Scanning Tunneling Microscopy Simulations of Nitrogen- and Boron Doped single layer and bi-layer graphene

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The control of the doping of few layer graphene and carbon nanotubes represents a challenge that could lead to a production of carbon nanosystems with precise structural and electronic properties or chemical reactivity. Nowadays however, the first experimental data on chemical modification of carbon nanosystems with boron and nitrogen raise fundamental questions on the atomic configurations of the 'defect sites'. What are the most stable chemical modification atomic configurations ? Does the final configuration depends on the production method ? What are the chemical and physical properties of those configurations ? In this contribution, we present density-functional theory based simulations on the electronic properties and on the scanning tunneling microscopy (STM) signature of single layer and bi-layer graphene.

For monolayer graphene [1], the shift of the Fermi level away from the Dirac point and the position of the localized states associated with the defect is studied for several atomic configurations (substitution, pyridine like systems, adsorption, …). The associated STM patterns and STS spectra are deduced within the Tersoff-Hamman approach. For example, for metallic nanotubes, a shift of the Fermi level together with a localized donor (acceptor) states are observed for nitrogen (boron) substitution. Semiconducting tubes tend to become metallic under n and p substitutional doping. Finally, STM fingerprints of the localized states have been computed. We compare also our data with the few available experimental works.

Bi-layer (and multilayer) graphene are known to present electronic properties close the Fermi level dependent on the number of layer and their stacking [2]. For example, the well described massless fermion behavior of single layer graphene is destroyed by the interaction with a second layer, except in the case of rotationally disordered stacking. As a consequence the symmetry of the STM pattern depends on the layer stacking. Here, we show that the substitutional doping on bilayer graphene could also lead to a modification of the STM pattern symmetry, as a result of the asymmetry of the charge on the layer of the doped systems.

References

[1] B. Zheng, P. Hermet, L. Henrard. ACS Nano, **7** (2010) 54165
[2] S. Latil, L. Henrard. Phys. Rev. Lett., **97** (2006) 036803
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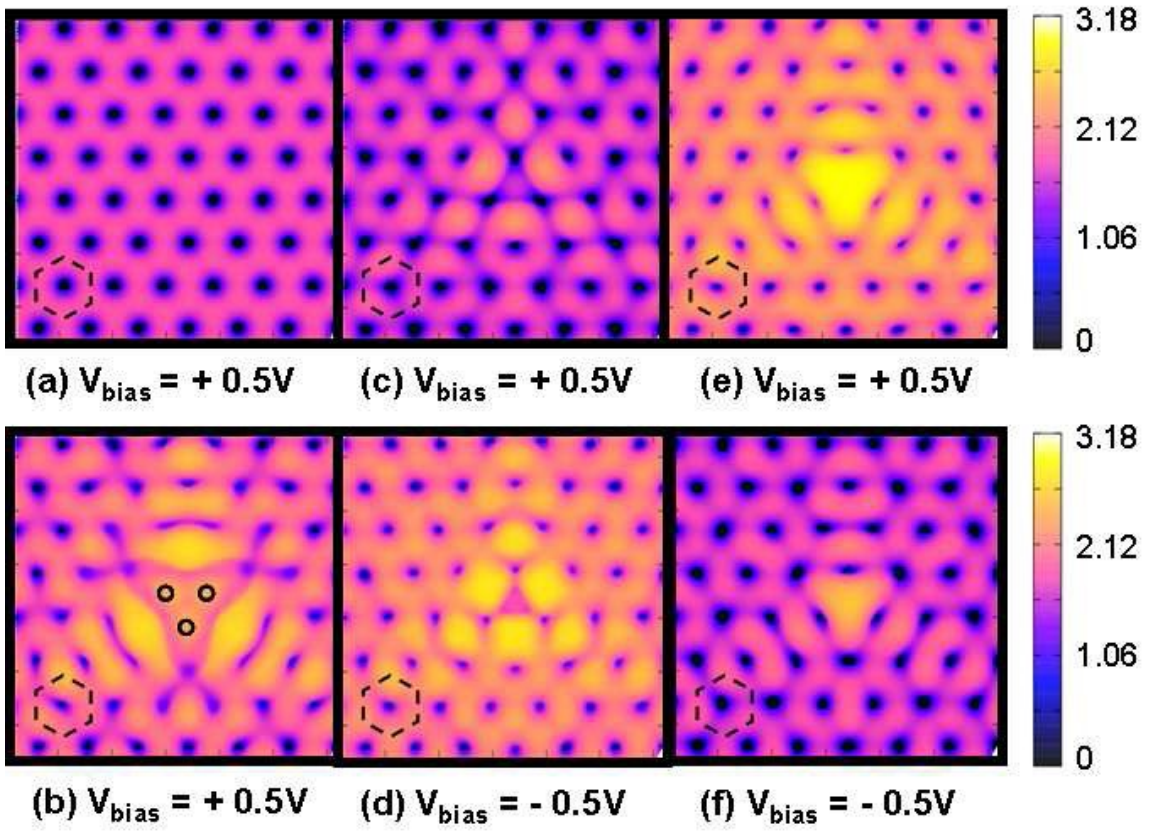
Figures



Computed STM images of pristine and doped graphene: (a) pristine, (b) pyridine (locations of 3N are denoted by black circles), (c,d) N-substitution, (e,f) B-substitution. One dashed hexagon is represented on the different images to highlight the atomic network. The color scales for height are in Angstroem. (From Ref 1)