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Published in:
Carbon

Link to article, DOI:
[10.1016/j.carbon.2016.01.084](https://doi.org/10.1016/j.carbon.2016.01.084)

Publication date:
2016

Document Version
Early version, also known as pre-print

[Link back to DTU Orbit](#)

Citation (APA):

Jacobsen, K. W., Falkenberg, J. T., Papior, N. R., Bøggild, P., Jauho, A-P., & Brandbyge, M. (2016). All-graphene edge contacts: Electrical resistance of graphene T-junctions. *Carbon*, 101, 101-106. <https://doi.org/10.1016/j.carbon.2016.01.084>

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All-graphene edge contacts: Electrical resistance of graphene T-junctions

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Abstract

Using *ab-initio* methods we investigate the possibility of three-terminal graphene “T-junction” devices and show that these all-graphene edge contacts are energetically feasible when the 1D interface itself is free from foreign atoms. We examine the energetics of various junction structures as a function of the atomic scale geometry. Three-terminal equilibrium Green’s functions are used to determine the transmission spectrum and contact resistance of the system. We find that the most symmetric structures have a significant binding energy, and we determine the contact resistances in the junction to be in the range of 1 – 10 k Ω μ m which is comparable to the best contact resistance reported for edge-contacted graphene-metal contacts[1, 2]. We conclude that conducting all-carbon T-junctions should be feasible.

1. Introduction

Two-dimensional (2D) materials are being vigorously investigated as a platform for nano-scale electronics due to their potential use *e.g.* in flexible electrodes[1], high performance electronics, photovoltaics and spintronics[3]. Graphene plays a key role, not only because it was the first 2D material to be isolated and experimentally characterized[4], but also because of its

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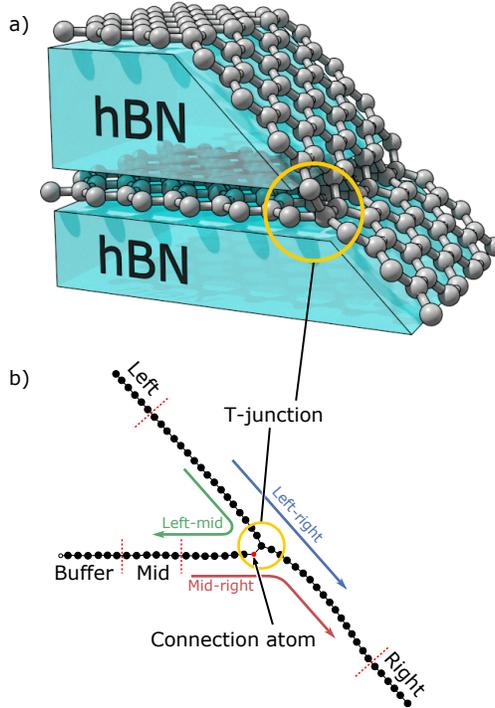


Figure 1: **a)** Sketch of a possible experimental realization where the GTJ is partly encapsulated in a stack of hexagonal boron-nitride. **b)** Schematic of the graphene T-junction system (side view) consisting of 3 semi-infinite graphene electrodes (“Mid”/“Buffer”, “Left”, “Right”) used in the DFT-EGF calculation. In the calculations that include passivation, the connection atom was substituted with other elements. The structure shown here is the result of a nitrogen substitution in the ZZ geometry.

extraordinary electronic properties, which can be harnessed by various types of nanostructuring and chemical functionalization[5, 6, 7, 8, 9, 10, 11, 12].

Recently graphene has played a role as contact electrode to semi-conducting transition metal di-chalcogenides (TMDC) encapsulated in insulating hexagonal boron-nitride (hBN) layers[2]. In these devices graphene is connected to the external circuit via one-dimensional edge-contacts to 3D metal electrodes[2, 13]. In the fabrication process the hBN-G-hBN stack is etched with a slope of approximately 45° resulting in a graphene edge being exposed to subsequent metal electrode deposition.

