Carbon-based nanoelectronics: insights from calculations

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Carbon-based nanomaterials such as graphene, graphene nanoribbons, and carbonaceous molecular wires are the basis of carbon-based nanoelectronics. For their true potential to be realized, a precise control and understanding of the conformational or chemistry related electronic signatures in these carbon-based systems is crucial. By using state-of-the-art experimental techniques, planar and vertical functional carbon-based electronic units can now be built with atomic precision, which has opened the door to exploring their electronic and transport properties at the nanoscale.

In this talk, I will present some density-functional theory (DFT) based studies of electronic and transport properties of carbon-based nano-structures that we have performed in collaboration with our experimental colleagues.

On one hand, we have studied a family of carbon-based molecular wires composed of different functional groups vertically attached to an extended organic platform. We have shown that, depending on the length and chemistry of the functional group, these molecules can behave as switches or rotors.[1,2,3]

On the other hand, we have extensively investigated the influence of chemical doping in graphene nanoribbons. Our studies show that, changing the nature and position of the dopants, the electronic properties of the nanoribbons can be finely tuned.[4,5] Remarkably, we have found that substitutional boron atoms can induce magnetism in armchair graphene nanoribbons.[6]

References

[1] T. Jasper-Tönnies *et al.*, Phys. Rev. Lett. 119, 066801 (2017)

[2] T. Jasper-Tónnies *et al.*, J. Phys.: Condens. Matter 31, 18LT01 (2018)

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Figures

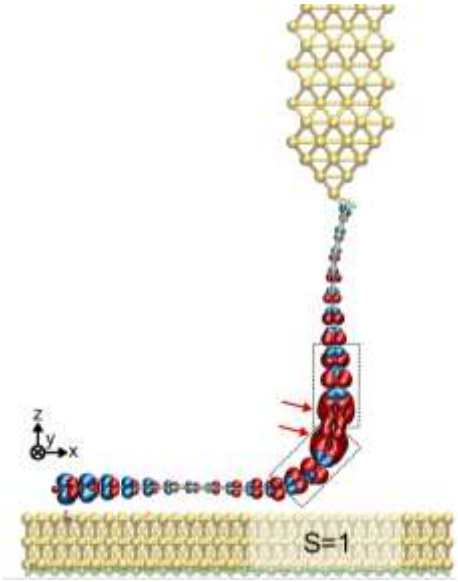

Figure 1: DFT optimized structure of a 7-armchair graphene nanoribbon doped with a pair of boron atoms, and contacted by a scanning tunneling microscope (STM) tip. Magnetization isosurfaces are shown over the atomic structure.