

Graphene-based Photonic Crystal: Ab-initio Calculation

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Photonic crystals are one of the modern, rapidly developing areas in solid state physics. Photonic crystals have a strictly ordered arrangement forming structural elements in one, two or three dimensions. Forming elements are generally considered monodisperse in geometric and identical in the dielectric parameters [1]. Photonic crystals with dielectric, metal or semiconductor constituent elements have different photonic band and transmittance spectrum. Attenuation of electromagnetic waves is also different in all these photonic crystals.

In these computing experiments, we consider periodically arranged stacks that form a two-dimensional photonic crystal. Stacks consist from the graphene planes, which separated by an insulator (SiO_2) (fig.1). We attempt to study the influence of the geometric parameters of stacks on the band gap, density of states, dielectric function. Electron response of solids to the impact of the electromagnetic field closely related to the structure of the energy bands. We calculated the electronic spectrum of the model atomic systems, the spatial distributions of the valence electrons density (fig.1), the distributions of the Coulomb potential and the static dielectric function using its own software complex [2].

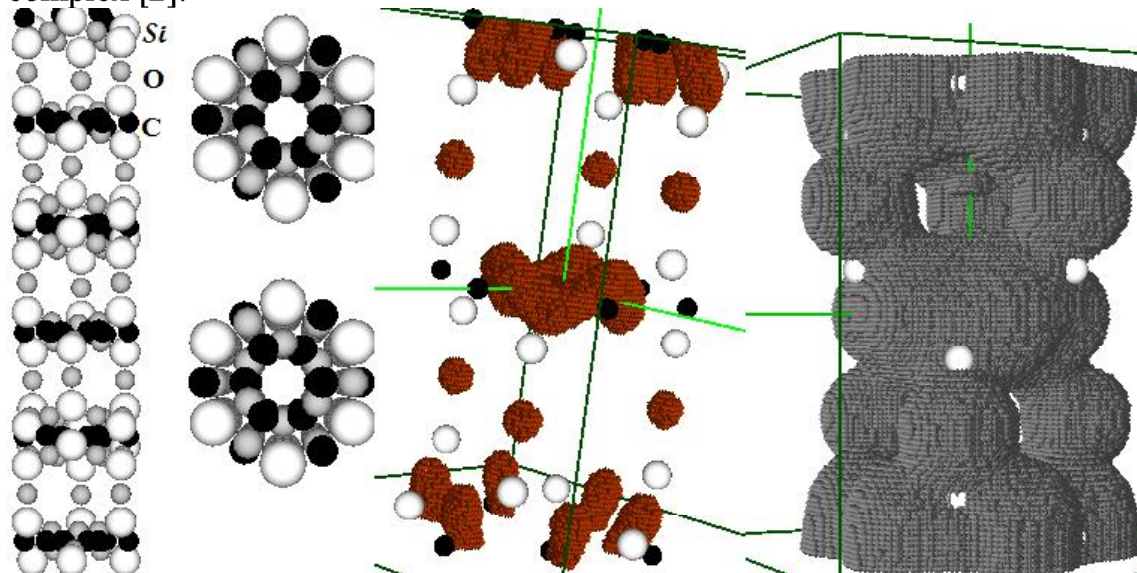


Fig.1. The model of photonic crystal that includes the periodically arranged stacks consisting the graphene planes and the SiO_2 slab with the electron density.

1. Yablonovitch E. Inhibited Spontaneous Emission in Solid-State Physics and Electronics // *Phys. Rev. Lett.* – 1987. – V.58. – P.2059-2062.
2. Balabai R.M. Electronic properties of functionalized graphene nanoribbons // *Ukr. J. Phys.* – 2013. – V. 58, № 4. – P.389-397.