While these studies have so far focused on planar devices it is relevant to investigate various ways of extending the 2D structures into 3D circuitry.

To this end, and inspired by the experimentally realized 1D edge contacts[2], we here use first principles calculations to investigate graphene T-junctions (GTJ), where the bulk metal electrode is replaced by graphene as illustrated in Fig. 1 and 2. The out-of-plane bonding is possible due to the sp^2 nature of graphene, which can hybridize further to sp^3 and thus allows the formation of a “standing” sheet (or ribbon). The electronic properties of the graphene T-junctions are only limited by the junction itself as the long range ripples are an intrinsic detail in graphene[14]. Formation of such a T-junction requires the edge atoms of one layer to form covalent bonds to the plane of another layer, which can either be done by fusing or by synthesis. Coalescing or fusing of separate carbon nanostructures can either be achieved through Joule heating[15, 16], ion[17, 18] or electron[19] irradiation, where the extraordinary ability of sp^2 carbon nanostructures to self-repair[20] can be exploited to reach well-defined, stable, low-energy configurations. In principle, the alternative approach of bottom-up synthesis can also lead to creation of complex hybrid all-carbon architectures with interconnections such as graphene carbon-nanotubes[1, 21], 3D interconnected graphene “foam”[22] and vertical T-junction-like “nanowalls”[23, 24]. While graphene-nanotube two-terminal systems have been investigated by first principles calculations[25], the electronic transport properties of T-junctions involving three semi-infinite graphene or graphene nano-ribbon (GNR) electrodes have not, to the best of our knowledge, been investigated. The paper is organized as follows: In Sec. 2 we describe the systems and computational method. In Sec. 3 we present the results for the energetics and structure of both infinitely wide junctions and narrow ribbon junctions to the graphene plane, and discuss the electronic transmission as a function of electronic energy (doping level or gate voltage) and electrical contact resistance. Finally, we summarize the results and present an outlook of future work and experimental realization of graphene T-junctions in Sec. 4.

2. Systems and methods

In order to predict the atomic structures and their binding energy we employ density functional theory calculations (DFT). Electronic transport is calculated by the Green’s function method[26] extended to the multi-terminal case, which in the present work involve three electrodes denoted “Left”, “Right” and “Mid”, see Fig. 1. The middle electrode corresponds to a graphene layer which for instance could be encapsulated in a hBN stack

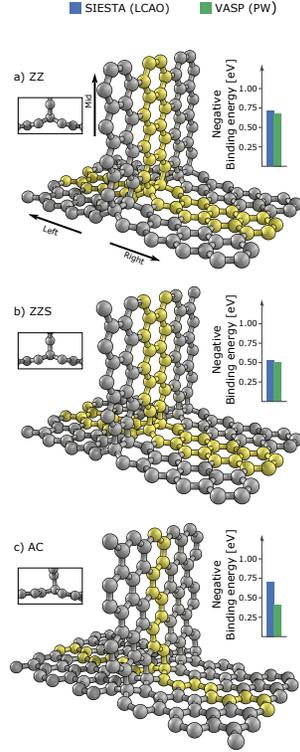


Figure 2: Sketch showing the three main principal structures of interest. The structures are periodic in the transverse direction and yellow indicates atoms belonging to the unit cell. The insets show the binding energy of the middle part as calculated with the SIESTA (blue bar) and VASP (green bar) codes which are in reasonable agreement. The insets show sideviews of the structures, clearly illustrating the sp^3 geometry at the junction.

as shown in Fig. 1. Here only non-gated graphene electrodes are considered, while in general care must be taken to account properly for gating effects of graphene electrodes[27]. The geometrical structure of the junction is, as we shall see, a main factor determining the resistance.

