Charge Transport in Pentacene-Graphene Nanojunctions

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Abstract

We investigate charge transport in pentacene-graphene nanojunctions employing density functional theory (DFT) electronic structure calculations and the Landauer transport formalism. The results show that the unique electronic properties of graphene strongly influence the transport in the nanojunctions. In particular, edge states in graphene electrodes with zigzag termination result in additional transport channels close to the Fermi energy which deeply affects the conductance at small bias voltages. Investigating different linker groups as well as chemical substitution, we demonstrate how the transport properties are furthermore influenced by the molecule-lead coupling and the energy level lineup.

Molecular junctions, consisting of single molecules that are chemically bound to electrodes, represent interesting systems to investigate and understand mechanisms of nonequilibrium transport processes at the nanoscale. Recent experimental\textsuperscript{1-10} and theoretical\textsuperscript{11-17} works have elucidated the conductance properties of molecular junctions and revealed a wealth of interesting transport phenomena such as Coulomb blockade, Kondo effects, negative differential resistance, vibronic effects and local heating, as well as switching and hysteresis.

Most experiments on single-molecule conductance have employed metal electrodes. Carbon-based materials, such as carbon nanotubes or graphene, represent another promising class of materials for electrodes. Studies of molecular contacts with carbon nanotubes have demonstrated a number of advantages\textsuperscript{18,19} as compared to metal electrodes, in particular, rigidity, mechanical stability and thus a more precise control of the molecule-electrode contact geometries. Graphene, furthermore offers excellent electronic properties,\textsuperscript{20} especially high electron mobility and, furthermore, may facilitate optical addressability of the nanocontact for optoelectronic applications.\textsuperscript{21} Electron transport through molecular films connecting graphene electrodes\textsuperscript{22} and molecular junctions with few layer graphene electrodes\textsuperscript{23} were recently reported. Furthermore, using electron beam lithography, all-carbon junctions consisting of a carbon chain between graphene electrodes were realized.\textsuperscript{24}

In this work, we study the conductance properties of molecule-graphene nanojunctions em-
ploying a combination of density functional theory (DFT) calculations and the Landauer transport formalism. Considering several different examples, we show that charge transport in molecule-graphene nanojunctions is strongly influenced by the edge structure of the graphene electrodes. In particular, for graphene electrodes with zigzag termination, edge states may result in additional transport channels close to the Fermi energy that affect the conductance at small voltages profoundly. These findings extend previous theoretical work on graphene-molecular junctions.\textsuperscript{25–27}

![Diagram](image)

Figure 1: Molecule-graphene junctions with a covalently bound pentacene bridge investigated in this work. (a) Overall structure of a junction. Two types of molecular bridges without (b,d) and with (c,e) CN-groups are considered. Two different geometrical arrangements of the molecular bridge have been analyzed: twisted geometries (b,c), where the molecular bridge is weakly coupled to the leads through amide-binding groups and nearly flat geometries (d,e), where the bridge is strongly coupled via oxygen atoms to the leads.

As prototypical systems, we consider molecular bridges based on pentacene as the central unit (see Fig. 1). The extended $\pi$-electron system of pentacene facilitates electron transport and makes this system, in combination with its optical properties, a promising material for molecular devices. Pentacene-based systems have been used, for example, in thin-film organic electronic devices.\textsuperscript{28,29} In the graphene-molecule junctions depicted in Fig. 1b and c, the molecular bridge is bound covalently via amide linker groups to two graphene nanocontacts. This binding group has been used successfully for molecular nanojunctions with carbon nanotubes.\textsuperscript{18} The coupling of
the molecule-graphene nanojunction to leads and an external circuit are modeled by self energies and absorbing potentials (vide infra). To analyze the influence of graphene edge states on the conduction mechanism, we investigate both zigzag-terminated graphene nanocontacts, as depicted in Fig.1 and armchair termination.

