Electrostatic doping and hybrid carriers in graphene on a polar $SrTiO_3$ (111) surface: theoretical investigation

Donghan Shin and A. A. Demkov[+]
Department of Physics, The University of Texas, Austin, TX 78759, USA

Graphene is a two-dimensional carbon sheet with a honeycomb lattice structure. It is a zero-gap-semiconductor that has a linear energy dispersion near the Fermi level [1,2].Doping graphene layers presents a difficult practical and fundamental problem. We consider theoretically, the possibility of electrostatic doping of graphene by the intrinsic field of a polar substrate. Density functional theory calculations are carried out for a graphene sheet placed on the (111)-oriented perovskite $SrTiO_3$ surface. We find that the Fermi surface moves well below the Dirac point of graphene, resulting simultaneously in a fast conducting channel in graphene, and a slow, large effective mass channel in the oxide surface. Electrostatic gating may allow one to explore peculiar states that, through the "no-crossing" reminiscent of polaritons, would represent a hybrid carrier that exists simultaneously in both materials. In Fig. 1 we show the near edge electronic structure and corresponding charge distribution of the system. Importantly, in addition to the field doping, we identify a more "obvious" mechanism of doping through the contact potential difference, which may have wider applications in the doping of two-dimensional materials.

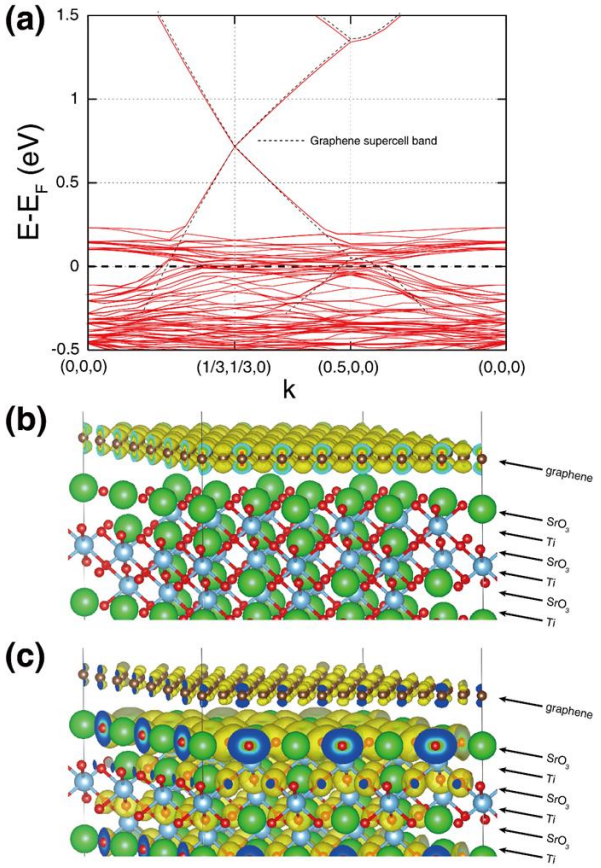

Figure 1. (a) Band structure of graphene on STO (111). A dashed line represents the Fermi level which is set to zero. Probability distribution calculated within the energy window (± 0.03 eV) corresponding to the band crossing point (b) and charge density corresponding to the Fermi level (c). It shows the charge density of graphene sheet and the surface of STO (111).

[+] Author for correspondence: demkov@physics.utexas.edu

[3] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, Science **306**, 666 (2004).

[2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. **81**, 109 (2009).