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Adsorption, functionalization and electrostatic multipolar interactions at CNT and graphene surfaces

Abstract

The functionalizing molecules (atoms) at a surface are considered for charge transfer between a molecule and substrate (CNT or graphenes). It is shown that at initial and intermediate stage of functionalization the intermolecular interaction can be described as electrostatic dipoles and quadrupoles ones. This model explains a homogeneous (sometimes periodic) distribution of adsorbed particles found in the experiments.

Keywords: adsorption, charge transfer, multi pole electrostatic interaction, graphenes, CNT Pacs 79.60.Dp

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Introduction

Carbon nanotubes (CNTs) are 1D nano materials, quantization along axis exists; CNT is considered as quantum wire or quantum dot.[1] Functionalization is powerful method for tuning CNTs quantum energy levels and physical properties. Functionalization of 2D graphene and bigraphene layers is also applied widely. The theory was developed[2] for energy spectra tuning in the semiconducting nanowires and 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[3] and conducting polymers at CNT surface was found by TEM.[4] The charge transfer[3] 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. It is shown that the electron-hole pairs can be presented as the dipole and quadrupole moments with long range interaction. We consider situation of enough small molecules with relatively large distance between ones. At short range distances, compared with the molecules size, the proposed method would be applied with higher error. The charge transfer is example of a general contact interaction of molecules with different electro negativity. Thus, in comparison with CNT and graphene we have electronegative molecules with F, Cl, O, N. P, S atoms and electropositive metals or metal-organic complexes. In further consideration we suppose the molecules (atoms) to be electropositive and the electronic clouds of the transferred charge to be negative, they are shown in Figure 1. A dipole vector[5] $d = qr$ is shown as arrow between centers of negative and positive charges in Figure 1. Following to[5,6] we write dipole-dipole interaction as:

$$U_{dd} = \frac{d^2}{R^3}\left[(\omega_1\omega_2) - 3(\omega_1\,\mathrm{n})(\omega_2 n)\right] \ldots\ldots\ldots \quad (1)$$

where R is the radius-vector between centers of the dipoles 1 and 2, $R = |\mathrm{R}|$, the unit vectors ω_2, ω_2 and n are directed along d_1 d_2 and R. Force between two particles for (1) is

$$F_{ij} = -\frac{dU_{ij}(\mathrm{R})}{dR} = -\frac{1}{dR}\left[\frac{A}{R^K}\right] = \frac{K}{R}U_{ij}(\mathrm{R}) \ldots\ldots \quad (2)$$

where factor A is function of all parameters except distance R. In (1) power $k = 3$ and $U_{ij} = U_{dd}$. In next formulae $k = 4; 5$ and $U_{ij} = U_{Qd}; U_{QQ}$. Positive F means repulsion. The dipoles configuration in Figure 1 gives according (1, 2) $F_{12} > 0$ and $F_{13} < 0$ because of $(\omega_1\,\mathrm{n}) = 0$ and $(\omega_1\omega_2) > 0$ but $(\omega_1\omega_3) < 0$. Increasing of the functionalizing molecules concentration leads to formation of different clusters[3,4] which can't be described in the present model. Only the small clusters with the multiple numbers N of the molecules can be described by (1) applying $d_N = Nd_1$. A renormalization of the charge transfer can arise depending on the cluster size (multiple numbers N). The nanobelts, nano spheres, nanocrystals are formed at CNT or nanowire surface[3,4] at higher concentration of the functionalizing molecules. These structures are periodic or almost periodic. The nanobelts are schematically depicted in Figure 2. We propose to describe the nanobelts with charge transfer as electric quadrupole. Definition of tensor of electric quadrupole moment is $Q_{ab} = \sum Q_a x_a x_b$ (5). In the main axes and after normalization $\mathrm{Sp}Q_{aa} = 0$ the quadrupole moment in axe-symmetric case is described by only one parameter Q.[5,6] In Figure 2 external arrangement of the positive ions gives $Q > 0$. Dipole-quadruple U_{Qd} and quadruple-quadruple U_{QQ} interactions are:[6]

