Conductance of graphene flakes contacted at their corners

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Abstract
Linear conductance of junctions formed by graphene flakes with the order of the nanometer-thick electrodes attached at the corners of the flakes is studied. The explored structures have sizes up to 20 000 atoms and the conductance is studied as a function of applied gate voltage varied around the Fermi level. The finding, obtained computationally, is that junctions formed by armchair-edge flakes with the electrodes connected at the acute-angle corners block the electron transport while only junctions with such electrodes at the obtuse-angle corners tend to provide the high electrical conductance typical for metallic GNRs. The finding in the case of zig-zag edges is similar with the exception of a relatively narrow gate voltage interval in which each studied junction is highly conductive as mediated by the edge states. The contrast between the conductive and insulating setups is typically several orders of magnitude in terms of ratio of their conductances. The main results of the paper also remain to a large extent valid in the presence of edge disorder.

Keywords: graphene, conductance, transport, edge, corner, gate voltage, flakes

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(Some figures may appear in colour only in the online journal)
the dc linear conductance of graphene flakes of various shapes and edges and with the electrodes connected at the corners of the flakes. Specific investigated samples have the shapes of trapezoids, triangles, rhombi and rhomboids, all with angles at the corners being integer multiples of 30°. We find that the conductance strongly depends on the angles at the corners to which the electrodes are connected. Acute-angle corners (30° and 60° studied here) in most cases do not enable good electronic transport. The opposite is true for electrodes attached at obtuse-angle corners (120° studied here): they often provide high conductance levels typical for metallic GNRs. We describe GNRs’ electronic structure using a tight-binding (TB) approximation with hoppings up to the third nearest neighbour (NN), as specified below in section 2. The model of the electrodes uses the first NN approximation and will be further described as well. The main results of the paper are explained in section 3, considering graphene flakes with shapes of symmetrical trapezoids and triangles. Section 4 supports the main results by a local density of states analysis. Section 5 provides a summary and discussion of the results. Comparisons with the results obtained within the first NN TB approximation (1NNTBA), further details and an examination of the model of the electrodes, and a section describing the results for samples with edge disorder are supplied as appendices. Supplementary information (SI) (stacks.iop.org/JPhysCM/27/435005/mmedia) contains results for graphene flakes of several additional shapes including a system with wide contacts to electrodes, further results within the 1NNTBA and a section with data for the flakes terminated by imperfect edges.

2. Models and methods

Our model of a GNR’s electronic structure employs one explicit electron per atom, the independent-electron approximation and a TB Hamiltonian with hoppings up to the third NN included (3NNTBA). According to [11], we set the hopping parameters to values \( t_0 = -2.97 \text{ eV} \), \( t'_0 = -0.073 \text{ eV} \) and \( t''_0 = -0.33 \text{ eV} \). A magnitude of \( t_0 \) is conveniently used as the energy unit. Interatomic overlaps are neglected. The edges of the flakes are assumed to be terminated by hydrogen atoms electrons of which do not explicitly enter the TB Hamiltonian; see for instance [12]. Although the TB modelling is a relatively basic-level one, it has, even in the 1NNTBA, in many cases been proven to provide a satisfactory description of the conductance properties of graphene structures on at least a semi-quantitative level, which is sufficient for the present study. Such models are frequently employed in theoretical studies of graphene samples [7, 13, 14] and carbon nanotubes [15].

In the present study the whole system including the electrodes is composed of identical atoms. Each of the two electrodes in our model is composed of a number (from tens to hundreds) of monatomically thin mutually non-interacting wires (figure 1). Within each wire the 1NNTBA with the parameter \( t_0 \) is used to describe the electronic structure. This simple model of the electrodes was found to be very convenient in [16] where it was used for GNRs and provided results in a semi-quantitative agreement with different models of the electrodes [14, 17]. The coupling of the wires to the GNR is again described by the first NN model using the parameter \( t_0 \). See appendix B, in which we consider a model with wires mutually coupled along a finite length.

![Figure 1](https://example.com/image1.png)

Figure 1. Schematic graphical representation of our model of the electrodes and their coupling to a graphene flake. In this example the flake has zig-zag edges and the electrode is attached to its 60° corner. The electrode itself is formed by a bunch of monatomically thin semi-infinite mutually decoupled wires. In typical setups we use 35–36 wires per electrode. Here we show only 12 of them for easier visualisation. The interatomic distances within each wire are \( a_i \), i.e. the same as is the NN distance in graphene. See also appendix B, in which we consider a model with wires mutually coupled along a finite length.

