Graphene nanoarchitectures: insights from theory and experiments

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Graphene-based materials *are* promising units for the development of novel electronic, spintronic or optoelectronic devices. For *their true potential to be realized, a precise* atomic-level *control and understanding of the conformational or chemistry related electronic signatures in these systems is* crucial. *By using state-of-the-art experimental techniques,* graphene nanoarchitectures *can now be built with atomic precision, which has opened the door to exploring their electronic properties at the nanoscale.*

In this talk, I will review some of our works on graphene nanoarchitectures, performed in close collaboration with our experimental colleagues. Using density-functional theory (DFT), we have investigated the electronic, magnetic and transport properties of graphene nanoribbons and nanoporous graphene, with special focus on the role of chemical doping and the creation of tunable pores in the carbon backbone. Our findings are compared with scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES).

Depending on the conformational details and the doping mechanism, various effects are observed and explained, such as semiconductor-to-metal transition, energy gap modification, tuning of topological properties, emergence of magnetism and control of electron confinement.[1-4]

References

[1] J. Li *et al.*, ACS Nano 14, 1895 (2020)
[2] M. Panighel *et al.,* ACS Nano 14, 11120 (2020)
[3] N. Friedrich *et al.,* Phys. Rev. Lett. 125, 146801(2020)
[4] J. Li *et al.,* Nat. Commun. 12, 5538 (2021)

Figures

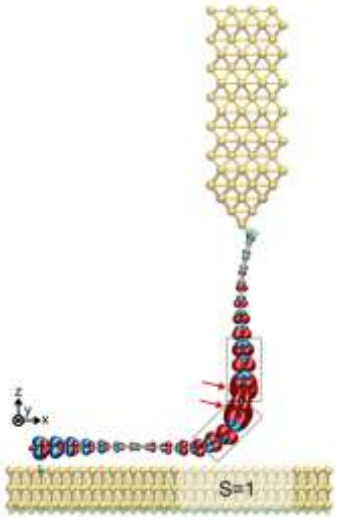

Figure 1: DFT optimized structure of a graphene nanoribbon doped with a pair of boron atoms, and contacted by a scanning tunneling microscope (STM) tip. Magnetization isosurfaces are shown over the atomic structure. Figure adapted from Ref. [3].