In addition to the basic pentacene molecular bridge, we consider CN-substituted molecular bridges (Fig.1f and e). The electron-withdrawing CN-group allows one to shift the location of the molecular energy levels relative to the Fermi energy of graphene and thus to vary the conductance at small voltages. Due to the almost perpendicular geometry of the molecular bridge with respect to graphene, the molecular junctions depicted in Figs.1b and c exhibit only weak coupling between the electronic $\pi$-orbitals of pentacene and graphene and thus low conduction. As an example for strongly coupled systems, we consider the systems depicted in Fig.1d and e, where the binding to the nanocontacts is achieved via oxygen atoms forming oxepine rings resulting in an overall planar geometry and a strong electronic interaction between the central pentacene molecule and the graphene nanocontacts.

The theoretical methodology used to study charge transport in the systems considered is based on a combination of DFT calculations to characterize the geometry and electronic structure of the systems and Landauer theory to simulate the transport properties. Closed shell DFT calculations using the B3LYP exchange correlation functional together with the 6-31G(d) basis set are used to model the different systems investigated in this work. To avoid dangling bonds, the graphene edges have been saturated using hydrogen atoms. During the optimization process, geometrical constraints have been imposed to prevent artificial distortions of the nanocontacts. All calculations were carried out using G09\textsuperscript{30} and TURBOMOLE\textsuperscript{31} codes. Following previous work,\textsuperscript{32} the Kohn-Sham matrix obtained for the relaxed junction is identified with the Hamiltonian of the system. To facilitate the transport calculations, the Hamiltonian matrix is partitioned into blocks that correspond to the molecular bridge $H_m$, left and right contacts $H_l$ and $H_r$ and coupling between them $V_{lm}$, $V_{ml}$, $V_{mr}$ and $V_{rm}$, respectively, as described by Benesch et al.\textsuperscript{32}. Direct coupling between the left and the right contacts is neglected. To model the effect that extended graphene contacts have in
the electron transport, we employ absorbing boundary conditions described by complex absorbing
potentials $-iW_\alpha (\alpha = l, r)$, which are added to the Hamiltonian in the graphene contacts. Thus, the
overall Hamiltonian $\tilde{H}$ reads

$$\tilde{H} = \begin{pmatrix}
H_l - iW_l & V_{lm} & 0 \\
V_{ml} & H_m & V_{mr} \\
0 & V_{rm} & H_r - iW_r
\end{pmatrix}. \quad (1)$$

The matrices describing the absorbing potentials are assumed to be diagonal, $(W_\alpha)_{ij} = w_{\alpha i} \delta_{ij}$. Following previous work, a polynomial function was employed to model $w_{\alpha i}$. Accordingly, the elements of the matrices, which correspond to the $i$th atom of the nanocontact, are described by the formula

$$w_{\alpha i} = a |x_i - x_0^\alpha|^4, \quad (2)$$

where $x_i$ is the $x$-coordinate of the atom, assuming that the $x$ axis is directed along the molecular bridge, and $x_0^\alpha$ is selected to be close to the point where the molecular bridge is connected to the nanocontact. To determine the empirical parameter $a$, test calculations over a wide range of values were carried out. On the basis of that, the value of $a$ was chosen from a stable parameter range, where the results do not depend on $a$ Kopf and Saalfrank.

The transport properties of the nanojunctions are described by the transmission function. On the basis of the model introduced above, the transmission function for an electron with energy $E$ is given by the expression

$$t(E) = \text{tr}\{\Gamma_r G_m \Gamma_l G_m^\dagger\}, \quad (3)$$

where the trace is taken over the molecular degrees of freedom. The transmission function close to the Fermi energy $E_f$ determines the conductance $\mathcal{G} = \frac{e^2}{\pi \hbar} t(E_f)$ at small bias voltages.

