Graphene nanoribbons with sublattice-asymmetric doping

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Modifying the electronic structure of graphene to induce, for example, band gap behaviour is a key step towards fully exploiting the unique properties of this material. Doping graphene with different impurity species is a common strategy, but most doping processes distribute impurities evenly between the two sublattices (shown by hollow and filled symbols in Fig 1) which compose the graphene lattice.

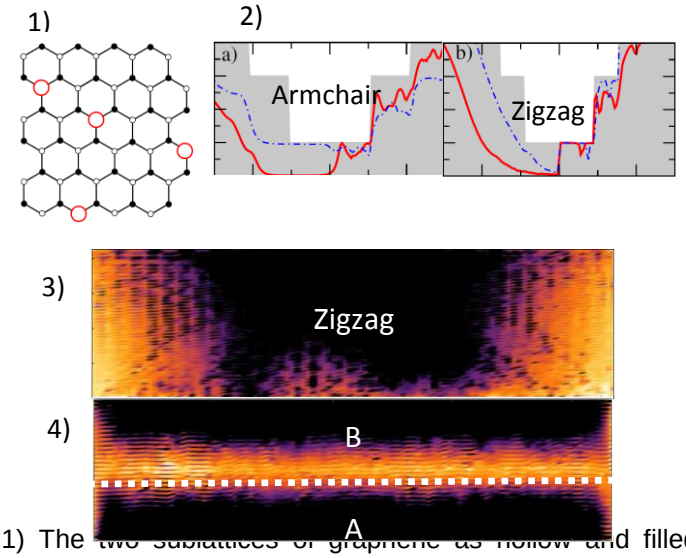
Images of the dopant placement [1] show that, in certain cases, the doping distributions spontaneously become asymmetric, i.e. most of the dopants are present on one sublattice. This resulting asymmetry has been predicted to create an electronic bandgap and an electron-hole asymmetry [2]. The corresponding electronic transport is robust against doping for one kind of carrier, e.g. for substitutional nitrogen dopants electron transport is more robust and hole transport is diminished compared to symmetric doping.

Our study models the electronic structure and transport properties of asymmetrically-doped graphene nanoribbons [3]. In particular, we focus on the role of edge geometry in determining whether a band gap is opened. We find that zigzag edge geometries prevent the formation of electronic band gaps due to the formation of impurity states near one edge, see Fig 2 & 3. We also investigate transport channels which form at the interface between different sublattice domains. Such channels are expected to display robust waveguiding features, and should be detectable by scanning tunnelling microscopy, see Fig 4. Lastly I will discuss some efforts we have made to calculate similar effects of localised disorder on extended graphene.

References

[1] L. Zhao et al., Science, 6045 (2011) 999-1003; A. Zabet-Khosousi et al., JACS, 4 (2014) 1391-7.
[2] A. Lherbier et al., Nano Letters, 13 (2013) 1446-1450.
[3] T. Aktor et al., Phys. Rew. B, 93 (2016) 035446.

Figures



1) The two sublattices of graphene as hollow and filled symbols. The red circles indicate positions of dopants all on the hollow sublattice. 2) a): Transmission through armchair ribbon for all dopants on one sublattice (red line), symmetric doping (blue line) and undoped ribbons (grey background). b): Same as a) but for zigzag ribbons. 3) Local electronic density of states in zigzag ribbons with asymmetric doping showing the formation of impurity states near the bottom edge, which is associated with the doped sublattice. 4) Local electronic density of states at an interface between two sublattice domains, i.e. in the top region all dopants are on one sublattice and in the bottom on the other. The white dashed line is an aid to the eye along the boundary between the two regions.