Thermoelectric Properties of Functionalized Graphene Grain Boundaries

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Abstract

Thermoelectric effect enables direct conversion between thermal and electrical energy and provides an alternative route for power generation and refrigeration. Hereby it is important to find materials with a high thermoelectric performance. In this sense, in the present work, we study the behavior of the thermoelectric properties of functionalized graphene grain boundaries by employing non-equilibrium Green’s Functions formalism combined with density functional tight-binding theory (NEGF-DFTB) approach. Our results show that H and O ad-atoms affect the phonon and electron transport properties of the grain boundaries but the thermoelectric figure of merit is slightly reduced. However, grain boundaries functionalized with nitrophenyl molecules improve the thermoelectric behavior. We have also found that physisorbed molecules do not alter their transport properties. We expect our results to shed light on the potential of 2D materials for engineering highly efficient nanoscale thermoelectric devices.

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1 Introduction

Thermoelectric (TE) materials as one key ingredient for sustainable and clean energy solutions have attracted increasing interest since the world’s demand for energy rapidly increase as in parallel fossil fuel supplies decrease. The ability of a TE material to convert heat into electricity is measured by the dimensionless thermoelectric figure of merit, $ZT$, defined as:

$$ZT = \frac{GS^2T}{\sigma_{ph} + \sigma_{el}}.$$  \hspace{1cm} (1)

Here, $G$ is the electronic conductance, $S$ is the Seebeck coefficient, $T$ is the absolute temperature, $\sigma_{el(ph)}$ is the electronic (phonon) thermal conductance, and $GS^2$ is usually defined as the power factor. The larger $ZT$ is, the better is the performance of a TE material [1]. So a promising TE material should simultaneously have a high power factor and low thermal conductance. In other words, one would like to ideally achieve an electron crystal and a phonon glass. In order for TE materials to become competitive with conventional refrigerators and generators, a large increase of $ZT$ is imperative. Traditional efforts to increase $ZT$ have been directed toward selective reduction of the phonon thermal conductance $\sigma_{ph}$, using either complex bulk materials (through disorder in the unit cell) or bulk nanostructured materials, while at the same time maintaining as optimal as possible the electronic properties encoded in the power factor $S^2G$. However, it is found that optimizing $ZT$ is a big challenge due to the strong interdependence among $G$, $S$, $\sigma_{el}$, and $\sigma_{ph}$: changing one often adversely alter the others. Fortunately, recent progress in nanofabrication technologies has helped to demonstrate that nanostructure materials can dramatically enhance $ZT$ due to a suppression of the thermal conductance caused e.g. by boundary scattering, while increasing the power factor by quantum confinement effects [2–4].

Since its discovery in 2004, graphene, $sp^2$-bonded carbon atoms arranged in a two-dimensional (2D) honeycomb lattice, has been at the focus of major research efforts due to its versatile electronic, mechanical and thermal properties which may lead to applications in a broad variety of fields [5, 6]. Large-area graphene sheets required by technology can be obtained by several
scalable production routes such as epitaxial growth on the SiC substrate and chemical vapor deposition (CVD) on metal surfaces [7]. However, similar to many other macroscopic materials, graphene exists in polycrystalline structures. In typical polycrystalline graphene, two 2D domains are separated by a 1D topological defect called grain boundary (GB), an intrinsic topological defect of polycrystalline materials [8]. For polycrystalline graphene grown in the laboratory, synthesis has been shown to produce interfaces with meandering structures comprised of pentagons, heptagons, and nonagons [9–11]. Intensive studies have been carried out to study the properties of GBs because of the relevance for the development of graphene-based nanoelectronics. By analyzing the symmetry between the Brillouin zones on the two sides of the GB, a theoretical approach was developed to predict the electronic transport properties through GBs, indicating that symmetric GBs have zero transport gap, but asymmetric GBs have finite gaps. In fact, Yazyev et al. showed that the electronic structure of GBs can range from metallic to semiconducting with a considerable transport gap [9]. It has also been found that grain boundaries in graphene cause weak localization and impede electrical transport [12]. Regarding phonon transport properties across graphene GBs, it has been reported, using non-equilibrium molecular dynamics [13, 14] and the non-equilibrium Green’s functions formalism [15, 16], that like any imperfections, grain boundaries can lower the thermal conductivity by introducing additional phonon scattering. Thus, the question may arise whether graphene GB can be engineered to tune its thermoelectric response.

