Inducing a Finite In-Plane Piezoelectricity in Graphene with Low Concentration of Inversion Symmetry-breaking Defects.

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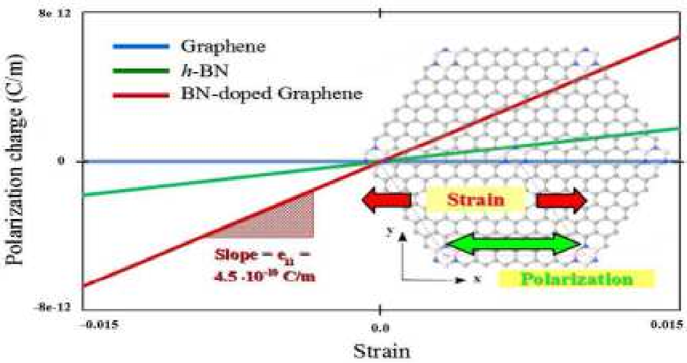
In this work[1], we adopt a quantum mechanical approach based on the periodic Density Functional Theory (DFT), to show that a finite in-plane piezoelectricity can be induced in graphene by breaking its inversion center with any in-plane defect, in the limit of vanishing defect concentration. We first consider different patterns of BN-doped graphene sheets of *D3h* symmetry, whose electronic and piezoelectric (dominated by the electronic rather than nuclear term) properties are characterized at the *ab initio* level of theory. We then consider other in-plane defects, such as holes of *D3h* or *C2v* point-symmetry, and confirm that a common limit value (for low defect concentration) of the piezoelectric response of graphene is obtained regardless of the particular chemical or physical nature of the defects ($e_{11} \approx 4.5\ 10^{-10}$ C/m and $d_{11} \approx 1.5$ pm/V for direct and converse piezoelectricity, respectively). This in-plane piezoelectric response of graphene is one-order of magnitude larger than the out-of plane previously investigated one[2]. All the calculations are performed using the CRYSTAL14 program[3].



1. Kh. E. El-kelany, Ph. Carbonnière, A. Erba, and M. Rérat, *J. Phys. Chem. C* **2015**, (submitted).
2. M. T. Ong and E. J. Reed, *ACS Nano* **2012**, 6, 1387-1394.
3. R. Dovesi, R. Orlando, A. Erba, C. M. Zicovich-Wilson, B. Civalleri, S. Casassa, L. Maschio, M. Ferrabone, M. De La Pierre, Ph. D'Arco, et al., *Int. J. Quantum Chem.* **2014**, 114, 1287-1317.