Each atom of the system is characterised by its on-site energy. In equilibrium and in the absence of any external field these energies are set to zeros for all the atoms of the entire system. The effect of the applied bias voltage \( U \) as well as of a gate voltage \( V_g \) are modelled by variations of the on-site energies of the atoms in the electrodes and/or in the graphene flake [16]. Variation in the gate voltage represents the shift of the chemical potential in the graphene flake away from the neutrality point and is considered within a 0.2 \( |t_0| \) wide interval around the Fermi level. We apply almost limingly small (still numerically finite) values of the bias voltages \( U \), compute resulting dc currents \( I \) through the junctions and consequently obtain the linear conductances \( G_{\text{lin}} = \lim_{U \to 0} I/U \). The considered model can now be briefly summarised: The Hamiltonian of the entire system is

\[
\hat{H} = \sum_{l,l'} H_{l,l'} a_l^\dagger a_{l'},
\]

with \( l \) and \( l' \) running over the atomic sites of the entire system (including the electrodes) and \( a_l^\dagger \), \( a_{l'}^\dagger \) being the creation and annihilation operators of an electron in the TB orbitals \( l \) and \( l' \), respectively. It is assumed that the TB orbitals form an orthonormal basis set: \( \langle l | l' \rangle = \delta_{ll'} \). The matrix elements of the Hamiltonian in our model are set to
function formalism [18], again in the same way as we used in [16]. A scattering approach and the Landauer-type formula were used also in our work [19] for systems with just two terminals; see equations (24) and (25) therein\(^1\). Here we use the multi-terminal generalisation of the method and instead of the simple scattering approach we employ the more general one based on the Green function technique, which allows us to obtain the wavefunctions.

3. Results

The conductance properties of a graphene-flake formed nanojunction depend on a number of parameters and conditions: on the intrinsic properties of the flake itself (its shape, size) and also on how and where the electrodes are attached to the flake. Among the plethora of possible scenarios we focus on several representative ones with the aim of studying junctions with the electrodes at the corners. We present our results in figures which display particular considered structures together with the linear conductance \(G_{\text{lin}}\) as a function of the chemical potential variation (here represented by the gate voltage) around the neutrality point. The results for a limited set of structures only are described in the text, which, however, should be sufficient to explain our main findings. The results for other structures can be found in the SI (stacks.iop.org/JPhysCM/27/435005/mmedia). In our description of the physical structure sizes we often employ the graphene NN distance \(a \approx 1.42\) nm as well as its lattice parameter \(b = a\sqrt{3} \approx 2.46\) nm.

3.1 Armchair edges

As representative structures with armchair (ac) edges we consider symmetrical trapezoids with acute angles of \(60^\circ\) at their base (left panel of figure 2). These flakes support four different basic attachments of the electrode pair: (i) both electrodes at the acute angles (AA–AA setups), (ii) one electrode at the acute angle and the other at the nearby obtuse angle (AA–OA setup), (iii) one electrode at the acute angle and the other at the opposite obtuse angle (the other AA–OA setup), (iv) both electrodes at the obtuse angles (OA–OA setup). The top three structures in figure 2 share the same base length \(L = 176\) a \(\approx 25.0\) nm. The equilateral triangle in this context can be considered as a limiting-case trapezoid. The two trapezoids at the bottom represent wider and overall larger structures \((L = 353 a \approx 50.1\) nm\) and allow us to observe the size-dependence of the computed results. The heights of the samples are \(14b, 32b, 88b, 23b\) and \(46b\) from the uppermost structure to the one at the bottom. The total numbers of atoms composing any given flake are typed on the images. Each electrode considered for figure 2 is 36 monoatomic wires thick. When possible, we choose the shape of the contact areas to be the same for the corresponding corners\(^2\). All trapezoids in figure 2 have (vertical) widths corresponding to metallic AGNRs [3, 4]. The right panel in the figure displays

1 Formula (24) in our work [19] has the density-of-states factors included in the definitions of coefficients \(A\) and \(C\).

