

Spontaneous electric polarization of a two-dimensional hexagonal lattice: Do we correctly understand the ground state of graphene?

S. A. Mikhailov

Institute of Physics, University of Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany
sergey.mikhailov@physik.uni-augsburg.de

The static dielectric constant of bulk (three-dimensional) insulators is related to the atomic polarizability α of constituting atoms by the known Clausius-Mossotti formula. We derive a similar expression for a two-dimensional crystal with the hexagonal lattice. The result shows that due to the local field effects the effective *macroscopic* polarizability λ of such a crystal becomes negative under the condition

$$\beta = \alpha/2a^3 > \beta_{\text{crit}} = 0.02925$$

where a is the lattice constant. For the carbon atom the calculated value of α_C is [1]

$$\alpha_C = 1.54 \text{ \AA}^3$$

while the lattice constant of graphene is 2.46 Å. The β -parameter for graphene

$$\beta_{\text{graphene}} \approx 0.05 > \beta_{\text{crit}}$$

is thus larger than the critical value of the sign inversion of λ .

A two-dimensional crystal with the negative macroscopic polarizability is thermodynamically unstable which means that intrinsic graphene should have a spontaneous electric polarization, i.e. to be in the ferroelectric ground state.

The spectrum of electrons in graphene is usually described within the tight-binding approximation [2] which was originally used for three-dimensional graphite [3]. However in three dimensions the sign inversion of the macroscopic polarization is not the case as follows from the Clausius-Mossotti formula. The two-dimensional crystals thus substantially differ from three-dimensional ones in this respect and the essentially single-particle tight-binding approximation should be applied to them with care. Since it neglects electron-electron interaction between π -electrons the predicted here effect cannot be obtained within the tight-binding approach even if the interaction was taken into account as perturbation. Theoretical results obtained for graphene so far may thus need to be reconsidered.

Since the atomic polarizability of B and N atoms are of the same order as that of carbon [4], the same conclusions are valid for boron-nitride monolayer crystals.

References

- [1] J. H. Miller and H. P. Kelly, Dipole polarizability of the neutral carbon atom and the dipole-dipole interaction between carbon atoms, *Phys. Rev. A* **5** (1972) 516.
- [2] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov and A. K. Geim, The electronic properties of graphene, *Rev. Mod. Phys.* **81** (2009) 109.
- [3] P. R. Wallace, The band theory of graphite, *Phys. Rev.* **71** (1947) 622.
- [4] A. Dalgarno and D. Parkinson, The polarizabilities of atoms from boron to neon, *Proc. Roy. Soc. London A*, **250** (1959) 422.