Graphene nanoarchitectures: insights from theory and experiments

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Nanostructuring graphene at the atomic scale is now possible by on-surface synthesis methods, which unite the sturdiness of covalently bonded networks with the easy tunability of molecular materials. These experimental advances have boosted the research attempts to create novel 0D, 1D and 2D carbon-based structures aimed at the development of new nanoelectronic or optoelectronic devices. However, before graphene nanostructures can be used in practical applications, an atomic level understanding and control of their properties is required. As such, *ab-initio* simulation has developed as an essential partner in the search of optimal graphene-based low dimensional materials.

In this talk, I will present some studies of graphene nanostructures, in particular graphene nanoribbons (GNRs) and nanoporous graphene (NPG), that we have perfomed in collaboration with our experimental colleagues.[1,2,3] Using density-functional theory (DFT), we have investigated their structural, electronic and transport properties, with special focus on the role of chemical doping and the creation of pores in the carbon backbone. Our findings are compared with scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission (ARPES) data. Depending on the conformational details and the doping mechanism, various effects are observed and explained, such as electron confinement, energy gap modification, or semiconductor-to-metal transition.

References

[1] J. Hieulle *et al.*, Nano Letters 18, 418 (2018).
[2] E. Carbonell-Sanromà *et al.*, Nano Letters 17, 50 (2017); J. Phys. Chem. C 122, 16092 (2018).
[3] Moreno *et al.*, Science 360, 199 (2018).

Figures

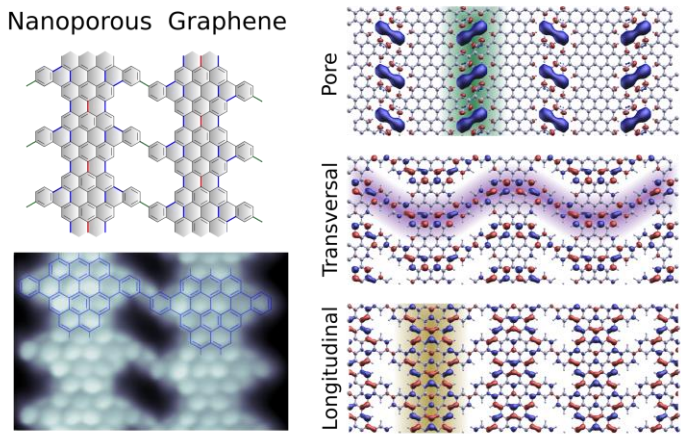

Figure 1. Left panels: schematic representation (top) and STM image (bottom) of nanoporous graphene. Right panels: DFT wave functions of pore (top), transversal (middle) and longitudinal (bands).