2 The largest trapezoid has sharper corners at its obtuse angles, compared to the smaller structures.
Importantly, we find that the conductance of the trapezoidal shapes in graphene is sensitive to the choice of the particular pair of the AA–OA attachment corners: both the nearby-corners case and the opposite-corners case yield similar curves; compare the dashed red and solid green plots in the figures. The similarity is reduced with increasing the relative length of trapezoids. This is an intuitively comprehensible feature because for long-narrow trapezoids the mutual positions of the contacts in the two $60^\circ - 120^\circ$ setups are quite different. In SI (stacks.iop.org/JPhysCM/27/435005/mmedia) we show that there is no such similarity in the case of ac-edge terminated long-narrow rhomboids. Note that the AA–OA junctions have not been calculated for the largest trapezoid, figure 2(e). Finally we refer to appendix A, which provides results employing the linear scale on the conductance axis (figures A1 and A2).

### 3.2. Zig-zag edges

For graphene flakes with ZZ edges we perform an analysis analogous to that in the previous section, now choosing electrodes 35 monoatomic wires thick. We again choose structures of trapezoidal shapes. The samples displayed in figure 3 are of two different lengths, 100 $b$ and 204 $b$. Their heights from the uppermost flake to the lowest one are 24.5 $a$, 56 $a$, 150.5 $a$, 41 $a$ and 80 $a$. Generally valid differences if compared to the ac-terminated flakes (figure 2) are that (i) The AA–AA junctions now provide a significant conductance within a narrow gate voltage window; this is an effect of the special

**Figure 2.** Results for the trapezoidal flakes with armchair edges. **Left panel:** graphical representation of the flakes. The red-coloured atoms in the corners are directly coupled to the electrodes. Each individual considered setup employs just two of the four coloured corners serving as the electrodes-attachment areas. The electrodes are 36-monoatomic wires thick. The numbers of atoms in each flake are displayed by labels 3168, …, 19 158. $a \approx 1.42$ nm is the NN distance in graphene. See the main text for more details. **Right panel:** linear conductances $G_{\text{lin}}$ plotted as functions of the gate voltage for the structures shown in the left panel in the same vertical order. $t_g$ is the nearest-neighbour tight-binding parameter used for the entire system and $e$ is the unit charge. Solid black curves: both electrodes at the $60^\circ$ corners. Dashed red curves: one electrode at the $60^\circ$ corner, the other at the nearby $120^\circ$ corner. Solid green curves: one electrode at the $60^\circ$ corner, the other at the opposite $120^\circ$ corner. Solid blue curves: both electrodes at the $120^\circ$ corners. Legends like $60^\circ - 120^\circ$ opp. apply globally within the whole figure. For graph (e) the two plots only have been calculated. The independent variable on the horizontal axes is $V_g + \Delta V_g$, with $\Delta V_g = +0.072 |t_g|/e$, as explained in section 2.
localised ZZ-edge state and can be found to be significant if TB hoppings up to the third NN are included; this high-conductance regime would not be found for AA–AA setups within just the 1NNTBA as we have checked and provided several comparisons in appendix A, most relevantly in figure A4(b).

(ii) The conductance ratios of the OA–OA setups and the remaining ones are now larger for most of the studied $V_g$ range.

(iii) The $G_{lin}$ spectra are significantly asymmetric around the Fermi level. (iv) Rapid oscillations are visible in the $G_{lin}(V_g)$ spectra within the high conductance window.

As mentioned above, the high conductance regime of the AA–AA setup found in the vicinity of the Fermi level comes from the contribution of the ZZ edge state. Figure 3 shows the rapid oscillations of $G_{lin}$ in this gate voltage range. The oscillations can be more clearly seen in the data obtained within the 1NNTBA and consequently more easily interpreted. We demonstrate such results in SI (stacks.iop.org/JPhysCM/27/435005/mmedia) for long-narrow rhomboids. The presence of the oscillations even at gate voltages arbitrarily close to the zero can be understood taking into account the effect of the electrodes and the coupling of their modes to the flake: the semi-infinite electrodes support modes at energies arbitrarily close to the Fermi level.

Away from the energies or in the absence of the ZZ-edge-induced peaks, the electronic transport between the corners is predominantly mediated by the bulk modes, not by the edge states. This is demonstrated by the 120°–120° plots (the OA–OA setups) in figure 3, which shows the almost uniform high conductances across the whole interval of gate voltages. In this way our data in terms of the conductance reflect the fact that the ZZ edge state does not exist at and close to 120° corners [8]. The transport between the 120° corners of the ZZ-edge structures is only marginally affected by the ZZ edge states.