We first focus on the two main symmetry directions of current flow in graphene (zig-zag and armchair) and consider three different principal structures corresponding to perfect match in the junction as shown in Fig. 2. We note that the structures have been rotated compared to Fig. 1 so that the “mid”-section is pointing out-of-plane of the graphene sheet going from “left” to “right”. The simplest possible connection is denoted “ZZ” according to the zig-zag edge of the attached “ribbon” as shown in Fig. 2a, and is mirror

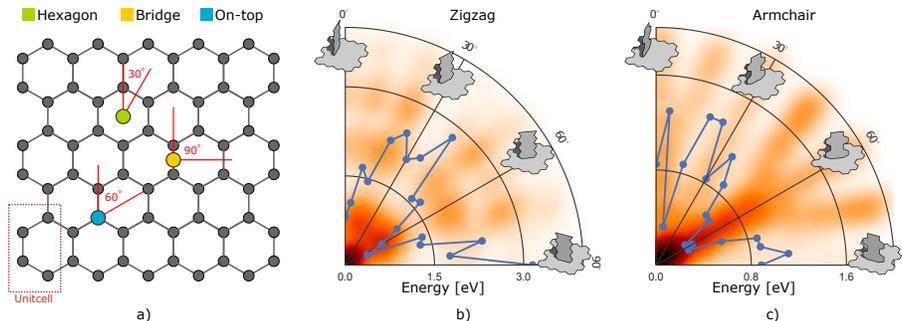


Figure 3: **a)** The setup for the starting configurations of the calculations of ribbon T-junctions. Each calculation was initiated with the ribbons placed one bondlength above the base sheet and with the bottom corner atom above one of the three sites, hexagon (green), bridge (yellow) or on-top (blue). The ribbons were rotated around the anchor points in steps of 5° between the directions indicated with red. **b), c)** The blue curve shows the mean energy of the three ribbons started at each angle (one for each site). It is shown atop a gaussian kernel density plot (red colors) of the two bottom rows of atoms in each of the relaxed ribbons translated to have the outermost atom in the same point and projected onto the plane. The orientation of the underlying graphene sheet is as in a). Both types of ribbons energetically favor the 0° and 60° directions, making the zig-zag ribbon similar to the ZZ(S) structure in Fig. 2, but the armchair ribbon different from AC in the same figure.

symmetric around the middle part and involves only hexagonal carbon rings. The second principal structure is a shifted zig-zag (ZZS) and is also mirror symmetric, but the middle part has been shifted one half of a unit cell resulting in 4- or 8-ring transition in the T-junction. The armchair junction (AC) in Fig. 2c has no mirror-symmetry between the electrodes. However, it is noted that the left-mid and the mid-right transitions have similar grain boundary types in the junctions. In Sec. 3.2 we will see how this similarity is reflected in the transmission through the junction. For all these structures we employ periodic boundary conditions (PBC) along the one-dimensional junction. We have also investigated junctions with an initial angle different from 90° between the “mid” section and the base sheet. When allowed to move freely, however, the “mid” section relaxes towards the symmetric configuration in all cases.

In order to examine the role of a less symmetric match in the T-junction we also investigate *rotated* junctions by attaching the nano-ribbons in the “Mid” position on top of an infinite graphene sheet (still containing “Left”/“Right” electrodes). Both zig-zag and armchair nano-ribbons are investigated by plac-

ing the bottom right carbon atom one bond-length above the graphene sheet consisting of 10×5 4-atom unit cells (indicated in Fig. 3). The attachment site on the graphene sheet is chosen among the three high-symmetry sites, *on-top*, *bridge*, and *hexagon*, as illustrated in Fig. 3a. For each attachment site, the ribbons are rotated in steps of five degrees within the angles as indicated in the figure.

In summary, with the use of periodic boundary conditions, we examine T-junctions formed by infinite graphene sheets as shown in Fig. 2 and finite-width ribbons intersecting with an infinite graphene layer as depicted in the small illustrations in Fig. 3.

