

Charge transfer engineering in graphene nanoribbons using metallic contacts and organic adsorbed layers

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Graphene is a very promising material for electronics due to its extremely high electron mobility. Its two-dimensional structure is especially well suited for the current microfabrication techniques. On the other hand, most electronic devices are not built from semi-metals such as graphene but rather from semiconductors. Fortunately, graphene can be made semiconducting after being engineered into nanoribbons [1, 2], and then can be incorporated into the fabrication of transistors [3, 4].

The electronic interactions between graphene nanoribbons (GNRs) and the indispensable metallic contacts remains a source of high interest since critical features at such a small length scale, for example the presence of metal induced gap states (MIGS), can have a dramatic impact on the final device performance. Beyond the effect of metallic electrodes, an interesting approach to control the electronic properties of GNRs through doping would be to use a self-assembled adsorbed layer (see Figure 1) [5]. In addition, this adlayer could also act as an additional conduction channel when properly connected to the electrodes.

Accordingly, we report the results of first principles density functional theory (DFT) calculations of finite GNRs in contact with Au and Pd electrodes. Our results make clear evidences of the molecular hybridization between frontier orbitals of GNRs and the metallic states. Moreover, we observe significant charge transfer from graphene to the electrode which extends into the nanoribbon beyond the zone located immediately under the contact. In the case of zigzag GNRs, the charge transfer is mainly accommodated by the ribbon's edge states (see Figure 2). By plotting the local density of states (LDOS) at the Fermi level (see Figure 3), we have evaluated the penetration length of MIGS. For the adsorbed organic layer, our first DFT calculations suggest that the chemical nature of the layer appears more important than the native structure (armchair, zigzag) of the GNRs on the magnitude of doping.

References

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Figures

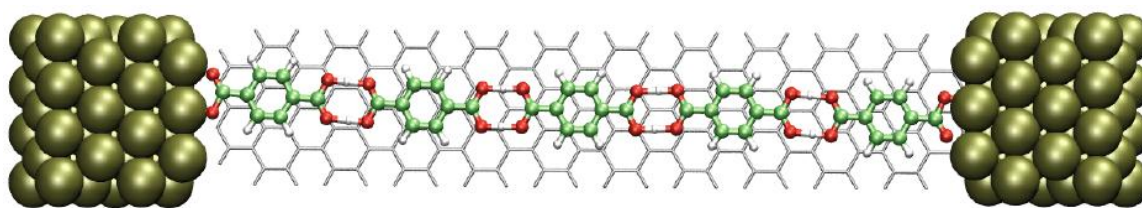


Figure 1: Terephthalic acid chain adsorbed on an armchair GNR between two metallic contacts.

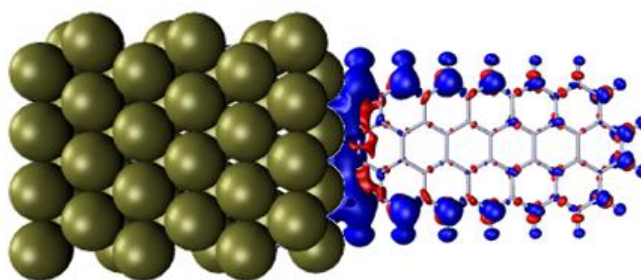


Figure 2: Change in the electronic density (red for positive, blue for negative) of a zigzag GNR in contact with an Au (111) electrode.

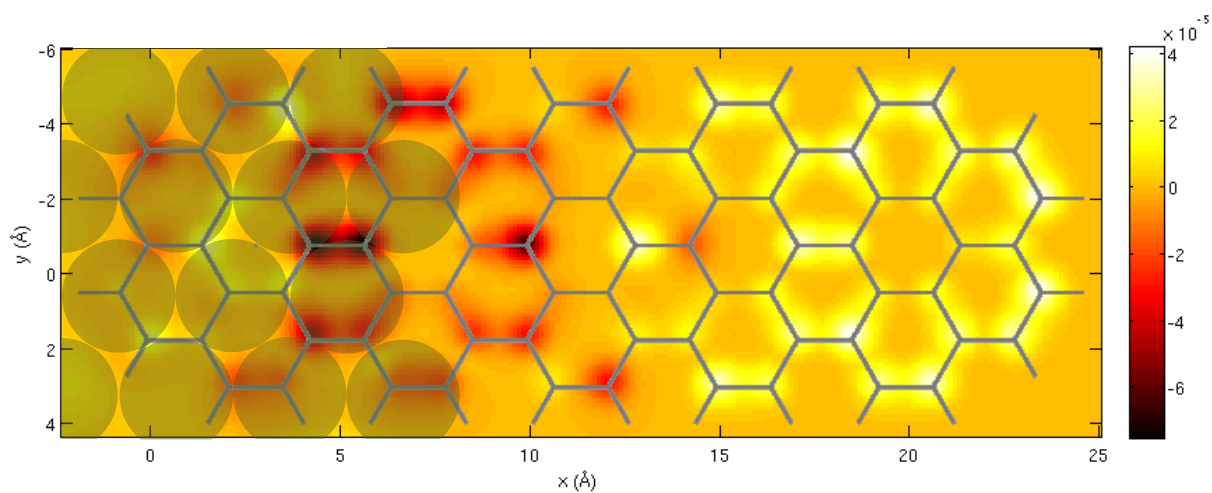


Figure 3: Variation in the LDOS of an armchair GNR at Fermi energy upon addition of an Au (111) contact (represented by darker circles).