At the end of this section we conclude that outside the narrow range of the ZZ-edge conductance window the linear conductance of the ZZ-terminated trapezoid is typically vanishing unless the two electrodes are attached at the OA corners. Outside the ZZ-edge conductance window the contrast between the conductances of the OA–OA and AA–AA setups is several orders of magnitude. The other similarity to the case of the ac-edge terminated trapezoids is that the results for the two AA–OA setups are very close to each other (red and green plots in figure 3). Contrary to the ac edges, the proximity of the two AA–OA curves is now also found for long-narrow structures; additional examples of this feature can be found in SI (stacks.iop.org/JPhysCM/27/435005/mmedia) in the case of rhomboidal flakes. Although we do not analyse this effect we can say that it is related to the electronic modes which are used for the transport: the edge states and the bulk states. Finally, we again refer to appendix A, in particular figures A3 and A4, which use the linear scale on their conductance axes.
Besides the trapezoids, we have also addressed graphene flakes of several other shapes, including rhomboids, rhombi and equilateral triangles. All of these features 60° and 120° angles at their corners. Not surprisingly, they provide basically the same picture as the results for the trapezoids described above. Some of these results are shown in SI (stacks.iop.org/JPhysCM/27/435005/mmedia). As a different example, here we consider a flake with an isosceles triangle shape with 30° acute angles, the ac edge at the base and the ZZ edges along its sides. In other words, in the 30° angle corners the two crossing edges are of different types (ac and ZZ). Based on the above findings, we intuitively expect a large contrast between the conductances of the setups –30° and 30° –120°. The quantitative results shown in figure 4 confirm this expectation, with the exception of the isolated resonances and, more significantly, with the exception of the 0.025 |t]| narrow high-conductance channel, which is the signature of the presence of the ZZ edge, although now only a single one at each acute-angle corner. We can expect that results for the case of a ZZ base would be similar to those in figure 4.

3.4. Contact size effect

Naturally, the conductance depends on the size of the contact area, which in our model is represented by the electrode’s thickness and is quantified by the number of the monoatomic wires per electrode. We have seen that graphene flake junctions can be highly conductive, especially for the OA–OA contacts, even if the contact area corresponds to just 35 or 36 atoms. For these contact sizes the AA–AA setups have usually been found to be relatively insulating for most of the applied gate voltages, the exception being the ZZ-edge mediated transport window. In this section we study if and how the predominantly insulating behaviour is modified due to increased contact areas. We opt to study this effect on equilateral-triangle-shaped flakes. The results are shown in figures 5 and 6.

4. LDOS analysis

The current-blocking versus conductive behaviour reported above can be understood by studying the electronic modes of the graphene flakes. We use the local density of states (LDOS) of isolated flakes as a tool. We start from the definition of the density of states of an isolated flake projected onto an atomic site \( l \):

\[
\rho_l(E) = \sum_i |\langle l | \psi_i \rangle|^2 \delta(E - E_i),
\]

with \( |l| \) being the atomic orbital at the site, \( \psi_i \) is \( i \)th eigenfunction of the isolated flake and \( E_i \) the associated eigenenergy.
corner. The corners of the armchair flake, as shown in figure 2, to the
angle) reaches a maximum of only about 5 on the given
corner (solid line) within the central range of energies rel-
state contribution, the values of LDOS at the
and the corresponding peak in the LDOS. Apart from the edge
presence of the special localised edge state [3] at zero energy
as our analysis confirms, see the discussion in section 3.2. Our
LDOS data for the ZZ case confirm the absence of the edge
situation is more complicated because of the
relevant for the electronic transport studied here. In the ZZ case
graph (b) in figure 7 shows the LDOSs for the ZZ-terminated trapezoid composed of 6306
atoms of the chosen corner (36 atoms in case (a) and 35 atoms
in case (b)). In the ac case the LDOS at the 120° corner (solid red line) is clearly larger than the LDOS at the 60° corner
(dashed black line) within the central range of energies relevant
for the electronic transport studied here. In the ZZ case (figure 7(b)) the situation is more complicated because of the
presence of the special localised edge state [3] at zero energy
and the corresponding peak in the LDOS. Apart form the edge
state contribution, the values of LDOS at the 120° corner are
again much larger than the LDOS at the 60° corner. The contribution of the edge state to the electronic transport between
the corners of the flakes studied here is specifically limited or
suppressed in some cases: this state does not exist at and close
to the 120° angles of the graphene flakes, as shown in [8] and
as our analysis confirms, see the discussion in section 3.2. Our
LDOS data for the ZZ case confirm the absence of the edge
state: the solid red plot in figure 7(b) (corresponding to the
120° angle) reaches a maximum of only about 5 on the given
interval while the dashed black curve (the 60° angle) has its
maximum at about 68 (beyond the axis scale).

