Sublattice asymmetry of substitutionally doped impurities in grapheme

J. A. Lawlor, M. S. Ferreira, S. R. Power and C. G. Bezerra

Trinity College Dublin

Ireland

Motivated by the recently oberved asymmetry in the spatial distribution of substitutional nitrogen impurities in graphene[1,2,3,4], we explain why substitutional impurities may favour one of the sublattices of graphene even though both are absolutely equivalent. We show that oscillations in the local density of states that arise as a result of the presence of substitutional impurities [5] are responsible for breaking the sublattice symmetry displayed by pristine graphene. While these oscillations are normally averaged out in the case of randomly dispersed impurities, in graphene they have either the same periodicity of the lattice or are very close to it. As a result, the total interaction energy of randomly distributed impurities embedded in a conduction-electron-filled medium does not vanish and is lowered when their spatial distribution is sublattice-asymmetric. Furthermore, we argue that this effect should be more ubiquitous and seen with a plethora of other impurities if suitable substrates are identified.

References:

[1] Zhao et al., Science 999 (2011) 333.

[2] Lv et al., Scientific Reports 2 (2012) 586.

[3] Lherbier et al., Nanoletters 13 (2013) 1446.

[4] Zhao et al., Nanoletters 13 (2013) 4659.

[5] Lawlor et al., Phys. Rev. B 88 (2013) 205416.