Graphene in view of atomic-molecular approach

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Atom-molecular approach suggested in the paper concentrates attention on characteristics of graphene that follow from peculiarities of its atomic electronic structure, main of which is effective unpairing of odd electrons. The feature makes graphene stand in one row with fullerenes and carbon nanotubes, which opens large facilities of application of a number of conceptually original and practically efficient approaches developed for and checked over the latter to the graphene case [1]. This concerns the following fundamental properties of graphene

1. Chemical activity and chemical modification;
2. Magnetic behavior;
3. Mechanical strength and failure;

sp^2 Nanocarbons become partially radicalized when the length of their C-C bonds exceeds a limit value of 1.395Å, under which two odd electrons related to the bond are covalently coupled forming a classic pair of π electrons but over which the two electrons become effectively unpaired, the more, the bigger length of the bond. In the case of benzenoid-based structures, the number of the unpaired electrons constitutes ~0.6 *e* per the unit which is typical for fullerenes, carbon nanotubes, and graphene. All together the unpaired electrons of total number N_D quantitatively determine the molecule chemical susceptibility while their fractions on each atom N_{DA} quantify the atomic chemical susceptibility. Both quantities lay the foundation of the computational synthesis of both one-step and multi-step derivatives governed by strictly defined algorithm.

Weakening the interaction between odd electrons exhibited by their effective unpairing promotes the magnetic behavior of the molecule, once existing in the singlet ground state. The weakening increases with the molecule size thus providing quite a low values for the magnetic coupling constant *J* that becomes sufficient for a noticeable van Fleck's admixture of high spin states to the singlet one [2]. When the molecule size exceeds the electron mean free path, quantization of electron properties strongly increases the constant *J*, which removes high-spin contribution from the singlet state making it non-magnetic.

The molecular approach based on mechanochemical reaction is suitable for describing deformation and failure of graphene as well as exhibiting a peculiar tricotage-like behavior of the graphene molecule under uniaxial tension [3] as well as the effect of chemical modification.

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[2] E.F.Sheka and L.A.Chernozatonskii. *J. Exp. Theor. Phys*. **111**, 222, 2010.
[3] E.F.Sheka, N.A.Popova, V.A.Popova, E.A.Nikitina, L.Kh.Shaymardanova. *J. Mol. Mod*. DOI:10.1007/s00894-010-0816-3, 2011.