Tailoring the properties of a material primarily requires an understanding on how the material can be modified in a controlled manner. One possible strategy to influence the properties of GBs could be its functionalization with molecules or ad-atoms, which can act as electronically active dopants controlling the electronic and phonon transport of graphene GB and, hence, its thermoelectric behavior [17–19]. It has been shown that ad-atoms and molecules can endow pure graphene with various new or improved electromagnetic, physicochemical, optical, and structural properties [20, 21]. The importance of such local modifications is reflected in graphene’s measurable properties. For instance, it has been reported, by comparing STM images with DFT calculations, the presence of small molecules (hydroxyl-OH, amino-NH₂, and methyl-CH₃) on graphene after the synthesis process [22]. Huang et al. demonstrated that the electrical conductivity of graphene is enhanced by attaching nitrophenyl groups via covalent carbon-carbon bonds [23]. It has also been observed that degradation of charge transport across the
grain boundary is caused by their passivation by extrinsic contaminants like OH molecules or O and H atoms [18]. Nevertheless, up to now, there is lack of information about the influence of these compounds on the thermoelectric behavior of graphene grain boundaries. In the present work, we study the electron, thermal and thermoelectric transport properties of ad-atoms (Hydrogen and Oxygen) and chemisorbed molecules (Hydroxyl-OH, Methyl-CH\textsubscript{3}, and nitrophenyl-NO\textsubscript{2}C\textsubscript{6}H\textsubscript{4} (NPD)) on graphene grain boundaries. Methodologically, we employ a density functional tight binding (DFTB) approach combined with Green’s function techniques. In the next section, we describe the methodology and proceed then in Section 3 to discuss the results of the different functionalization approaches.

2 Methods

Neglecting electron-phonon interaction, which would need a separate self-consistent non-equilibrium study, both electronic and phonon transport channels can be considered as independent from each other. In the absence of phase breaking processes, the electronic and phononic transport properties can be computed within the Landauer approach in terms of the corresponding electronic $\tau_{el}(E)$ and phononic $\tau_{ph}(\omega)$ transmission coefficients. Using non-equilibrium thermodynamics and series expansions of the electrical current in the low bias, linear response regime, closed expressions for the different electronic transport coefficients appearing in Equation 1 can be written:

\[ G = e^2 L_{0}, \]
\[ S = \frac{1}{qT} \frac{L_{1}}{L_{0}}, \]
\[ \sigma_{el} = \frac{1}{T} \left[ L_{2} - \frac{L_{1}^2}{L_{0}} \right], \]

where $q$ is the electric charge of carriers, which is positive for holes and negative for electrons. The functions $L_m$ are given in terms of the moments of the electronic transmission function:

\[ L_{m} = \frac{2}{h} \int (E - \mu)^m \left[ -\frac{\partial f(E, \mu, T)}{\partial E} \right] \tau_{el}(E)dE, \]

with $f(E, \mu, T)$ being the Fermi-Dirac distribution function, $\mu$ the chemical potential, and $h$ is Planck’s constant.
For the phonon transport, the corresponding linear thermal conductance is given by:

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

(6)

with $k_B$ being the Boltzmann constant. The prefactor in front of the phonon transmission function is obtained by a linear expansion in the applied temperature difference $\Delta T$ of the quantity $N_B(T + \Delta T) - N_B(T)$, where $N_B$ is the Bose-Einstein distribution. Notice that, while for electrons, the relevant integration range is usually located around the Fermi energy of the system, computing the thermal conductance of the vibrational system requires an integration over the whole phonon spectrum. Both transmission coefficients $\tau_{el}(E)$ and $\tau_{ph}(\omega)$ can be computed in a similar way by using Green’s function techniques. We use the common partitioning scheme for both electron and phonons by dividing the system into three regions, namely left, right, and a central region, where scattering takes place. In our case, the central region includes the grain boundary part, whereas the left and right regions are taken as a unit cell of the 2D graphene domain in each side. The electron transmission coefficient $\tau_{el}(E)$ is then calculated as

$$\tau_{el}(E) = \text{Trace} (G^r \Gamma_L G^a \Gamma_R),$$

(7)

