Modelling chemical nanosensor devices based on graphene ribbons

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The search for novel nanoscale materials combined with the fabrication of ultra small circuit architectures are immediate priority for industry and research branches. Nanoelectronic devices based on carbon nanostructures, such as carbon nanotubes[1] and graphene[2], rise as a promising alternative to Si-based apparatus due to their extraordinary physical properties, for instance, outstanding mechanical strength[3] and electronic character strictly dependent on geometrical aspects[4]. The applicability of these materials also ranges the field of chemical and biological sensors at nanoscale offering promising applications in the realms of Medicine diagnosis and environmental pollution control. One has confirmed that graphene and nanotubes can discriminate low concentrations of contaminants and they can pose as suitable host materials for sensing a considerable number of different molecules and gases[5,6].

The experimental achievements in this field have progressed at fast pace, however its theoretical counterpart has not shared the same success, mainly due to the large computational complexity required to model highly doped structures. The theoretical description of more realistic systems turns into a big challenge since larger number of impurities and disordered features should be taken into account. For this reason, the main goal of this work is to improve the theoretical understanding of the physical properties of carbon-based hosts interacting with foreign structures. Different foreign entities such as nanoparticles, individual atoms, small molecules, polymers and metallic contaminants are attached to graphene hosts and the systems are theoretically addressed within robust semi-empirical approaches that are able to treat highly imperfect systems[7]. The electronic transmission of the sensors are also modulated by mechanical strain. The performance of the devices and their response to the application of external mechanical forces are probed in order to determine optimal physical conditions that can maximize the chemical sensibility of graphene hosts[8].

Preliminary results are shown in the figure below which displays the electronic transmission as a function of Fermi energy for pristine and doped graphene nanoribbon. Carbon monoxide is adsorbed on graphene's surface and one can notice that the presence of the impurity is detected by the transmission curve although the energy gap itself is not modified. In the following, the ribbon is uniaxially stretched by the aid of mechanical forces which elongate the ribbon with a mechanical strain of 7%. The system demonstrate remarkable sensibility to mechanical strain since its energy gap size is altered with the strain application. Still, carbon monoxide adsorption can be perceived by the ribbon.

References

[1] J.-C. Charlier, X. Blase, and S. Roche, Rev. Mod. Phys. **79**, (2007) 677 (2007);

[2] K. S. Novoselov, *et al.*, Science **306**, (2004) 666;

[3] C. Lee, X. Wei, J. W. Kysar, and J. Hone, Science **321**, (2008) 5887;

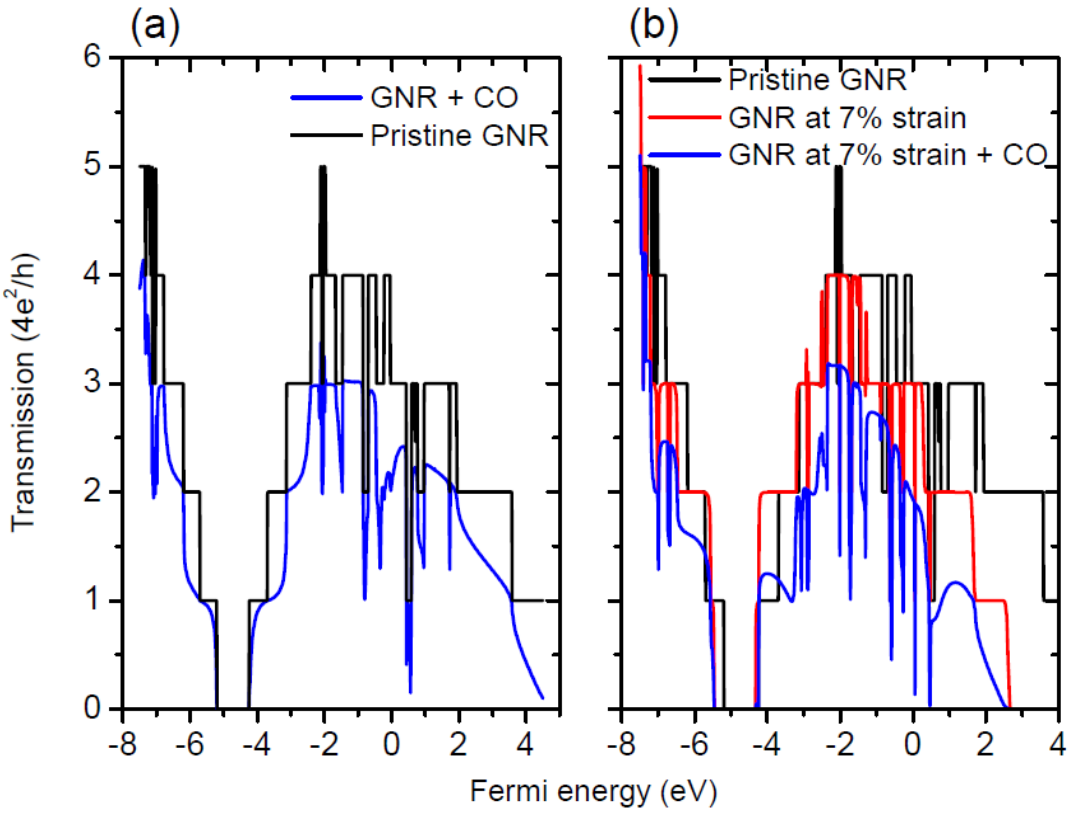
[4] A. H. Castro Neto, *et al.*, Rev. Mod. Phys. **81**, (2009) 109;

[5] F. Schedin, *et al.*, Nat. Mat. **6**, (2007) 652;

[6] Y. Dan, *et al.*, Nano Lett. **9**, (2009) 1472;

[7] C. G. Rocha, *et al.*, J. Phys.: Cond. Matt. **19**, (2007) 346201; C. G. Rocha, and M. S. Ferreira, Europhys. Lett. **82**, (2008) 27004;

[8] M. Poetschke, C. G. Rocha, L. E. F. Foa Torres, and G. Cuniberti, Phys. Rev. B **81** (2010) 193404.


(a)
(b)
GNR + CO
Pristine GNR
Pristine GNR
GNR at 7% strain
GNR at 7% strain + CO
Transmission (4e²/h)
Fermi energy (eV)
0
1
2
3
4
5
6
-8
-6
-4
-2
0
2
4