

New specific properties of graphene: from stability to electronic properties

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Since the isolation in 2004 graphene continues to attract significant attention from the scientific community. Despite of the fact that graphene is under detailed investigation more than 10 years it still serve as a source for unusual effects.

Here I will show that multilayer graphene surface can be used a base for formation of diamond nanofilms [1] facilitated by chemical adsorption of adatoms on the multilayer graphene surface, and explain how the pressure of phase transition is reduced and formally turns negative. For the first time we obtain, by *ab initio* computations of the Gibbs free energy, a phase diagram (P, T, h) of quasi-two-dimensional carbon—diamond film versus multilayered graphene. It describes accurately the role of film thickness h and shows feasibility of creating novel quasi-2D materials [2]. In such “chemically induced” phase transition both chemistry and compression concurrently serve as the driving factors for diamond film formation. I will continued to discuss this effect through the ultrastiff films with hexagonal diamond (lonsdaleite) type structure and further show that under the particular external conditions and using particular adsorbate atoms films with the specific structure can be formed [3]. Developed theory successfully described experimental results of formation of diamond nanoclusters in the amorphous carbon. We estimated dependence of phase transition pressure upon the cluster size, it was found that diamond particles with the radius up to 20 nm can be formed only by hydrogenation [4].

In the second part of the talk I will be focused on the new effect in graphene electronic properties. It is known that a homogenous mechanical distortion of graphene cannot induce electrical dipole due to graphene lattice central symmetry center (no piezoelectric effect). This rule however does not apply to the second order electronic flexoelectric effect induced by the strain gradient, especially by the bending of graphene sheet, which is one of the most intriguing properties of graphene. Moreover, all graphene based nanostructures will succeed such property. We show a correlation between atomic scale characteristic (pyramidalization angle) and macroscopic characteristic (curvature) of material and substantiate that slight variations in atomic structure will lead to significant changes of macroscopic characteristics of material by the example of dipole moment. We established the linear dependence of flexoelectric dipole moments on the local curvature for different carbon networks with various atomic arrangements by combining direct *ab initio* calculations with, wherever possible, analytical phenomenological equations. Using the obtained universal flexoelectric coefficient, the large dipole moment values of various carbon nanocones are predicted and their scaling with cone dimensions is elucidated. Our analysis suggests the possibility of predicting the electric dipole moments of complicated low-dimensional graphene-based systems using only their atomic geometry [5].

References

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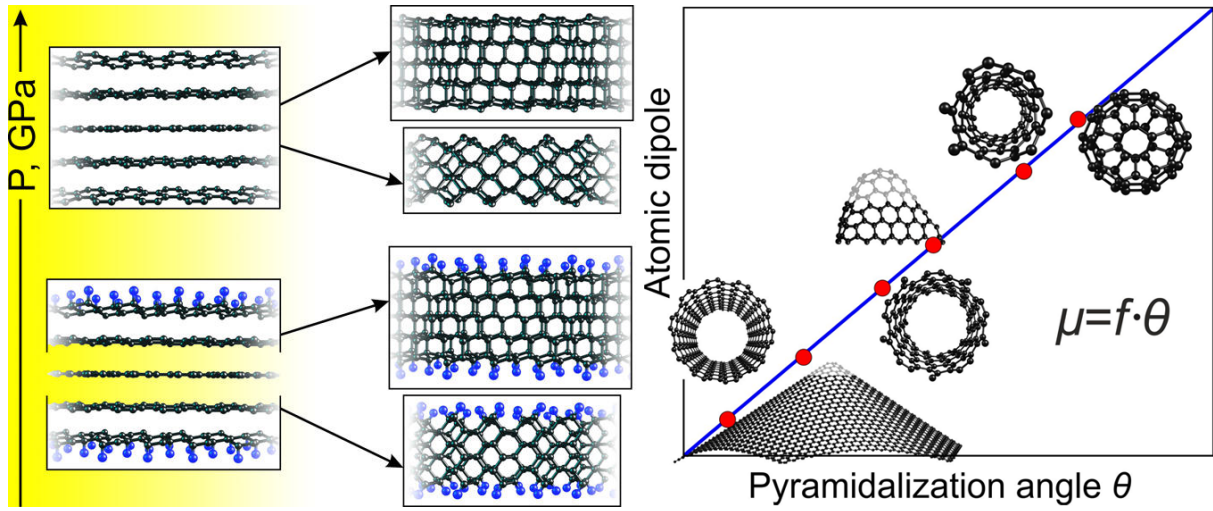


Figure 1: New nanoscale effects in graphene. Left: The chemically induced phase transition as a way to form diamond films of nanometer thickness from multilayered graphene. Right: Flexoelectric effect in graphene based nanostructures, computed atomic dipole moment for carbon nanostructures as function of pyramidalization angle.