

# Electronic and structural distortions in graphene induced by carbon vacancies and boron doping

Faccio, R.,<sup>1</sup> Fernández-Werner, L.,<sup>1</sup> Pardo, H.,<sup>1</sup> Goyenola, C.,<sup>1</sup> Ventura, O. N.,<sup>2</sup> and Mombrú, A. W.<sup>1</sup>

<sup>1</sup>*Crystallography, Solid State and Materials Laboratory (Cryssmat-Lab),  
DETEMA, Facultad de Química, Universidad de la República,  
Gral. Flores 2124, P.O. Box 1157, Montevideo, URUGUAY*

<sup>2</sup>*CCBG, DETEMA, Facultad de Química, Universidad de la República, URUGUAY*

We present an ab initio - DFT/GGA - study on the structural and electronic distortions of modified graphene by creation of vacancies, inclusion of boron atoms, and the coexistence of both, by means of total energy and band structure calculations. In the case of coexistence of boron atoms and vacancy, the modified graphene presents spin polarization only when B atoms locate far from vacancy. Thus, when a boron atom fills single- and di-vacancies, it suppresses the spin polarization of the charge density. In particular when B atoms fill a di-vacancy a new type of rearrangement occurs, where a stable BC<sub>4</sub> unit is formed inducing important out of plane distortions to graphene. All these findings suggest that new chemical modifications to graphene and new type of vacancies can be used to modify its electronic properties. [1] Faccio, R. et al. J. Phys. Chem. 2010 (in press)