2.1. Computational methods

The DFT calculations were performed using the software packages SIESTA[28] and VASP[29]. The former utilizes a localized basis set (LCAO), which allows much faster calculations than the more accurate plane-wave basis in VASP, which provides a quality check on the total energies of the LCAO method. A SZP basis set was chosen for SIESTA after noting only negligible differences in the resulting relaxed geometries and transmission spectra when comparing to a DZP basis set. The plane-wave calculations used a cut-off of 400 eV. The PBE-GGA functional for exchange-correlation[30] was used for both methods, as well as an atomic force tolerance of 0.04 eV/Å. Additionally, the SIESTA calculations used confinement radii determined from an energy shift of 275 meV with a real-space grid cutoff energy of 300 Ry. The PBC of the principal structures along the 1D junction was utilized in k -point sampling by a Monkhorst-Pack grid of $15 \times 1 \times 1$ ensuring relative energy convergence. In the subsequent transport calculations, the three electrodes (“left”, “right”, and “mid”) were all treated as semi-infinite while the system was modelled as periodic in the transverse direction. The transport calculations were performed using the TranSIESTA[26, 31] method extended with a recently implemented N -electrode capability following Saha et al. [32]. This allows the description of proper boundaries for the three semi-infinite graphene leads. All electrodes are described using surface self-energies from separate bulk calculations. Here we focus on low bias properties and only present equilibrium transport calculations while full non-equilibrium calculations are presented elsewhere[31]. We extended the “Mid” electrode using “buffer” atoms[26] in order to obtain a bulk electrode potential profile for this. Transmission calculations are performed using 100 k -points and post-processed using the interpolation technique described by Falkenberg

and Brandbyge [33] in order to obtain well converged smooth transmission functions.

3. Results

3.1. Energetics

All three structures shown in Fig. 2 have a negative binding energy, and could thus be experimentally feasible. The total energy calculations were consistent when comparing energies from SIESTA with VASP after relaxing the atoms, as is shown as bars to the right of the structures in Fig. 2.

We investigate the rotation of ribbons perpendicularly attached to a graphene sheet, but attached to the sites shown in Fig. 3a and allowing the atoms to relax. In the calculation, one row of atoms in the base sheet was fixed in space while all other atoms – including the entire ribbon – was free to relax. The zig-zag and armchair ribbons were both four rows of atoms wide. Only negligible rotation is observed of the carbon atoms in the GNRs the furthest away from the base sheet, thus allowing us to define a starting angle. The averaged energy of the three ribbon configurations is shown in Fig. 3b,c. The blue line is the mean energy for the three relaxed structures at each starting angle subtracted the minimum energy configuration of the entire set of structures. The angles in Fig 3b,c indicate the initial rather than the final angle of the relaxed structure, which may be slightly different. In order to examine the relaxed direction a density map of atoms is shown as the background of the energy plot. All relaxed configurations have been translated and projected to the graphene plane.

We see that the zig-zag ribbons preferentially will be oriented in the directions similar to the principal periodic structure in Fig. 2a, and are thus corresponding to a geometric transition similar to that of pristine graphene. Note that the armchair ribbons also have the lowest energies when oriented along the armchair direction of the base sheet and are thus *not* similar to the periodic armchair structure described earlier, cf. Fig. 2c. In this configuration, the ribbons are situated symmetrically, but in a way that cannot be periodic without inducing a substantial strain in the graphene layers. Fig. 3c seem to break the 60° -rotation symmetry as the energies at 0° and 5° are much larger than the ones around the other armchair direction. This is caused by one of the three calculated structures in each case that quickly relaxed in to a local minimum with very high energy, thus raising the average energy considerably.

3.2. Transmission

The transmission spectra shown in Fig. 4 show conductance per junction length for each of the three principal systems and between each of the three electrodes defined in Fig. 2. The gray transmission curve is that of pristine graphene. The geometric symmetries of the periodic zig-zag structures (ZZ, ZZS) are reflected in the transmission spectra as the left-mid (blue) and the mid-right (green) curves are identical. Interestingly, it is found that the transmission T through the base sheet (*i.e.* left-to-right) is lower than that from the base and into the mid-terminal for all principal structures. In contrast to the ZZ and ZZS structures the armchair (AC) transmission spectrum display a bandgap-like feature for low energies, but yield the highest transmission into the mid-electrode from left (green curve in Fig. 4 AC) of all the structures.