Finally, we note that while in the graphs with $G_{lin}$ we have applied a uniform horizontal shift $\Delta V_g = +0.072$ $|t_B|/e$ to the
calculated data (see section 2 for explanation), no such shift is
used for the LDOS data.

5. Discussion and conclusions
In this work we studied stationary zero-temperature quantum
transport through junctions formed by non-rectangular gra-
phene flakes with approximately a nanometer or several nano-
meter-thick electrodes attached at the corners of the flakes.
Such structures are perfectly compatible with a hexagonal
graphene lattice. Typical shapes are rhomboids, rhombi, trap-
ezoïds and triangles. They feature corners with angles being
integral multiples of 30°. Many of these structures have all
their edges of the same kind: either armchair (ac) or zig-zag
(ZZ). Isosceles triangles with 30° acute angles provide combi-
nations of ac and ZZ edges. The studied flakes have sizes up
to almost 20000 carbon atoms. Assuming a low bias voltage
regime we computed the linear conductance as a function of a
gate voltage applied to the flake. The computational meth-
ology was based on a tight-binding model with hoppings up
to the third nearest neighbour included and on the scattering
approach. The latter technique was employed in stationary
calculations in our recent work [16].

The main finding of the present work is that the conduct-
ance strongly depends on the size of the angles at the corners
to which the pair of the electrodes is attached. In particular, for
flakes with ac edges we can say that junctions with both elec-
trodes connected at obtuse-angle (OA) corners provide 1–5
orders of magnitude higher conductance compared to setups with the electrodes attached at acute-angle (AA) corners. The OA–OA junctions often provide high conductance values typical for metallic graphene nano-ribbons. On the contrary, a pair of the electrodes attached at acute angles forms a relatively insulating junction. The contrast between the conductances of OA–OA and AA–AA setups extends beyond one order of magnitude within a 0.15 $|t_0|$ wide interval of the chemical potential tuned around the Fermi level, $t_0$ being the nearest-neighbour hopping parameter of the tight-binding model. Exceptions are a few narrow isolated resonances at which AA–AA setups also yield a high conductance. The quantitative values depend on the dimensions of a particular flake.

For graphene flakes with ZZ edges the situation is complicated by the existence of the well-known edge state at the Fermi level. This mode couples with the electrodes and also provides the high conductance for AA–AA setups, but only within a 0.025 $|t_0|$ narrow interval of the chemical potential close to the Fermi level. For the remaining part of the spectra in the ZZ cases we again find a huge contrast between the conductances, which can be even 1–2 orders of magnitude larger than for ac edges. The spectral range in which the high contrast is found is also significantly wider that in cases of flakes with ac edges.

We have found that the reported behaviour does not change qualitatively within a range of electrodes’ thicknesses, from sub-nanometer values to several nanometers. Another important feature of real samples is the presence of edge defects and their impact on the electronic transport. It is known that AGNRs in particular are more affected by the presence of the edge disorder. On the contrary, flakes with ZZ edges are much more robust in this respect thanks to the presence of the edge state [12], see also [20, 21]. Although we did not address this problem in a systematic manner, we at least examined two representative trapezoidal flakes with imperfect edges, an ac-edge terminated trapezoid with random edge defects as well as a ZZ analogue. We provide details in appendix C and additional material in SI (stacks.iop.org/JPhysCM/27/435005/mmmedia). Our findings fully confirm the aforementioned properties: in particular for graphene flakes with ZZ edges the effects reported in the present paper remain preserved to a large extent even in the case of significant edge disorder. In the case of ac edges we observe a significant drop in the conductance of the junction, which would otherwise be highly conductive with perfect edges. Even in the ac case, the conductance of the OA–OA setup remains several orders of magnitude larger compared to the AA–AA setup within a range of gate voltages. We expect that experimental confirmation of the effects reported here could be realised using proper carbon nano-ribbon or nanotube electrodes, possibly also providing a mechanical support for the graphene flake.

