Modelling of Functionalization of Boron Doped Graphene for Sensor Applications

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The forefront of research on graphene has moved from the study of the synthesis and properties of the pristine material to investigations of chemically modified systems including doped graphene. Introduction of selected dopants into the honeycomb lattice allows for tuning of the physical-chemical properties of the material. Particularly, boron doped graphene (BG) is turning out to be an excellent candidate for a wide range of applications. It represents not only an important platform for the development of graphene-based electronics but it has also shown remarkable performances as sensor to detect different kinds of substances. [1-2]
Our on-going work is focused at exploring the potential usefulness of BG for sensor and bio-sensor applications with a close collaboration between simulations and experiments. The starting point is the Lewis acid property of BG to incoming Lewis bases [3], a chemical strategy (socket-plug strategy) that allows to realize a subset of the unique properties of graphene both in free-standing and supported BG [4].
A first way to realize bio-sensors is to use the socket-plug strategy to covalently attach receptor molecules to boron atoms in the BG layer. These receptors will be capable of binding specific analytes and will have the ability to transfer charge to the graphene surface. More precisely, if in the non-bound state the geometry of the receptor is such that the interaction with the π-orbitals of the graphene is too far for charge transfer, upon binding of the analyte its geometry will change and will allow the interaction with the π-orbitals, thus transferring charge and generating a signal in terms of graphene resistivity (see Figure 1).
A second way is to employ the socket-plug strategy to promote surface chemical bonds between a metal nanoparticle substrate and BG in order to create a boron-doped-graphene-coated plasmonic copper nanodevice that exploits the change in the dielectric function at the interface between graphene and metal upon binding of the analyte to realize a sensor for small molecules (see Figure 2).

References

[1] R. Lv et al., PNAS, 112 (2015) 14527
[2] Y. Xu et al., Electrochim. Acta, 216 (2016) 219
[3] V. Cantatore and I. Panas, Carbon, 104 (2016) 40
[4] V. Cantatore and I. Panas, Carbon, Just Accepted

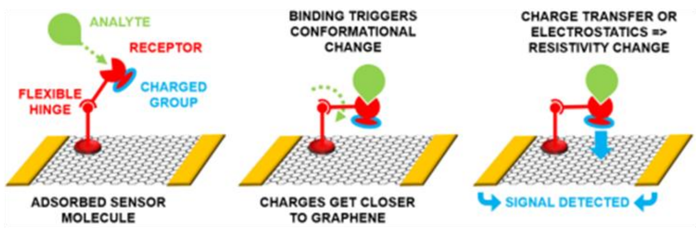

Figure 1

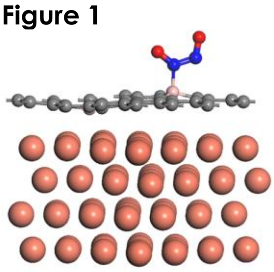
Figure 2