We can compare the left-right transmission $T_{\text{left-right}}$ through the ZZ structure to that found for hydrogenated kinked graphene[12]. This can be done by realizing that the row of atoms in the mid-part closest to the junction can be exchanged by hydrogen atoms while the rest of the mid-atoms can be removed. Since the junction atoms are allowed to relax we locally have an sp^3 -configuration directly comparable to the hydrogenated kinks acting as transmission barriers. There are minor numerical differences in normalized transmission but the trends remain the same: hole transport slowly grows to around $0.03 G_0/\text{\AA}$ at -2 eV, while the electron transmission grows more rapidly to $0.1 G_0/\text{\AA}$ at 2 eV.

As previously stated, there are similarities in the atomic transitions from left-to-right and from mid-to right in the AC structure. One could thus expect $T_{\text{left-right}}$ and $T_{\text{mid-right}}$ to differ from $T_{\text{left-mid}}$ and this is also what is found in Fig. 4 AC. The $T_{\text{left-right}}$ and $T_{\text{mid-right}}$ transmission spectra are rather similar even though the angle the electrons have to pass through differs greatly.

For the sake of completeness, we have also briefly investigated the effect of forcing the “mid” part into an non-orthogonal angle with the base graphene. As previously mentioned, the ZZ(S) T-junctions relax towards the symmetric structures shown in Fig. 2 and to avoid this, we have in one case fixed the “mid” terminal part to move doing these relaxations. With an imposed angle of 55° between the “mid” and “right” terminals in an ZZ configuration, only minor changes in the transmission spectrum was observed. The left-to-right and left-to-mid transmissions remained almost unaffected while the mid-to-right lowered a bit to have roughly the same behavior as left-to-right.

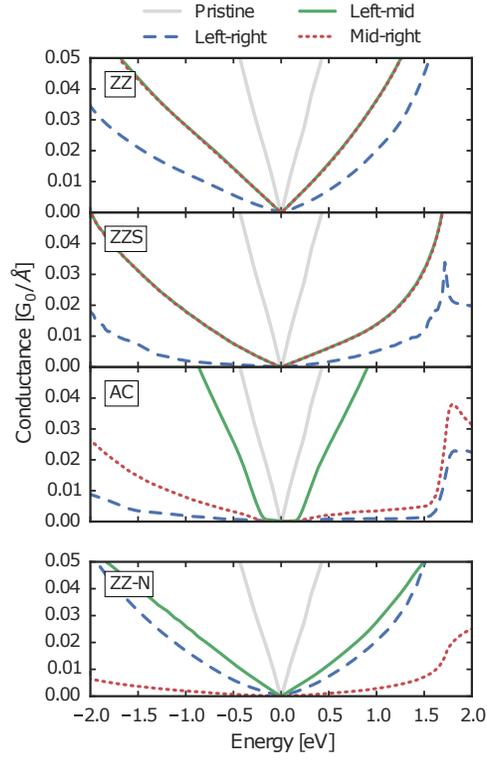


Figure 4: Transmission through the T-junctions for the structures in Fig. 2 (Fermi energy, $E_F = 0$). The bottom frame shows the transmission spectrum for ZZ-N where nitrogen replaces carbon as connecting atoms in the arm of the ZZ junction (cf. red atom in Fig. 1b).

