FUNCTIONALIZATION AND ELECTROSTATIC MULTIPOLES AT CNT AND GRAPHENE SURFACES

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Carbon nanotubes (CNTs) are 1D nano materials, quantization along axis exists; CNT is considered as quantum wire or quantum dot. Functionalization is powerful method for tuning CNT’s quantum energy levels and physical properties. Functionalization of 2D graphene and bigraphene layers is also applied widely. The theory was developed for energy spectra tuning in the semiconducting nanowires and {\bf polarons} formation as the result of functionalization by molecular layers with (i) radial degree of freedom, (ii) conformational transition in the molecules and (iii) incommensurate structures.

Periodic distribution of metals, metal-organic and conducting polymers at CNT surface was found by TEM. The charge leads to electron and hole (pair), spatially separated in neighboring substrate (CNT) and a molecule or atom.

The aim of this work is theoretical consideration of initial stages of functionalization with the charge transfer. The functionalizing molecules (atoms) at a surface are considered for charge transfer between a molecule and substrate (CNT or graphenes), the electron-hole pairs are formed. The molecules (atoms) can be electropositive with the electronic negative clouds of the transferred charge or electronegative with the transferred positive holes. It is shown that at initial and intermediate stage of functionalization the intermolecular long-range interaction can be described as electrostatic dipole’s and quadrupole’s ones. We consider situation of enough small molecules with relatively large distance between ones. This model explains a homogeneous (sometimes periodic) distribution of adsorbed particles found in the experiments. At short-range distances, compared with the molecules size, the proposed method would be applied with higher error.

For separately adsorbed atoms or molecules we write dipole-dipole interaction which depend on orientation at the CNT or bigraphene surface. The same dipoles orientation leads to repulsing, the opposite one leads to attraction. They correspond to experimentally observed structures. Increasing of the functionalizing molecules concentration leads to formation of different clusters which can't be described in the present model.

The nanobelts, nanospheres, nanocrystals are formed at CNT or nanowire surfaces at higher concentration of the functionalizing molecules. These structures are periodic or almost periodic in experiment. We propose to describe the nanobelts with charge transfer as electric quadrupole (tensor of electric quadrupole moment). It is shown an indifferent equilibrium of a dipole exists between the nanobelts; a weak attraction to the nanobelts at short distances is realised. The nanobelts (quadrupole) are repulsed. These interactions create the stable periodic nanobelts structure as atomic (molecular) condensate at a CNT surface.