where the retarded Green’s function $G^r$ is obtained from the Hamiltonian $H$, $G^r = (EI - H - \Sigma^r_L - \Sigma^r_R)^{-1}$, and the broadening functions $\Gamma_{L/R} = i[\Sigma^r_{L/R} - \Sigma^a_{L/R}]$ with $\Sigma_{L/R}$ being the electrode self-energies. The phonon transmission coefficient $\tau_{ph}(\omega)$ is calculated in a similar way by the substitution $H \rightarrow K$ and $EI \rightarrow M \omega^2 I$, where $M$ is a diagonal matrix including the atomic masses and $K$ is the dynamical matrix. Here, both the electronic Hamiltonian matrix as well as the interatomic force constants are obtained using the density functional tight-binding (DFTB) method as implemented in the DFTB+ software package [24]. The advantage of the DFTB approach, when compared to full density functional methods, is its computational efficiency, since it is based on a generalized tight-binding formulation with parametrized electronic matrix elements. In order to compare the influence of the kind of ad-atom and molecule, all the calculations shown in Section 3 were performed for a concentration equivalent of four elements, i.e., four atoms or four molecules. To avoid spurious effects related to the specific choice of initial positions for the ad-atoms or molecules, an average over four random choices of the initial positions was additionally performed.
3 Results and Discussion

In this work, we have studied two possible grain boundary models, symmetric (model I) and asymmetric (model II), as shown in Figure 1a). In order to generate these GBs we have considered graphene sheets oriented in different angles. For the symmetric model, we have two graphene sheets with the same orientation (8°) but in opposite direction, clockwise and counterclockwise, whereas, the asymmetric model has been built with a graphene sheet oriented in the armchair direction and another in the zigzag (10° in the clockwise) direction. As it can be seen in Figure 1a, for model I, the grain boundary is composed by pentagons and heptagons, and, for model II, we also find a nonagon. It is worth mentioning that those geometries have been reported in experimental works [10, 8]. Concerning the transport properties, the phonon thermal conductance, $\sigma_{ph}$, for both graphene GBs is lower than the corresponding to pristine graphene for the whole range of temperatures explored in this study (up to 800 K), see Figure 1b. This is obviously expected, since the presence of local structural defects induces additional phonon scattering. Moreover, when comparing $\sigma_{ph}$ for the two GBs in Figure 1b, we see that the model II has the smallest phonon thermal conductance. This can be related to the more disordered structure of the GB region in model II. A similar situation is found when looking at the electron transport signatures of both models. This is shown in Figure 1c, where we plot the linear conductance $G$ at 300 K as a function of the chemical potential of the system. $\mu = 0$ corresponds to the charge neutrality point, while by varying $\mu$ the effect of doping of the graphene layer can be mimicked. Notice that for values of the chemical potential close to zero, the GB model II displays a small pseudo-gap of the order of 0.1 eV, while model I behaves closer to the pristine graphene with two linear branches in the conductance. The presence of a band gap in asymmetric graphene GB has been extensively discussed in Ref. [9]. Its presence is also reflected in the Seebeck coefficient $S$, shown in the inset of Figure 1b, where $S$ for GB model II takes larger values around the charge neutrality point. This is related to the fact that the Seebeck coefficient can be shown — by performing a Sommerfeld expansion at low temperatures — to be proportional to the log-derivative of the transmission function [25]. As a result, strong variations in the transmission over a narrow energy window can lead to jump in the thermopower of the system. To have a more systematic overview, we have calculated the dependence of the figure of merit $ZT$ on the chemical potential and on the temperature for pristine graphene and the two GB models. This is displayed as a 2D plots in Figure 1d (graphene),
Figure 1  a) Atomistic representation of the two graphene grain boundary models investigated in this study: symmetric (model I) and asymmetric (model II). Panels b–f compare pristine different transport coefficients of pristine graphene with the two GB models. b) Phonon thermal conductance and transmission (inset); c) Electronic conductance and Seebeck coefficient (inset) at 300 K, d–f) Figure of merit $ZT$ as a function of the temperature and the chemical potential for pristine graphene (d), GB model I (e), and GB model II (f). The color bar indicates the value of $ZT$. 
e (model I), and f (model II), respectively. In the case of graphene, $ZT(T, \mu)$ has mirror symmetry with respect to the line $\mu = 0$, the values of the figure of merit are however very low for temperatures up to 800 K due to the very high thermal conductivity of pristine graphene [26]. Less symmetric patterns appear for models I and II, mainly with increasing temperature; yet the figure of merit does not reach values much larger than those for pristine graphene, $\sim 0.04$, since the presence of the GBs turns out to simultaneously affect in a detrimental way both the electronic and phononic conductances.

