Intercalation and Doping Effects on the Electronic Properties of Mono- and Bilayer Graphene

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Abstract

A possible approach to achieve monolayer quasi-freestanding graphene on a substrate is the intercalation of alkali metal atoms. Cs intercalation between graphene and Ni(111) is investigated by density functional theory, incorporating van der Waals corrections [1]. Direct contact between graphene and Ni(111) perturbs the Dirac states. Cs intercalation restores them, however, at to lower energy. The projected densities of states in Figure 1 show that the C atoms carry no magnetic moment and that the spin polarization of Ni(111) does not extend through the intercalated atoms to the graphene sheet. As engineering of the band gap of graphene is crucial for electronic applications [2], we study the properties of doped bilayer graphene. In the case of the top band structure in Figure 2 one layer is doped with B and the other with N. There are two buried Dirac cones at the K point that can be attributed to the B (unoccupied cone) and N (occupied cone) layers. Introducing an additional B-N pair into the B-doped layer gaps the Dirac cones and reduces the band gap, see the bottom band structure in Figure 2.

References

[1] Alattas, M. and Schwingenschlögl, U. *Sci. Rep.* 6 (2016) 26753
[2] Castro Neto, A. H., et al. *Rev. Mod. Phys.* 81 (2009) 109-162

Figures

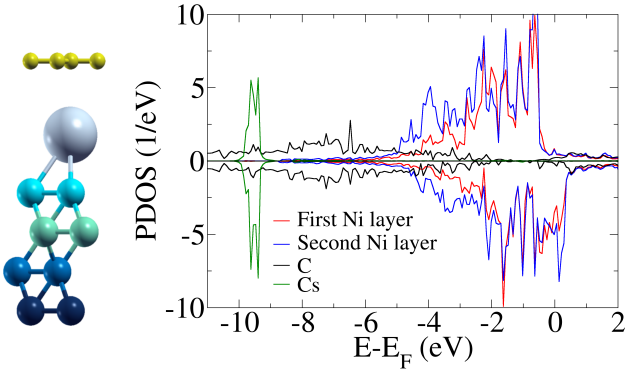

Figure 1: Atomic structure of graphene on Ni(111) with intercalated Cs and the obtained projected densities of states. The two spin channels are plotted separately.

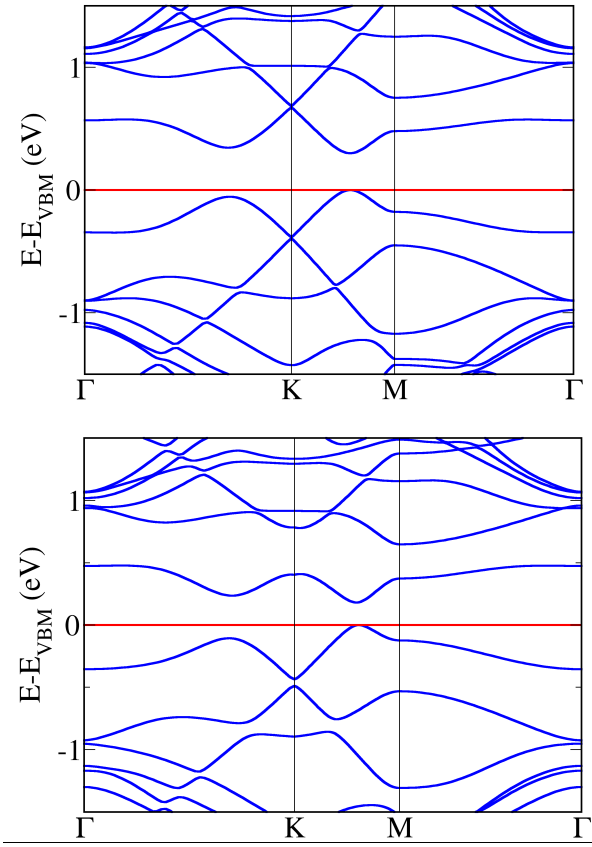

Figure 2: Electronic band structure of bilayer graphene. Top: One layer is doped with B, the other with N. Bottom: One layer is doped with B and a B-N pair, the other with N.