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Appendix A. 1st versus 3rd nearest neighbor model

All the results in main text were obtained within the 3NNTBA. In addition, we performed several calculations in which TB hoppings up to only the first NN were included (1NNTBA). In this section we compare the results by the 1NNTBA and 3NNTBA approaches, and in this way evaluate the effect of the extended hopping range on the conductance. The wires forming the electrodes are always modelled within the 1NNTBA. The examined systems are an ac-terminated trapezoid composed of 6324 atoms (figure 2) and a ZZ-terminated one composed of 6306 atoms (figure 3). The comparisons are provided only for the AA–AA and OA–OA attachments. As opposed to the main text, in this appendix we use the linear scales on the conductance axes.

An overall view of the results for the ac case is shown in figure A1, where we display both the conductance within the 1NNTBA (solid green plots) as well as the results with the extended hoppings included (dashed red plots). The conductance spectrum in the immediate neighbourhood of the Fermi level is shown in a zoomed view in figure A2. We see that the extended TB hopping range modifies the results only quantitatively.

We now turn to the case of the ZZ-edge terminated trapezoidal flake. The results are shown in figures A3 and A4. As we can see, in this case the extended TB hopping range has a noticeable effect on the conductances within an about 0.02 $|t_0|/e$ narrow gate voltage window. Most importantly, the AA–AA setup exhibits rapid oscillations of the conductance within this range (figure A4(b), red plot), in this way opening the high-conductance window. Despite this effect, in most of the 0.3 $|t_0|/e$ wide central gate voltage window the AA–AA setup remains insulating (figure A3(b), red plot). Similar rapid oscillations of the conductance are also found for the highly conductive OA–OA setup (figure A4(a), red plot). In this case the oscillations partially decrease the conductance within the narrow central window. The conductance remains on average significant, as was also found within the 1NNTBA.

Appendix B. Electrodes composed of interacting wires

As specified in section 2, each of the two electrodes in our model is composed of a bunch of identical mutually non-interacting monoatomic wires; see figure 1, which shows a schematic graphical representation of such an electrode and its contact to the graphene flake. It may be questioned whether this model of the electrodes is sufficiently realistic. We note that in theoretical studies of electronic transport in GNRs very simple models of electrodes are often used, for example an electrode being just a continuation of the GNR [6, 7, 14, 17]. Despite the substantial difference between our model and the referenced ones we have shown [16], using AGNRs as
examples, that our results are in semi-quantitative agreement with those employing different models. We also provide similar evidence in SI, see section 1 and figure 1 therein (stacks.iop.org/JPhysCM/27/435005/mmedia).

In addition, here we perform an explicit test of how our result would change if the wires were mutually interacting. To achieve this we assume a model in which the atoms of the wires within a $20\alpha$ vertical distance from the flake surface become mutually coupled using the 3NNTBA model with the same parametrisation as used for the graphene flake. That is, we assume an augmented central system formed by the flake and by the finite pieces of the electrodes (FPEs). The FPEs are those parts of the electrodes in which the wires are mutually coupled. All the couplings within the augmented system are treated on an equal footing using the 3NNTBA model. In this more complex model we still employ the semi-infinite mutually decoupled wires. They are fixed to the ends of the FPE, not to the flake. The couplings within the FPE, although not describing any real system, provide us with a verification example as to whether or not the internal structure of the electrodes is important for the effects studied in the present paper. As a test case we choose the ZZ-edge terminated trapezoidal flake shown in the left panel in figure 3, the second structure from the top. The results shown in figure B1 clearly demonstrate that the different model of the electrodes has only a marginal impact on the results reported in our present work. We can draw the conclusion that the effects reported in the present paper can be found for various types of electrodes assuming that they have an order of nanometer thickness.

Figure A1. Linear conductances compared for the 1NNTBA (solid green line) and 3NNTBA (dashed red line) models. The examined structure is the ac-terminated trapezoid composed of 6324 atoms (figure 2). The functions for the 3rd NN model have been horizontally shifted by $\Delta V_g = +0.072 [\text{meV}]$, as specified in the main text, section 2. Graph (a) shows the results for the electrodes attached at the $120^\circ$ angles. Graph (b) shows the analogous results for the $60^\circ$ angles. The models of the electrodes are identical to those used for the results in figure 2. See also figure A2 for a detailed view of the low-$V_g$ interval of the present graph. Note that for the figures in this section we use the linear scales also on the vertical axes.

