Effect of alkali metal adsorption on the graphene band structure

Akhmatov Z A[1,2,@] and Akhmatov Z A[2]

[1] Vladikavkaz Scientific Centre of the Russian Academy of Sciences, Markus 22, Vladikavkaz, North Ossetia-Alania 362027, Russia
[2] Kabardino-Balkarian State University, Chernyshevskogo Street 173, Nalchik, Kabardino-Balkaria 360004, Russia

[@] ahmatov.z@bk.ru

We investigated the effect alkali metal adsorption on the graphene band structure using first-principles density-functional theoretical calculations. It is shown that when potassium atoms are adsorbed on the graphene surface, an energy gap appears in its electronic spectrum. It was also observed that the band gap strongly depends on the number of adsorbed atoms, namely, with an increase in the number of adsorbed atoms, the band gap in graphene can either increase or disappear. For example, when there is one potassium atom per 32 carbon atoms in the graphene lattice, the band gap is $\Delta E = 0.1$ eV. An increase in the number of potassium atoms to two leads to the disappearance of the energy gap, while for three potassium atoms it is $\Delta E = 0.22$ eV. All calculations were performed using the Quantum Espresso program [1], based on the density functional theory, plane waves, and pseudopotentials [2].

Acknowledgments
This work was supported by grant No. MK-927.2022.1.2 from the President of the Russian Federation.

[1] Giannozzi P, Baroni S and Bonini S 2009 *J. Phys.: Condens. Matter* **21** 1–19
[2] Blöchl P 1994 *Phys. Rev. B* **50** 17953–79