



***Ab initio* modeling of novel 2D materials**

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Borophene, a recently synthesized two-dimensional monolayer of boron atoms, is expected to exhibit anisotropic metallic character with relatively high electronic velocities [1]. At the same time, very low optical conductivities in the infrared-visible light region have been reported. Based on its promising electronic transport properties and *a priori* high transparency, borophene could become a genuine LEGO piece in the 2D materials assembling game. Such early suggested properties demands for an in depth investigation of borophene electronic structure. Moreover, borophene is naturally degraded in ambient conditions and it is therefore important to assess the mechanisms and the effects of oxidation on borophene layers. Optical and electronic properties of pristine and oxidized borophene have been investigated using first-principles techniques [2]. Optical response of the oxidized layer is found to be strongly modified suggesting that optical measurements can serve as an efficient probe for borophene surface contamination.

Two-dimensional conjugated polymers exhibit electronic structures analogous to that of graphene with the peculiarity of π - π^* bands which are fully symmetric and isolated. Realistic 2D conjugated polymer networks with a structural disorder such as monomer vacancies (unavoidable during bottom-up synthesis) are investigated using both *ab initio* and *tight-binding* techniques [3] in order to check their suitability for electronic applications. As expected, long mean free paths and high mobilities are predicted for low defect densities. At low temperatures and for high defect densities, strong localization phenomena originating from quantum interferences of multiple scattering paths are observed in the close vicinity of the Dirac energy region while the absence of localization effects is predicted away from this region suggesting a sharp mobility transition [3].

Electronic structure and transport properties of N-doped graphene with a single sublattice preference are investigated using both first-principles techniques and a real-space Kubo-Greenwood approach [4]. Such a breaking of the sublattice symmetry leads to the appearance of a true band gap in graphene electronic spectrum even for a random distribution of the N dopants. In addition, a natural spatial separation of both types of charge carriers at the band edge is observed, leading to a highly asymmetric electronic transport. For such N-doped graphene systems, the carrier at the conduction band edge present outstanding transport properties including long mean free paths, high mobilities and conductivities. Such a transport behavior can be explained by a non-diffusive regime (quasi-ballistic transport behavior at the conduction band edge), and originates from a low scattering rate. The presence of a true band gap along with the persistence of carriers traveling in an unperturbed sublattice suggest the use of such N-doped graphene in G-FET applications, where a high I_{ON}/I_{OFF} ratio is expected. The present *ab initio* simulations should encourage more investigation and specific transport measurements on N-doped graphene samples where such an unbalanced sublattice doping is observed.

- [1] *Synthesis of borophenes: anisotropic, two-dimensional boron polymorphs*
A.J. Mannix, *et al.*, *Science* **350**, 1513 (2015).
- [2] *Electronic and optical properties of pristine and oxidized borophene*
A. Lherbier, A.R. Botello-Méndez, and J.-C. Charlier, *2D Materials* (2016), in press.
- [3] *The electronic and transport properties of 2D conjugated polymer networks including disorder*
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Nanoscale **8**, 1642 (2016).
- [4] *Electronic and transport properties of unbalanced sublattice N-doping in graphene*
A. Lherbier, A.R. Botello-Méndez, and J.-C. Charlier, *Nano Lett.* **13**, 1446-1450 (2013).