New monolayer penta-nanostructures: first-principles calculations

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Abstract

In this paper, a first principle study is performed to investigate the electronic and optical properties of new penta-(C_4B_2, C_2B_4, and C_2N_4) monolayers based on the density functional theory (DFT) and using the Wien2k code. The results of evaluating electronic properties demonstrate that the penta-(C_4B_2, C_2B_4, and C_2N_4) monolayers are semiconductors with gap energies of 0.2 eV, 1.2 eV, and 3.1 eV, respectively. Moreover, a number of optical parameters such as reflectivity, dielectric function, and energy loss function versus energy variations are calculated. The results of the optical calculations show that, in the x-polarization of the electric field, the optical band gap corresponds to the electronic band gap, and the plasmon energy is more in conformity with the free electron model. Furthermore, the effective number of electrons with an energy of about 15 eV for penta-(C_4B_2, C_2B_4, and C_2N_4) monolayers is found to be 21, 20, and 20 electrons, respectively, which is small compared with the free electrons due to the localization of a number of electrons.

Keywords: electronic properties, optical properties, reflectivity, dielectric function, energy loss function

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