3.3. Passivation

Wang et al. suggest[2] that graphene edges exposed after etching might be passivated with H, F or O. They further treat the edges with an O_2 plasma to change chemical composition[34, 35]. After such processing the edges may be oxygen terminated while other contaminants remaining from the edges should have been removed. To investigate the effects of this edge termination on the transport through the junction we substituted the edge atoms (see connecting atom in Fig. 1b) of the principal T-junction structures with H, F, O or N. We found, as expected, that H and F passivated edges did not bind to the graphene base sheet. On the other hand we found that while O only bonds in one case (ZZ), N binds to both in the ZZ and ZZS structures. A negative formation energy has been obtained for N on a clean zig-zag edge, originating from a N_2 gas[36] making incorporation during hBN etching a possibility. Most importantly, both O and N in the connection introduce an angle between the mid part and the base sheet around 45° , see Fig. 1b which shows the relaxed ZZ-N structure. The same size as the angle in the hypothetical structure based on the hBN-G-hBN setup due to the etch[2] as illustrated in Fig. 1. As seen from Fig. 4 (ZZ-N) the introduction of N in the junction and the resulting angle breaks the left-mid and right-mid symmetry in the transmission spectrum. Now left-mid transmission is significantly higher than that of right-mid while the left-right transmission is nearly unchanged compared to the C-only junction (ZZ). Even though the symmetry breaking due to the nitrogen completely changes the transmission, the magnitude of the transmission does not vary much between the various configurations. We note that similar high left-mid/left-right transmissions were obtained for O passivation.

For all the relaxed structures with a negative binding energy, similar calculations, *i.e.* the same number of atoms, were made, but without a connection between the mid part and the base sheet. That is, the atoms were lifted off the graphene sheet such that no contact was possible between the two. This setup was then relaxed, and the energy was used as reference for the binding energy. None of the edge-passivated structures had lower energies when forming a T-junction and are thus unlikely to occur.

3.4. Junction resistance

In order to determine the resistance of the contact between the graphene sheet and the attached “Mid” graphene terminal, we calculated the mean junction resistance for electrons with energies on each side of the equilibrium

Fermi energy ($E_F = 0$) in the $0\text{ eV} - 0.5\text{ eV}$ range, and likewise for holes, in the $-0.5\text{ eV} - 0\text{ eV}$ range. This can be compared to the pristine graphene result for both principal structures and their ribbon counterparts. The result is shown in Fig. 5. Note that since the armchair ribbons have a bandgap we average from the valence/conduction band edges for holes/electrons in this specific case. This explains why some of the AC ribbon resistivities are smaller than their corresponding values for the infinite structures. In general, it is seen that the infinite structures are much more electron-hole-symmetric than the ribbons and have lower resistances. This can clearly be seen in the combined mid-right/left-mid resistance,

$$R_{\text{combined}} = \left(\frac{1}{R_{\text{MR}}} + \frac{1}{R_{\text{LM}}} \right)^{-1}$$

which takes into account both sides of the base layer through the junction.

In an experimental realization of the T-junction it is likely that the connection between the two parts consists of many different bonding configurations due to disorder, defects and the specific orientation of the sheets. In such a case, the transmission would be dominated by the most transparent interface and would probably average to some effective resistance over the junction length.

4. Discussion and Conclusions

Using *ab initio* calculation methods, we find that three-dimensional graphene T-junctions are energetically feasible when no passivation is present in the connection. For N and O passivation some of the junctions are stable, but unlikely to occur because of their relatively high formation energy. The analysis of junctions created between graphene ribbons and an infinite base sheet using a large ensemble of possible starting configurations, revealed a preferential junction orientation along the armchair direction. Interestingly, this was regardless of whether the ribbons were of zigzag or armchair type.

Utilizing the three-terminal Green's functions transport capabilities of TranSIESTA, we find that the transmissive properties of the junctions depend heavily on the specific connection geometry, but that the transmission from the base graphene sheet to the middle terminal is larger than the one through the base sheet. The contact resistance of various metals end-contacted to graphene encapsulated in hBN have been measured[2]. The