Figure A2. A detailed view of the results from figure A1.

Figure A3. Linear conductances compared for the 1NNTBA (solid green line) and 3NNTBA (dashed red line) models. The examined structure is the ZZ-terminated trapezoid composed of 6306 atoms (figure 3). The curves for the 3NNTBA model have been horizontally shifted by $\Delta V_g = +0.072 [\text{meV}]$, as specified in the main text, section 2. Graph (a) shows the results for the electrodes attached at the $120^\circ$ angles. Graph (b) shows the analogous results for the $60^\circ$ angles. The models of the electrodes are identical to those used for the results in figure 3. See also figure A4 for a detailed view of the low-$V_g$ interval of the present graph.

Figure A4. A detailed view of the results from figure A3.
Appendix C. Impact of the edge disorder

In order to qualitatively assess the impact of the irregular edges on the main effects reported in the present paper, we perform calculations for two representative junctions. The first is based on the ac-edge terminated trapezoid shown in the left panel in figure 2, the second structure from the top. After the introduction of several random edge defects (including defects close to the corners) the structure consists of 6245 atoms (an image is provided in SI, figure 7 therein (stacks.iop.org/JPhysCM/27/435005/mmedia)). The perturbations are made in such a way that every carbon atom at the border has either two or three nearest-neighbour carbons. Similar to structures with regular edges, here we also assume that the edges are terminated by hydrogen atoms [12]. All three bonding parameters $t_B$, $t_B'$ and $t_B''$ remain the same as for models with perfect edges. Similarly, we keep all the equilibrium on-site energies at zeros. Due to the defects present even at the corners the electrode’s thickness has been slightly reduced to 34 monoatomically thin wires for each of the two electrodes. The calculated linear conductances for the AA–AA and OA–OA setups are shown in figure C1 and should be compared to figure 2(b), which uses the same colour coding. Graphs directly comparing the perfect and imperfect border cases and an image of the structure can again be found in SI, figure 7 therein (stacks.iop.org/JPhysCM/27/435005/mmedia).

(ii) the average magnitude of $G_{\text{lin}}$ has been decreased by about a factor of 10, i.e. the high conductance of the OA–OA setup has been lost, (iii) the $G_{\text{lin}}$ profile for the AA–AA setup has also got a more oscillatory character, (iv) the $G_{\text{lin}}(V_g)$ profile for the AA–AA setup now exhibits signs corresponding to the ZZ edges; see the central double peak in the black plot in figure C1 just above the zero energy. The latter feature is not surprising because some of the defects in the ac edges provide pieces of ZZ-type termination. Despite these modifications the conductance of the AA–AA setup is on average still several orders of magnitude below those of the relatively conductive OA–OA setup.

The second junction with imperfect edges is based on the ZZ-edge terminated trapezoid shown in the left panel in figure 3, the second structure from the top. The flake with the
defects is made up of 6219 atoms, the electrodes are 33 wires thick and the other conditions and treatment are the same as in the ac case described above. The results are presented in figure C2 and should be compared to figure 3(b). As in the ac case, additional graphs as well as an image of the flake can be found in SI, figure 8 (stacks.iop.org/JPhysCM/27/435005/mmedia). We observe that the disorder introduced to the ZZ edges has a noticeable impact on the linear conductance function. This impact is smaller than in the ac case, fully in line with the findings of [12]. Most significantly, the narrow window of the ZZ-edge state-induced high conductance (just at the Fermi level) becomes even narrower, which is easily comprehended because the ZZ edges are now frequently interrupted by the defects. Away from the Fermi level the conductance of the OA–OA setup is also high and, interestingly, almost unaffected by the disorder (compare the blue plots in figures 3(b) and C2). At these gate voltages the $G_{\text{tot}}(V_g)$ profile of the (insulating) AA–AA setup is also little impacted by the ZZ edge defects (compare the black plots in figures 3(b) and C2).

We can finally conclude that the main effects reported in the present paper are to a significant extent also found to be operational for flakes with edge disorder.

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