

MODIFICATION OF ELECTRONIC PROPERTIES OF GRAPHENE BY INTERACTION WITH SUBSTRATES AND DOPANTS

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Abstract

First-principles calculations have been carried out to investigate structural and electronic properties of graphene on SiC and diamond substrates and for a study of doping of fluorographene with various surface adsorbates.

New insight is given into the problem of the decoupling of the graphene layers from SiC substrates after epitaxial growth. Mechanisms of hydrogen penetration between graphene and SiC(0001) surface, and properties of hydrogen and fluorine intercalated structures have been studied. Energy barriers for diffusion of atomic and molecular hydrogen through the interface graphene layer with no defects and graphene layers containing Stone-Wales defect or two- and four-vacancy clusters have been calculated. It is argued that diffusion of hydrogen towards the SiC surface occurs through the hollow defects in the interface graphene layer. It is further shown that hydrogen easily migrates between the graphene layer and the SiC substrate and passivates the surface Si bonds, thus causing the graphene layer decoupling. According to the band structure calculations the graphene layer decoupled from the SiC(0001) surface by hydrogen intercalation is undoped, while that obtained by the fluorine intercalation is *p*-type doped.

Further, structure and the electronic properties of single and double layer graphene on H-, OH-, and F- passivated (111) diamond surface have been studied. It is shown that graphene only weakly interacts with the underlying substrates and the linear dispersion of graphene π -bands is preserved. For graphene on the hydrogenated diamond surfaces the charge transfer results in *n*-type doping of graphene layers and the splitting of conduction and valence bands in bilayer graphene. For the F- and OH-terminated surfaces, charge transfer and doping of graphene do not occur.

Finally, the possibility of doping fluorographene by surface adsorbates have been investigated. The structure and electronic properties of fluorographene with adsorbed K, Li,

Au atoms, and F4-TCNQ molecule are described. It is shown that adsorption of K or Li atoms results in electron doping of fluorographene, while Au atoms and F4-TCNQ introduce deep levels inside the band gap. The calculated value of the fluorographene work function is extremely high, 7.3 eV, suggesting that *p*-type doping is difficult to achieve.

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