Electronic and transport properties of graphene based systems with divacancies

Marta Pelc[1,2], Leonor Chico[2], Włodzimierz Jaskólski[1], Andres Ayuela[3]

[1]Instytut Fizyki UMK, Grudziądzka 5, 87-100 Toruń, Poland
[2]Instituto de Ciencia de Materiales de Madrid, CSIC, Cantoblanco, 28049 Madrid, Spain
[3]Centro de Física de Materiales de Madrid, CSIC-UVP/EHU,
Departamento de Física de Materiales, Fac. Químicas, UPV/EHU,
and Donostia International Physics Center (DIPC), 20080 Donostia,
martap@fizyka.umk.pl

Abstract

There is a growing interest on structural defects in graphene, either extended in defect lines or separated as mono- and multi-vacancies. The appearance of these defects has been experimentally observed in different graphene-based systems [1,2] and can significantly modify the electronic, magnetic and transport properties [3-6]. Such defects naturally appear during the growth process but have also been introduced on purpose using electron or ion irradiation [7]. Among those defects, vacancies are well-known to show atoms in topologies such as pentagons, heptagons and octagons.

We here deal with the particular case of divacancies, where the hexagonal graphene structure usually reconstructs into an octagon accompanied by two pentagons (the so-called 5-8-5 defect), as shown in the Fig. 1. Since such defects can spontaneously appear in graphene systems or be created intentionally, we theoretically study these vacancies in semiconducting graphene nanoribbons and carbon nanotubes. We investigate the influence of such defects on the electronic and transport properties of graphene nanoribbons and carbon nanotubes. We consider the orientation of vacancies before and after reconstruction, and vary the nanoribbon width or roll up the ribbon into a zig-zag nanotube. We also consider ribbons with pairs of such defects.

In our calculations, we focus on the armchair ribbons as they have no edge states that could mix with the defect-localized state. We perform calculations within the π-electron tight binding approximation (TB) with hopping parameter t =-2.7 eV. For non-periodic systems, like a single defect in a perfect ribbon, we use the Green function matching technique to calculate the local density of states (LDOS) and conductance. Band structures and the corresponding wave functions are obtained for superlattices with periodical 5-8-5 defects using the TB Hamiltonian direct diagonalization.

We find that the presence of divacancies leads to the appearance of gap states. In different cases, we have obtained one or two states appear in the gap. We have observed that in some particular cases, they may act as acceptor or donor states (see Fig. 2). The gap states we observe are mainly localized on the defect. By varying the hopping parameters, we investigate the source of these states, what shows that they originate from the octagonal ring states [8]

References

[1] A. Lherbier, S. M.-M. Dubois, X. Declerck, Y.-M. Niquet, S. Roche and J.-C. Charlier, Phys. Rev. B 86, 075402 (2012).

[2] J. M. Carlsson and M. Scheffer, Phys. Rev. Lett. 96, 046806 (2006).

[3] M.Pelc, L. Chico, A. Ayuela and W. Jaskólski, Phys. Rev. B, **87**, 165427 (2013).

[4] W. Jaskólski, M. Pelc, L. Chico and A. Ayuela, IEEE Conference on Nanotechnology, **1**, 1 (2012).

[5] R. R. Nair, M. Sepioni, I-Ling Tsai, O. Lehtinen, J. Keinonen, A. V. Krasheninnikov, T. Thomson, A. K. Geim and I. V. Grigorieva, Nature Phys. **8**, 199 (2012).

[6] S. Kattel, P. Atanassov, and B. Kiefer, J. Phys. Chem. C, **116**, 8161 (2012).

[7] M. M. Ugeda, I. Brihuega F. Guinea and J. M. Gomez-Rodriguez, Phys. Rev. Lett. **104**, 096804 (2010)

[8] M. Pelc, W. Jaskolski, A. Ayuela, and L. Chico, Acta Phys. Pol., **124**, 777-780 (2013).

Figures

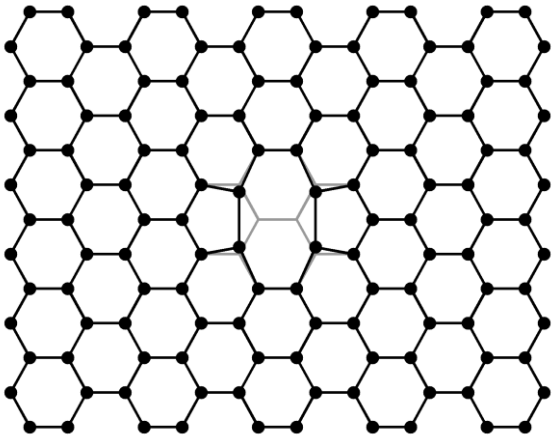

Fig. 1. A model of a graphene nanoribbon with a divacancy reconstructed into an octagonal topological defect accompanied by two pentagons.

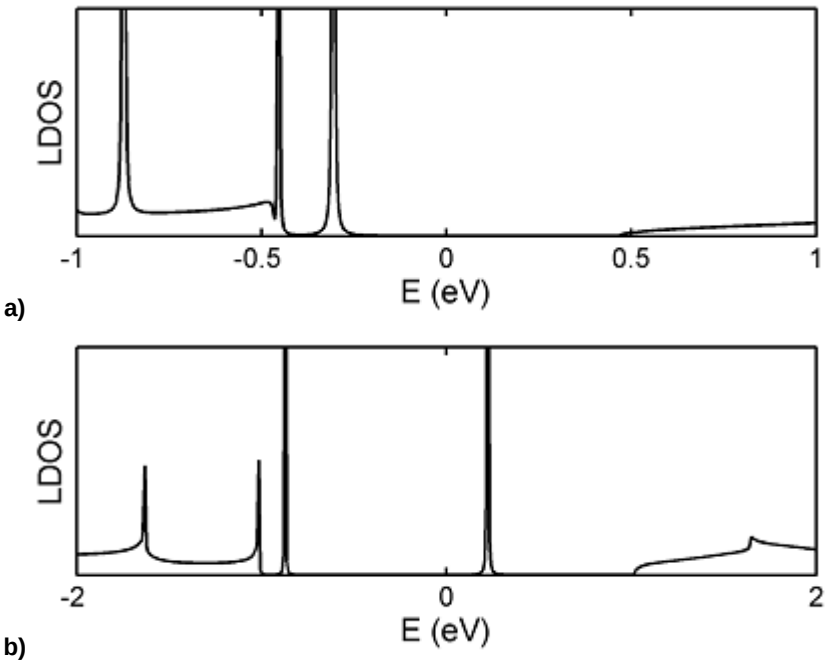

Fig. 2. Local density of states (LDOS) on the 5-8-5 defect introduced in a 9-AGNR (a) and CN (5,0) (b). In the case of the nanoribbon we observe only one gap state, while in the LDOS of the nanotube we observe appearance of two states, which play the role of an occupied acceptor state and an unoccupied donor state.