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Gap Opening by Asymmetric Doping in Graphene Bilayers

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Abstract – Graphene bilayers are metallic systems and seem to be very promising materials for electronic applications because they can be made semiconducting by the application of an external electrical field. In fact, the gap can be tuned by that field, which allows tailoring the electronic structure for specific applications. In this work, we explore using ab initio calculations another route for tuning the gap of graphene bilayers. We show that by controlling the doping with donor and acceptor species in separate sheets of the bilayer, a gap can be opened and tuned in a similar way to an external electrical field.

Graphene has attracted the attention of the scientific community due to its potential applications in nanoeletronics. However, for electronic applications, it is important to make graphene a semiconductor. For this reason, graphene bilayers seem to be very promising materials for such applications because they can be made semiconducting by the application of an external electrical field [1]. In fact, the gap can be tuned by the electrical field, which is very attractive because it allows tailoring the electronic structure for specific applications.

In this work, we explore theoretically another route for tuning the gap of graphene bilayers. We show that by controlling the doping with donor and acceptor species in separate sheets of the bilayer, a gap can be opened and tuned in a similar way to an external electrical field. Our ab initio calculations are based on the density functional theory within the generalized gradient approximation (GGA) for exchange-correlation effects and Vanderbilt ultrasoft pseudopotentials for electron-ion interactions, with a plane-wave basis.

We explore two specific realizations:

(1) Potassium adsorption in one of the sheets (Fig. 1).
(2) Boron and Nitrogen as substitutional donors in separate sheets. In this case we also study the stability of this configuration using total energy calculations.

We obtain similar results for both situations. An example of a band structure obtained for the second situation is shown on Fig. 2. We also investigate the gap magnitude dependence with respect to the dopant concentration.

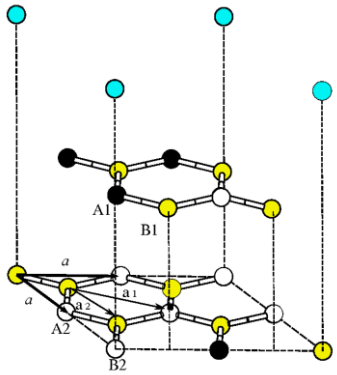

Figure 1: Simulation cell for the first situation (Potassium adsorption in one of the sheets)

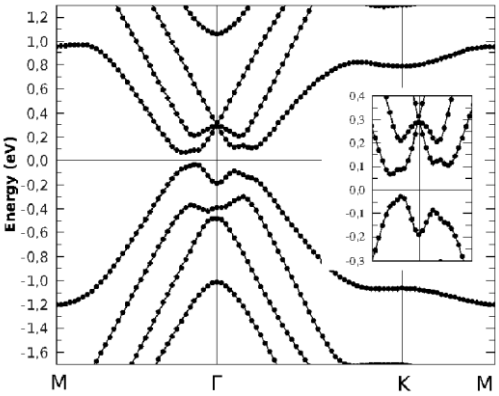

Figure 2: Example of a band structure for the second situation. It shows similar features to the external field application experimental result [1], including the order of magnitude of the gap.

References

[1] Ohta et al., Science **313**, 951 (2006).