Spontaneous electric polarization of the graphene lattice

S. A. Mikhailov

Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

Taking into account electron-electron interaction of π-electrons in intrinsic graphene we show that the hexagonal graphene lattice should be spontaneously electrically polarized, i.e. the ground state of graphene is ferroelectric.

The spectrum of π-electrons in graphene is usually described within the single-particle tight-binding approximation. The spontaneous-polarization effect resulting from electron-electron interaction is not taken into account in this approach. The tight-binding theory was first proposed and originally used for three-dimensional graphite [1] for which the ferroelectricity described above is not the case. While being perfectly correct for three-dimensional crystals, the tight-binding approach thus turns out to be not working for two-dimensional materials like graphene. Theoretical results which have been obtained for graphene so far and which are based on the single-particle tight-binding spectrum may thus need to be reconsidered.

The same conclusions are valid for bilayer graphene, boron nitride and other two-dimensional crystals.

This work was supported by Deutsche Forschungsgemeinschaft.

[1] P. R. Wallace, Phys. Rev. **71,** 622 (1947).