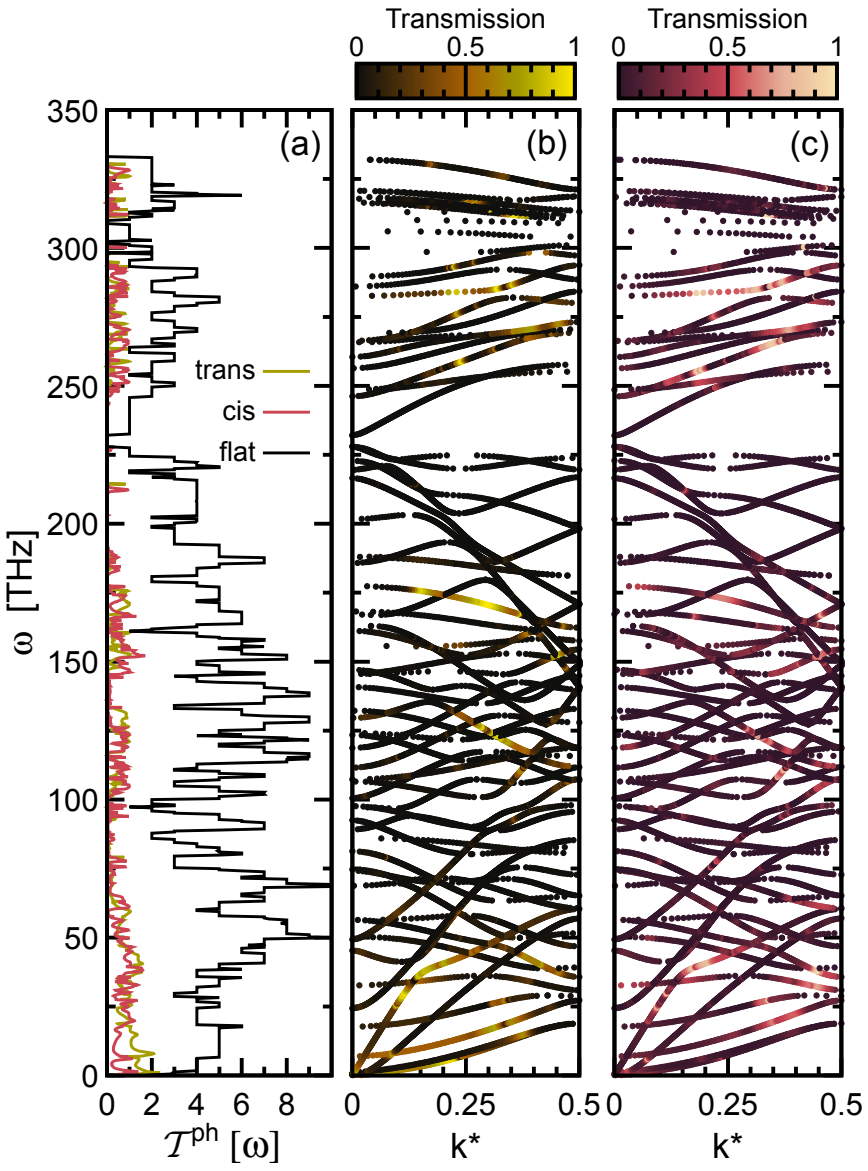

Figure 1: (a) $\mathcal{T}^{ph}(\omega)$ for a molecular junction featuring a (E)-stilbene (yellow curve) and a (Z)-stilbene molecule (red curve) with armchair GNR contacts. The transmission for a pristine, continuous armchair GNR is also shown for comparison (black curve). (b) Single-mode analysis for the (E)-stilbene and (c) for the (Z)-stilbene molecular junction.

The thermoelectric figure of merit and the electronic transport coefficients are shown in Figure 3 for the *trans*- and *cis*-stilbene molecular junctions and for a pristine graphene nanoribbon. Left and right panels show, respectively, the results for zigzag and armchair terminated nanoribbons. As it can bee seen, ZT is increased by the inclusion of the molecular junction over all considered chemical potentials in the case of the zigzag nanoribbon and