$$U_{Qd} = -\frac{3Qd}{2R^4}\left[(\omega_1\,\mathrm{n}) + 2(\omega_1\omega_2)(\omega_2\,\mathrm{n}) - 5(\omega_1\,\mathrm{n})(\omega_2\,\mathrm{n})^2\right] \ldots\ldots\ldots (3)$$

$$U_{QQ} = -\frac{3Q^2}{4R_0^5}[1-5(\omega_1 \text{n})^2 - 5(\omega_2 \text{n})^2 + 2(\omega_1\omega_2)^2 + 35(\omega_1 \text{n})^2(\omega_2 \text{n})^2 - 20(\omega_1 \text{n})(\omega_2 \text{n})(\omega_1\omega_2)] \quad \ldots..(4)$$

Here Q is the nanobelts quadrupolar moment, R is the distance between centers of a quadrupole and a dipole or between two quadrupoles, n, ω_1, ω_2 are unit vectors. $n \| \mathbf{R}$. In (3) $\omega_l \| d_1$ In (4) ω_1, ω_2 direction is along the quadrupole axes. For the dipole and quadrupole in Figure 2 $\omega_1 \perp \omega_3$ and $A_{Qd} \simeq +12Qd\,(\omega_3 \text{n}_{31}) < 0$, at large distances $A_{Qd} \rightarrow 0$. According to (3,2) an indifferent equilibrium of the dipole between the nanobelts and weak attraction at short distances exist. Two nanobelts repulsion in Figure 2 is due to $A_{QQ} = 6Q^2 > 0$ or $F_{12} > 0$ in (4,2).

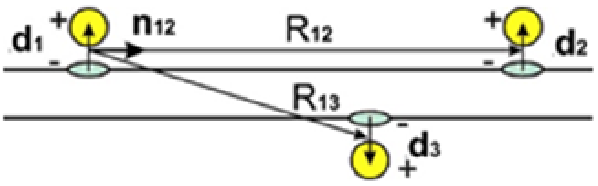

Figure 1 The adsorbed molecules or atoms (yellow spheres) at substrate (CNT, graphene) with transferred electrons (blue ellipses) gives repulsion of dipoles $d_1 \|\| d_2$. Opposite dipoles d_1; d_3 are attracted at semiconducting CNT or bi graphene.

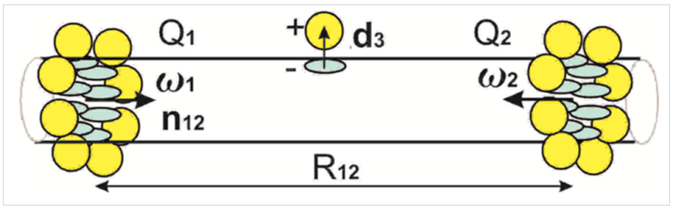

Figure 2 The quadrupoles Q_1, Q_2 formed by nanobelts of the adsorbed atoms at CNT sur-face are repulsed according (4). The intermediate dipole is unstable due to nanobelts attraction.

Another case of quadrupoles formation is intercalation into bigraphene or graphite, see Figure 3. Adsorption, functionalization and electrostatic multipolar interactions at CNT and graphene surfaces 3. It seems, to provide the charge transfer into two planes it be better to have higher valence of intercalating atoms. Values $(\omega_1 \text{n}) = 0$ and $A_{QQ} = (3=4)Q^2$ in (4,2) means repulsing.

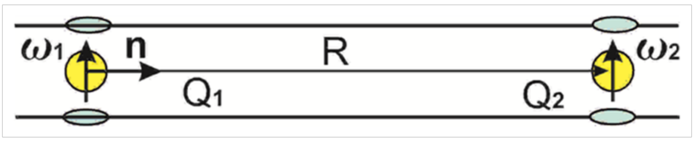

Figure 3 The quadrupoles formed by the inter-collated molecules are repulsed into bi graphene.

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Conflict of interest

The author has no conflicts of interests in this work.

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