In Eq. (3), $G_m$ denotes the Green’s function projected on the molecular bridge

$$G_m(E) = [E - H_m - \Sigma_l(E) - \Sigma_r(E)]^{-1}. \quad (4)$$
The matrix $\Gamma_\alpha \equiv -2\text{Im}\{\Sigma_\alpha\}$, which characterizes the energy-dependent width of the molecular resonance states, is proportional to the imaginary part of the self energy $\Sigma_\alpha$. The self energy $\Sigma_\alpha(E)$ describes the coupling of the molecular bridge to the graphene leads and is given by the expression

$$
\Sigma_\alpha(E) = V_{m\alpha}[E - H_\alpha + iW_\alpha]^{-1}V_{\alpha m}, \quad \alpha = l, r.
$$

(5)

Figure 2: Transmission through a weakly coupled pentacene-graphene junction. The upper panel depicts the transmission function for the pentacene bridge (solid line). The eigenenergies of the bridge (dash-dotted line) are also shown. The lower panel demonstrates the influence of CN groups on the transmission. The differences between zigzag nanocontacts (dashed lines) and armchair nanocontacts (dotted line) are also shown. The inset highlights the edge induced peak with and without CN substitution.

We first consider the amide-linked nanojunction with the basic pentacene bridge (see Fig.1b). Fig. 2 (top) shows the transmission function of this junction in the range of energies close to the Fermi level. The transmission function exhibits a series of peak structures, which can be classified into two types: (i) isolated resonance peaks with a maximum transmission value of unity, in the following referred to as regular or molecular resonances, and (ii) a small double peak structure close to the Fermi energy (see also the inset in Fig.2). The former are associated with
Figure 3: Energy spectrum of the molecular junction depicted in Fig. 1c. The highlighted area contains 8 edge states (including HOMO-3 and HOMO-4) and one molecular state (LUMO+4), see text for details. Through CN-functionalization of the pentacene bridge, the molecular state (LUMO+4) is embedded into the family of edge states. The energies of the states depicted correspond to peaks at $E = -0.2$ eV and $E = +0.2$ eV in Fig. 2 (bottom, dashed line).

resonant electron transport through the discrete energy levels of the molecular bridge and thus appear at energies close to the eigenenergies of the molecular levels. The width of these peaks varies significantly, depending on the coupling of the specific molecular level to the graphene leads. The latter double peak structure close to the Fermi energy, on the other hand, cannot be related directly to electronic states of the molecular bridge. Furthermore, this peak structure does not correspond to direct tunneling between the graphene nanocontacts because this mechanism was explicitly excluded in our treatment (cf. Eq. ???). As discussed in detail below, we assign the double peak structure close to the Fermi energy to an additional transport channel caused by the edge states of the graphene nanocontacts (in the following referred to as edge induced transmission channel).

It is worthwhile to mention that similar surface induced transport channels have also been found in carbon-nanotube-based molecular junctions\cite{35,36} as well as in molecular junctions with metal electrodes\cite{37,38} where they are known as a metal-induced gap states. Due to the proximity of the peak structure to the Fermi energy, it dominates the conductance at small bias voltages.

In the nanojunction considered in the top panel of Fig. 2, the amplitude of the edge-induced transmission peak is rather small. The amplitude can be strongly enhanced if molecular levels exist close to the Fermi energy. This is demonstrated in the bottom panel of Fig. 2 which shows the transmission function for the CN-substituted pentacene bridge. The CN-substitution causes an
overall shift of the molecular levels to smaller energies. As a consequence, the energy level associated with the LUMO of pentacene approaches the Fermi energy. As a result, the edge-induced transmission peaks acquire additional intensity that increases their maximal value to almost unity. Furthermore, the interaction between the molecular resonance state and the edge-induced transmission peaks results in a splitting of the double peak.

To further analyze the edge-induced transmission channel, we have investigated the electronic states of the overall nanojunction, as represented by their molecular orbitals, in a range of energies close to the Fermi level (see Fig. 3). These states can be classified in two groups: (a) states localized preferentially in the graphene contacts and (b) molecular states mostly localized on the bridge (see, e.g. LUMO+4 in Fig. 3). A detailed analysis of the (a)-type states shows that many of them are localized at the edge of the graphene contacts (see, e.g. HOMO-3, HOMO-2 in Fig. 3). These states are closely related to the well-known edge states of zigzag-terminated graphene nanoribbons. Due to their localization at the molecule-graphene interface, they interact strongly with the molecular states and induce the additional transport channels. This can be seen, for example, in the spectrum depicted in Fig. 3 bottom, where the near-degenerate pair of states HOMO-2 and HOMO-3 correspond to the induced transmission peak of the CN-substituted pentacene at $E = -0.2$ eV (see Fig. 2). On the other hand, the molecular state LUMO+4 in Fig. 3 represents a regular transmission channel and corresponds to the peak at $E = +0.2$ eV (see Fig. 2).

