Investigation of the Electro-optical Properties of Graphene with BC_3 Substrate

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Received: 02.08.2017 Final revised: 03.10.2017 Accepted: 01.11.2017

Abstract

In this article, the electronic and optical properties of graphene with BC_3 substrate are investigated. The calculations are performed on the basis of full potential linearized augmented plane waves in the framework of density functional theory. The total energy calculations of AA and AB configurations show that the AB stacking configuration is more stable than AA stacking configuration. The monolayer graphene has zero band gap while graphene with BC_3 substrate has a small band gap of 0.15 eV at K point. The intrinsic properties of graphene such as linear dispersion of electronic bands near the K point and high carrier mobility are retained in the graphene with BC_3 substrate. The dielectric function of graphene with BC_3 substrate can be considered as the superposition of dielectric function of graphene and BC_3 monolayer where the interaction between graphene and monolayer BC_3 leads to the shift of peak positions. These results can be used in designing new opto-electronic devices such as field effect transistors.

Keywords: Graphene, Monolayer BC_3, Density functional theory, Band Structure, Dielectric function

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