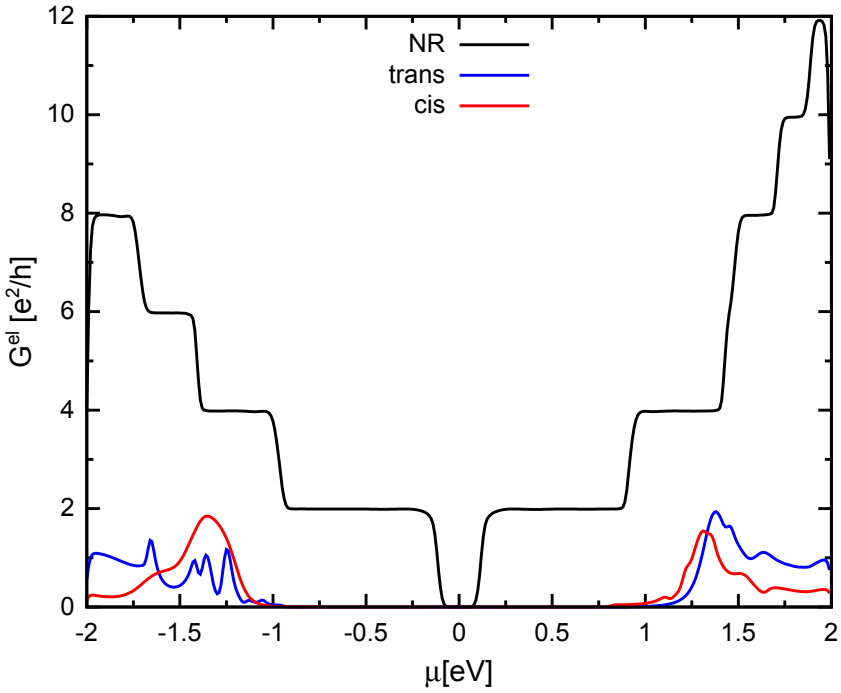

Figure 2: $G^{el}(e)$ at $T = 100$ K for an armchair GNR with a nanogap bridged by a (E)-stilbene (blue curve) and a (Z)-stilbene molecule (red curve). The conductance for a pristine, continuous armchair GNR is also shown for comparison (black curve).

for $|\mu| > 0.25$ eV in the armchair one. This effect is driven by the increase in the Seebeck coefficient since the reduction of electronic and thermal conductances as a consequence of the molecular junction are of the same order, thereby compensating each other. Notice that the large values attained by the Seebeck coefficient could result in phonon self-heating driven by electron-phonon interactions.[3,4] Although this effect can influence thermal conduction in the system, its study is beyond the scope of the ballistic framework used in this study. Regarding *trans*/*cis* isomerism effect, it is observed that depending on the chemical potential both type of junctions can lead to higher ZT values, in line with the trend discussed for the electronic conductance in the manuscript.

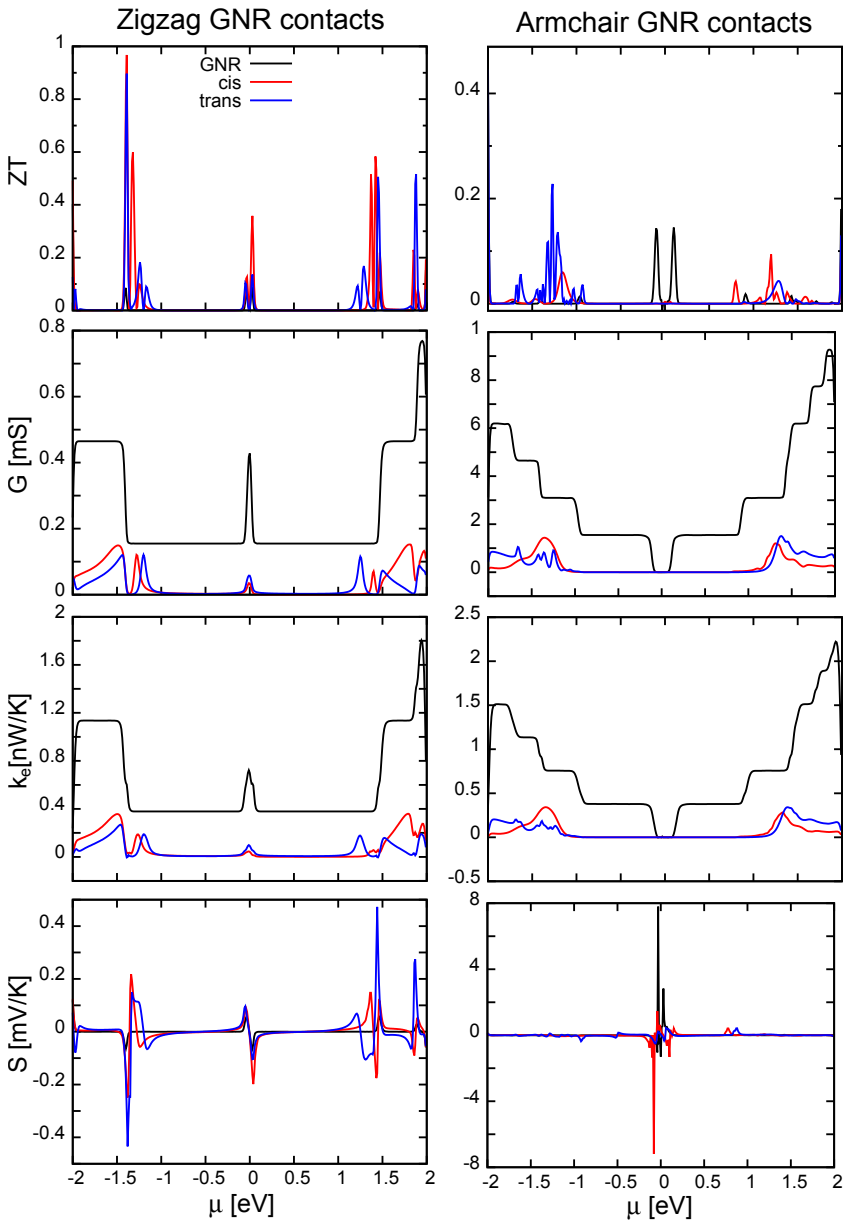

Figure 3: Thermoelectric coefficients for a pristine graphene nanoribbon (black lines) and a *trans*- (blue lines) and *cis*-stilbene (red lines) molecular junction. Left (right) column panels show results for a zigzag (armchair) nanoribbon.

References

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