To unambiguously show that the edge-induced transmission channel appears as a consequence of the existence of edge states in zigzag-terminated graphene nanocontacts, we have compared these results with the ones obtained for molecular junctions based on armchair-terminated graphene nanocontacts. As is well-known, armchair edges of graphene do not possess edge states. As a consequence, the transmission functions for both kinds of molecular junctions should differ, and the edge induced transmission channel should be missing in the armchair-terminated graphene nanocontact. As shown in Fig. 2 bottom, where the transmission function for a CN-substituted pentacene-graphene junction with armchair-terminated graphene nanocontacts is depicted, the edge-state-induced transmission channels are indeed not present for this type of molecular junc-
tion, whereas all of the regular peaks similar to those found in the zigzag-terminated graphene nanocontact appear. This result thus unambiguously demonstrates that these additional transmission channels are induced by graphene edge states.

In the molecular nanojunctions considered above, the overall coupling between the $\pi$-electron systems of pentacene and the graphene leads is rather small due to the twisted (almost perpendicular) orientation of the molecular bridge with respect to the graphene nanocontacts (see Fig.1b and c). To study charge transport for stronger molecule-lead coupling, we have also investigated the molecular junctions d and f depicted in Fig.1. In these junctions, the pentacene bridge binds to graphene via oxygen atoms forming oxepine rings, which facilitates a nearly planar structure and therefore a stronger coupling. The transmission functions (see Fig.4) again show a peak structure with regular peaks related to molecular resonances and edge-induced transmission channels close to the Fermi level. However, the peaks are significantly broader than those found in the amide-bound molecular junctions due to the stronger coupling between the graphene nanocontacts and the pentacene bridge. Furthermore, the overlap of some of the peaks results in values of the transmission function that are larger than unity. The larger coupling also induces a significantly higher transmission amplitude of the edge-induced transmission peaks close to the Fermi level. In the CN-substituted junction (see Fig.4 bottom), this is further enhanced by the presence of a molecular resonance close to the Fermi level, a result already found for the amide-bound CN-substituted junction. Interference between this molecular resonance and the edge-induced structures results in a complex triple peak structure, a characteristic feature that can be observed in the transmission function at the Fermi energy (see Fig.4 bottom).

In summary, we have investigated charge transport in molecule-graphene nanojunctions. The results obtained for different pentacene-based nanojunctions reveal the unique properties of graphene as material for electrodes. In particular, we have shown that charge transport is strongly influenced by the edge structure of the graphene electrodes. Graphene electrodes with zigzag termination have edge states that result in additional transport channels close to the Fermi level that strongly affect the conductance at small bias voltages. While the influence of graphene edge states on transport
Figure 4: Transmission through strongly coupled pentacene-graphene junctions. The upper and lower panel depict results without and with CN-substitution of the molecular bridge, respectively (see models d and e in Fig.1). The arrows show how regular and induced channels interact in the strong coupling regime to form complex peak structures in the transmission function.

in nanojunctions has been discussed before, the present results show, to the best of our knowledge for the first time, the importance of edge state effects in molecule-graphene nanojunctions in the resonant transport regime based on first principles calculations. Our results also show that the transport properties are strongly influenced by the effective coupling between the molecular bridge and the graphene nanocontacts as well as the position of the molecular energy levels, which can be controlled by the choice of different linker groups and appropriate functionalization of the pentacene molecular bridge, respectively. These findings may facilitate further experimental studies and possible future applications in nanoelectronic devices.

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