Novel Electronic States in Graphene Nanostructures

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A precise control and understanding of conformational or chemistry related electronic signatures in graphene nanostructures is crucial for their use in electronic and optoelectronic applications. In this talk, I will present some studies of electronic properties of graphene nano-structures that we have performed in collaboration with our experimental colleagues. Different aspects, such as the influence of the conformation or the effect of chemical doping, have been addressed.[1,2]

In particular, we have investigated the emergence of novel electronic states in carbon-based macromolecules and graphene nanoribbons. Our studies show that such peculiar states have similar origin as the image states of graphene, which exist in the vacuum region above and below the graphene layer.[3] Image states do not follow the atomic lattice modulation and behave as nearly-free electrons (NFE). When graphene is rolled into nanotubes or fullerenes, these states overlap giving rise to the emergence of 1D NFE bands or 0D Super-Atom Molecular Orbitals (SAMOs)[4].

Interestingly, we find that for graphene nanostructures there exist image states related to the 1D edge of graphene. Through the combination of scanning tunneling microscopy (STM) and density functional theory (DFT), we reveal the existence of a 0D-SAMO resonance in the central empty region of a planar carbon-based macromolecule.[5] Moreover, based on DFT calculations, we predict the emergence of 1D-NFE states in graphene nanoribbons, and we propose a way to confine them by modulating the width of the ribbons periodically, thus effectively creating 0D Super Atom States.

References

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[2] Carbonell-Sanromá et al. Nano Lett. 17, 50 (2017)
[3] V. M. Silkin et al., Phys. Rev. B 80 (2009), 121408(R)
[4] M. Feng et al., Science, 320 (2008), 359
[5] J. Heuille et al., Nano Letters 18, 418 (2018)

Figures

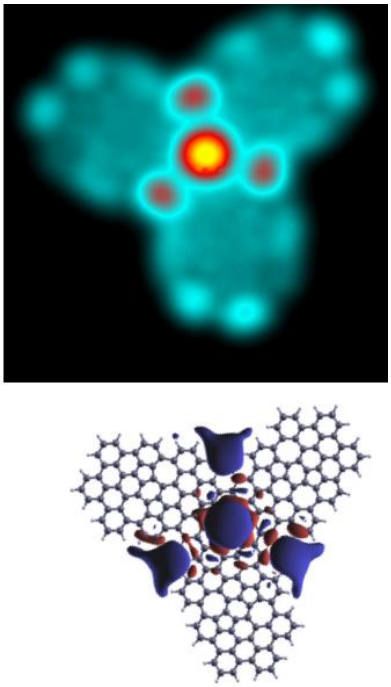

Figure 1: Electronic state with large weight in the pore region of the carbon based macromolecule. Upper panel: constant height dI/dV map. Lower panel: DFT wavefunction amplitude isosurface.