### 3.1 Ad-atoms on Grain Boundaries

We have then considered two kind of light ad-atoms, hydrogen (H) and oxygen (O). After relaxation, we have found that H atoms prefer to be located on top of carbon sites (C-H bond length is 1.14 Å), while O atoms are attached to bridge (B) sites (C-O bond length is 1.49 Å) for both GBs, see Figure 2, in good agreement with other published results [19]. As shown in Figure 2a and c, the phonon transmission of these grain boundaries is reduced over the whole spectrum of frequencies by the inclusion of ad-atoms, when compared with pristine graphene. H and O ad-atoms strongly affect out-of-plane modes which correspond to $\omega < 750$ cm$^{-1}$. The analysis of the projected vibrational density of states (not shown) reveals that the lighter H atoms have a stronger influence at high frequencies ($\omega \in [1000 - 1500]$ cm$^{-1}$) and O atoms at lower frequencies ($\omega < 900$ cm$^{-1}$). Notice that the major contribution to the phonon transmission function, shown in the insets of Figure 2a and c for models I and II, respectively, comes from a spectral region between 250 cm$^{-1}$ and 750 cm$^{-1}$. Since this is also the range where oxygen functionalization shows up in phonon transport, we see that attaching oxygen atoms has a stronger influence on the thermal conductance of the grain boundaries.

Similar effects have also been reported for the thermal conductivity of graphene sheets [19]. Interestingly, H- and O-functionalization has a stronger influence on the electronic transport of model I (Figure 2b) than for model II (Figure 2d), where the transmission is barely modified in the latter case with respect to the non-functionalized grain boundary. This indicates that the charge transport in model II for these ad-atoms is mainly determined by the intrinsic structural disorder of the grain boundary. This situation will change when the GB will be functionalized with small molecules, as discussed in the next section. The Seebeck coefficients for both models are however barely affected by the ad-atoms, see the inset of Figure 2b and d. The discussed behavior of
Figure 2: Transport coefficients of the graphene grain boundaries upon functionalization with H- and O-atoms. Panels a) and c) show the temperature dependence of the phonon thermal conductance in the GB models I (a) and II (c). The insets show the corresponding phonon transmission functions. Panels b) and d) display the electronic transmission and the Seebeck coefficient (insets) at 300 K for GB model I (b) and II (d). In all figures, the lines correspond to pristine grain boundaries (solid lines), hydrogen ad-atoms (○), and oxygen ad-atoms (□).
the phonon and electronic transport coefficients shows up in the computed figure of merit, displayed in Figure 3: the highest $ZT$ values attainable for the functionalized GB models I and II are found for small values of the chemical potential $\mu$ (around the charge neutrality point); yet, they are smaller than the corresponding values for the pure GB model, i.e. despite the reduction of the phonon thermal conductance upon functionalization, the figure of merit decreases because the electronic conductance is also (negatively) affected.

3.2 Chemisorbed Molecules on Grain Boundaries

We have selected a set of molecules which have been probed to be chemisorbed on graphene [21–23, 27]. We found that Hydroxyl-OH (C-O bond length is 1.49 Å), Methyl-CH$_3$ (C-C bond length is 1.58 Å), and Nitrophenyl-NO$_2$C$_6$H$_4$ (NPD), (C-C bond length is 1.58 Å) are covalently bonded to carbon atoms on the grain boundaries on T sites (Figure 4). We also studied Ammonia (NH$_3$) and Dibromine (Br$_2$), but they did not covalently bind to the grain boundaries, so that their impact on the thermal and electrical transport through the system was negligible, and we thus do not discuss them further at this point.