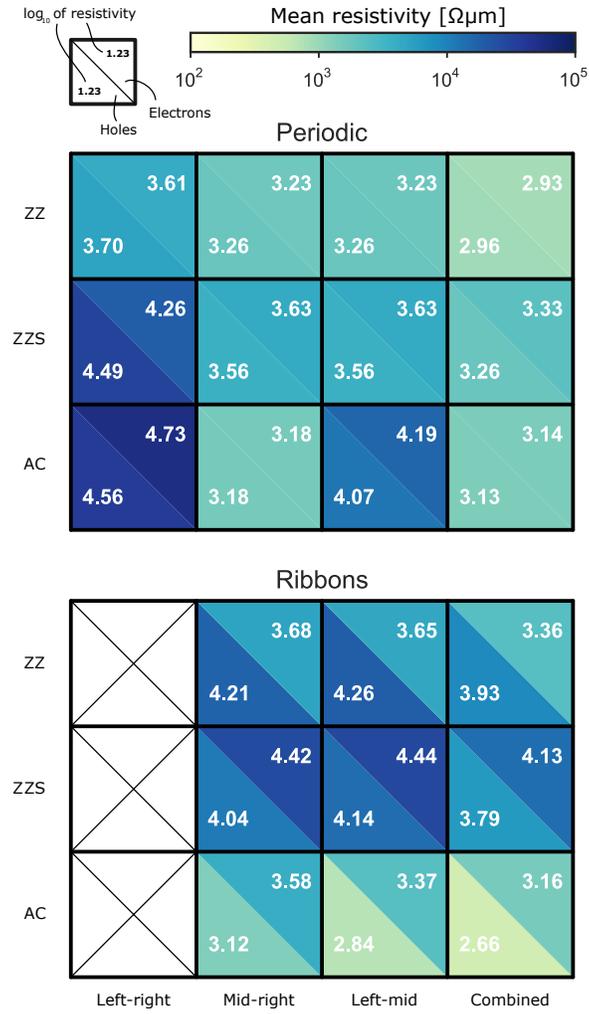


Figure 5: Resistance times length in the T-junctions compared to similar ribbons. The resistivity is taken as the mean value of electrons with energies between 0 eV and 0.5 eV on both the hole and the electron side.

lowest are obtained using Cr ($\sim 0.1 \text{ k}\Omega \mu\text{m}$), followed by Ti ($\sim 10 \text{ k}\Omega \mu\text{m}$) and Al, Pd ($\sim 100 \text{ k}\Omega \mu\text{m}$).

Our results show that not only are such T-junctions feasible, but also in some configurations exhibit superior contact properties. More importantly, the emerging van der Waals technique[37, 2] provides an ideal platform for creating such edge-plane contact architectures in a controlled and possibly scalable manner. Since a number of techniques to form seamless junctions between carbon nano-structures have been demonstrated experimentally, the T-junction architecture opens for a number of exciting possibilities. While we show that the behavior of the all-graphene junctions is already rich, structurally similar materials that should immediately be possible to join and combine in T-junctions include hexagonal boron nitride and boron-carbon-nitrogen alloys[38], where a mix of boron, carbon and nitrogen atoms allows for tunability of the electrical properties, paving the way for bandgap engineered T-junctions. A T-junction with a single sheet of graphene terminated with a few atomic rows of hBN grown by in-plane heterostructures[39] would be a compelling 1D equivalent of a field effect transistor, with the shortest channel imaginable. In fact, the topological similarity with several transistor geometries combined with in-plane heterosynthesis suggests that other 1D analogues of conventional semiconductor components should be possible to realize. Finally, control of the edge chemistry[40] opens for a wide range of possibilities in terms of tailoring the structural and electrical properties of such junctions.

Acknowledgement

The authors thank Bjarke Sørensen Jessen, Lene Gammelgaard, and Filippo Pizzocchero for sharing their experimental insight and ideas, and Dr. Gemma Solomon for valuable comments. Furthermore, the authors thank the Danish e-Infrastructure Cooperation (DeIC) for providing computer resources, EC Graphene FET Flagship (contract number 604391), and the Lundbeck foundation for support (R95-A10510). The Center for Nanostructured Graphene (CNG) is sponsored by the Danish National Research Foundation (Project DNRF103).

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