Gap Opening by Asymmetric Doping in Graphene Bilayers

RO-DRIGO CAPAZ, MARCOS MENEZES, Instituto de Física, UFRJ, Brazil, JORGE FARIA, Instituto de Física, UFMT, Brazil — Graphene bilayers are very promising materials for nanoelectronic applications because they are metallic systems which can be made semiconducting by the application of an external electrical field. More importantly, the gap can be tuned by that field, which 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 graphene bilayer, a gap can be opened and tuned in a similar way to an external electric field. Our calculations are based on the density functional theory and pseudopotentials, with a plane-wave basis. We explore specific realizations with potassium and nitrogen as donors and boron as acceptors, with similar results. We also investigate the dependence of the magnitude of the gap with respect to dopant concentration.

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