In Figure 4a and c we show the influence of chemisorbed molecules on the phonon transmission functions of GB model I and II. For both GB models, the largest influence of the functionalization is seen in the low frequency domain ($\omega \leq 400$ cm$^{-1}$) as well as at higher frequencies $\omega > 1100$ cm$^{-1}$. Still, GB model II turns out to be less sensitive to changes in the type of molecule, similar to the previously discussed case with ad-atoms, i.e. functionalization reduces the phonon transmission, but the effect is only weakly dependent on the specific chemical structure of the molecules. On the contrary, model I displays a stronger dependence on the functionalizing group in the above mentioned frequency ranges. We remark that covalently bonded molecules mostly influence the out of plane vibrational modes in the grain boundary region. This is illustrated in the insets of Figure 4b and d, where we show the contributions of out of plane modes to the phonon transmission spectrum for the pristine grain boundaries as well as for the CH$_3$ and NPD functionalization (the OH functionalization is barely different from CH$_3$ and is omitted in the inset for the sake of clarity). Mainly for GB model I the transmission component of these modes is overall suppressed, the effect being dramatic below 200 cm$^{-1}$. On the contrary, in the GB model II the considerably weaker influence of the molecules is reflected in the smaller reduction of the phonon transmission (although a strong reduction is still seen below 200 cm$^{-1}$).
Figure 3: Dependence of the figure of merit ZT on the chemical potential at 300 K for ad-atoms on GB model I (a) and GB model II (d). In all figures, the lines correspond to pristine grain boundaries (solid lines), hydrogen (○), and oxygen (□). Panels b, c, e, and f show surface plots of the figure of merit while varying both the chemical potential and the temperature for GB model I with H (b) and O (c) ad-atoms, and for GB model II with H (e) and O (f) ad-atoms.
Figure 4 Phonon transmission and phonon thermal conductance for functionalized grain boundaries: GB model I (a and b) and GB model II (c and d). In all plots, the transport coefficients for the pristine grain boundaries are shown with solid lines, Hydroxyl-OH (□), Methyl-CH\textsubscript{3} (◊), and Nitrophenyl-NPD (○). The insets in panels b) and d) show the component of the phonon transmission function corresponding to the out of plane modes to highlight the impact of the functionalization on these vibrational modes. Notice that the strongest modification of the transmission in this case takes place at low frequencies, below 200 cm\textsuperscript{-1}. 
The discussed features of the phonon transmission are then reflected in the corresponding thermal conductance functions as shown in the panels c and d of Figure 4. Deviations from the conductance of non-functionalized GB clearly increase with temperature as higher frequency modes, which are stronger affected by the chemisorbed molecules, become thermally activated.

Concerning the electron transport properties, displayed in Figure 5, the linear conductance is also suppressed upon functionalization, but the effect is less pronounced for model II, similar to the case of ad-atoms. Interesting is now that for model I the molecular functionalization also opens a small pseudo-gap in the spectrum (notice that this only happened for model II in the case of ad-atoms). As a consequence, the Seebeck coefficient, shown in the inset of Figure 5a, increases. By looking at the 2D plots of the figure of merit as a function of the temperature and the chemical potential for both GB models, see Figure 5c, d, and e for model I and Figure 5f, g, and h for model II, one can realize that functionalization with the NPD species can induce an increase of the figure of merit by about a factor of two if the chemical potential is shifted out of the charge neutrality point to positive values (model I) or negative values (model II). For the other molecules the tendency is rather to slightly reduce $ZT$ from its value for pristine grain boundaries (see Figure 1).

4 Conclusions

The thermoelectric response of graphene grain boundaries upon functionalization with ad-atoms and covalently bound small molecular species has been theoretically investigated by using density functional tight-binding methods combined with Green’s function approaches. Pristine grain boundaries suppress both electron and phonon transport due to the increased scattering probability, although the effect can vary in dependence of the structural symmetries of the grain boundaries. The investigated ad-atoms and molecules lead to further suppression of the electronic and phonon conductances. In particular, ad-atoms have a detrimental effect on the figure of merit by reducing it from the values it has in pristine grain boundaries. On the contrary, functionalization with nitrophenyl can increase $ZT$ by about a factor of two. However, the absolute values of $ZT$ in all cases (pristine as well as functionalized grain boundaries) remain very low, so that additional strategies need to be considered if these systems are going to find any application in thermoelectricity. For instance, reducing the dimensionality of the system from
Figure 5. Panels a) and b) show the dependence of the electronic conductance and Seebeck coefficient (insets) at 300 K on the chemical potential for GB model I (a) and GB model II (b) upon functionalization with small molecules: GB models (solid line), OH (□), CH$_3$ (♦), and NPD (农副). The surface plots of the figure of merit (ZT) as a function of the temperature and the chemical potential are also shown for GB model I and II with OH (c and d), CH$_3$ (e and g), and NPD (e and h).
2D to quasi 1D by considering graphene nanoribbons, may lead to additional ways of influencing both thermal and electronic transport due to finite size effects and the corresponding modifications of the electronic and vibrational spectra. Addressing this possibility in connection with target functionalization of the grain boundaries will be the scope of future work.

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Thermoelectric Properties of Functionalized Graphene Grain Boundaries


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