Electronic band structure of bilayer graphene intercalated by potassium atoms

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Using the electron density functional theory, the electronic band structure of potassium-intercalated bilayer graphene has been studied. The band structure was calculated using the Quantum Espresso program [1] based on the density functional theory, plane waves and pseudopotentials [2]. The Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional of the generalized gradient approximation (GGA) [3] was applied. It is shown that after the intercalation process, a band gap appears in the band structure of bilayer graphene. In addition, the energy gap changes nonlinearly depending on the intercalate concentration in the interlayer space of bilayer graphene. We also calculated the energy spectra of bilayer graphene containing vacancy defects, the presence of which leads to the appearance of mid-gap states.

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[3] Perdew J P, Burke K and Ernzerhof M 1996 *Phys. Rev. Lett.* **77** 3865–68