Ab initio study of surface states at the graphene/Al_2O_3(0001) interface

Ershov I.

Don State Technical University, 344000 Rostov-on-Don, Russia
e-mail: thijd@mail.ru

It is well known that for a practical usage, graphene should be fixed on a solid substrate. There are number of various methods for deposition of graphene on a substrate, including mechanical exfoliation of graphite, growth from SiC surfaces via Si sublimation, epitaxial growth, chemical methods, and others. Traditionally SiO_2 substrates have been used for investigations of graphene properties. However, there are number of reasons for studying graphene on a larger variety of substrates like CaF_2, TiO_2 and Al_2O_3 [1, 2]. Of particular intereSt are such effects as bonding, doping, electron and hole mobility and magnetic properties, which strongly depends on the type of substrate and its orientation.

In the present work the properties of the graphene/Al_2O_3(0001) interface were investigated within the framework of density functional theory (DFT) using ab initio pseudopotential method. We have modeled the system in the tri-periodic slab approximation. The slab consists of 20 inequivalent atomic layers including the passivating hydrogen layer. The periodicity of the slab allowed us to calculate band structure in the interface which helped to estimate the degree of interaction between graphene and the substrate. The analysis of the chosen one-electron Kohn-Sham orbitals in the vicinity of Fermi level allowed us to identify the positions and character of surface states of the substrate in the interface. The total energy of the system was calculated in order to estimate the binding energy of graphene with the surface.

The relaxation of the substrate surface atoms and graphene show that the distance between graphene and the topmost substrate layer amounts 3.2 Å. The latter is in good agreement with the lateSt experiments [1, 2]. The band structure analysis indicates that the band of the substrate surface states turned out splitted in the presence of graphene. The shift of the surface states curves in the valence band could be indicative of the change of work function in the system.

[1] S. Akcoltekin, M. El Kharrazi, B. Kohler, A. Lorke, M. Schleberger, *Nanotechnology* **20**, 155601 (2009).
[2] T. Tsukamoto, T. Ogino. *Jap. Applied Physics Express* **2**, 075502 (2009).