Quantum transport properties of gas molecules adsorbed on Fe doped armchair graphene nanoribbons

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Graphene, when doped with transition metals, is considered, both experimentally and theoretically, as a good candidate for the detection of gas molecules as CO, CO_2, NO or NO_2 [1]. This opens new perspectives for gas sensor set-ups considering that devices based on 2 dimensional graphene are more sensitive to detect molecules than solid-state gas sensors. The state of the arts on gas adsorption on Fe doped armchair graphene [2] nanoribbons (Fe-AGNR) is still in its starting phase and thorough investigations of the mechanism of the adsorption on graphene need to be done.

In the present work, the electronic and transport properties of molecules adsorbed on Fe-AGNR (see Fig. 1) are scrutinized using *ab-initio* calculations [3]. We observe that the adsorption of gas molecules on Fe-AGNR changes significantly the electronic properties of both the valence and the conduction band (see Fig.2). Besides, The adsorbed molecules change the local electron density of states of the graphene nanoribbons, modifying thus the conductivity, being one of the main output quantity of the gas sensors. We also observe that the adsorbed molecules induce specific impurity bands which play a role in the transport properties.

Finally, considering the observed variations of electrical conductance induced by the molecules, we propose several strategies to set-up gas sensors for CO, CO_2, NO and NO_2 molecules. These stategies are either based on the measurement of the conductance in the valence or the conduction band (using either p or n-doped Fe-AGNR) or to the spin polarization induced by the NO and NO_2 molecules.

References

[1] F. Schedin *et al.* Nature Materials 6, 652–655 (2007)
[2] A. W. Robertson *et al.* NanoLetters 13, 1468-1475 (2013)
[3] H. Zitoune et al. J. of Physics and Chemistry of Solids 153, 109996 (2021)

Figures

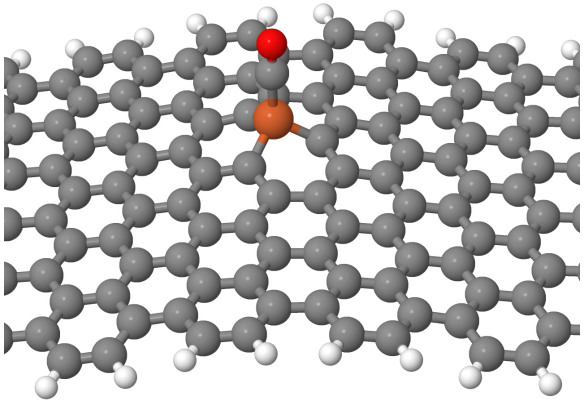

Figure 1: Armchair graphene nanoribbon with a CO molecule adsorbed on top of a Fe atom in substitution

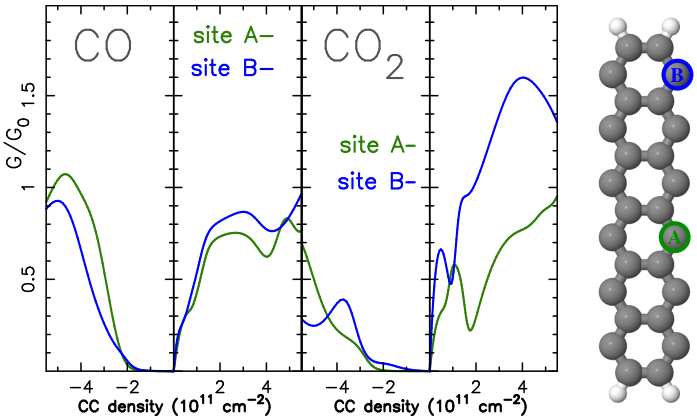

Figure 2: Electrical conductance as function of the charge carrier density