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FUNCTIONALIZED SEMICONDUCTING CARBON NANOTUBES: THREE MODELS FOR CARRIER SPECTRA

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Electronic spectra in functionalizing semiconducting carbon nanotube (CNT) are researched theoretically. The soft degrees of freedom are considered in the molecular system: radial deformation, misfit dislocations, and conformation. For each model the selfconsistent system of equations is derived. A system describes a charge carrier longitudinal quantization in CNT, interaction of a carrier in CNT and molecular electric dipoles, material equations for a soft degree of freedom and its reconstruction. It is shown that the functionalization reconstructs the CNT electronic spectra and creates different conditions of localization or tunneling for holes and electrons.

INTRODUCTION

Carbon nanotubes (CNTs) are nanomaterials with a small diameter of about 1 nm, length of about 1 μm and the mean free path of the charge carriers that exceeds 10 μm [1] which is important for quantization along CNT axis [2]. The optical properties and conductance of a nanoobject are determined by the set of quantum energy levels of its charge carriers [3] what has been observed for CNTs [4]. Functionalization is new powerful method for tuning CNTs quantum energy levels and a set of their physical properties [5]. The CNTs novel high-sensitive biosensors, electronic and optoelectronic devices are created due to functionalization. Chips based on CNTs and DNA [6] or surface self-organizing organic structures [7] are discussed.

Theory of energy spectra tuning in the semiconductor CNTs as the result of functionalization by enough thick molecular films were developed by the authors in [8, 9]. The spectrum is extremely sensitive to the state of the molecular subsystem. We considered the effect of the interaction of the uncompensated charge carried by an electron or hole in a quantum nanowire with the neighboring medium that has low mechanical rigidity and consists of molecules possessing an intrinsic electric-dipole moment. The nonlinear nonlocal equations describing the system were derived. Longitudinal quantization was reduced to the spectral problem for a nonlinear Schrodinger equation. The shift of the charge-carrier energy levels was calculated. Possibility of carrier localization was shown.

The aim of this research is to develop theoretical approach to the CNTs spectra tuning as a result of functionalization. The selfconsistent system of equations will be derived; it includes (i) the time-independent Schrodinger equation for a charge carrier in a semiconductor CNT; (ii) nonlinear equation for the molecular structure; (iii) the material equations for interaction of an extra carrier in CNT and molecular electric dipoles subsystem.

MODEL OF THE SYSTEM

The time-independent Schrodinger equation for an extra charge carrier in an intrinsic-semiconductor nanotube can be written as [3, 10]

$$\frac{\hbar^2}{2m_{ef}}\Delta\psi + U(\vec{r})\psi = W\psi. \qquad (1)$$

Here $\psi \equiv \psi(\vec{r}), m_{ef}$ and $\vec{r}$ are wave function, effective mass and the radius vector of the particle, Δ is the Laplace operator, *W* is the total energy, $U(\vec{r})$ is the potential energy. Approximation of infinite depth well is applied: $U(\vec{r}) \equiv U_0(\vec{r})$ where $U_0(\vec{r}) = 0$ inside CNT and $U_0(\vec{r}) = \infty$ outside one. Accounting the interaction

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with the surrounding medium $U_{int}(\vec r)$ the potential is given by relation

$$U(\vec r) = U_0(\vec r) + U_{\text{int}}(\vec r). \qquad (2)$$

This interaction can be relatively strong if functionalizing molecules have an intrinsic dipole moment $\vec d$. Summing the contributions from all the dipoles, one can get the interaction potential energy $U_{int} = e\phi$ within the nanotube by integration in respect to external space $\vec r\,'$. Here e is the carrier charge. In turn, a charge carrier determines the potential of the interaction with an individual dipole. Approximations of a long nanowire, relatively, thin layer and cylindrical coordinates ($\psi(\vec r) = \psi(x)\psi_\perp(y,z), x$ is the coordinate along the wire) allow to reduce the integral contributions to those of a local nature [8, 9]. The potential energy of the interaction of a charge carrier with the dipole subsystem is

$$U_{int}^{e0} = -4\pi n_0 de(R-r) \to -4\pi n_{S0} de. \qquad (3)$$

Here n_{S0} is the surface density of the molecules in the limit case of the thin functionalizing layer. The local value of the radial field strength is replaced with a value for an infinitely long wire taking the local value of the wave function

$$U_{int}^{d}(x) = -\vec E\vec d = -\frac{2\tau d}{\varepsilon r'};$$

$$\tau(x) = e|\psi(x)|^2 F_\perp;\ F_\perp = \int |\psi(y,z)|^2\,dydz. \qquad (4)$$

Here $\tau(x)$ is the local linear charge density and ε is the relative permittivity of the medium. The positive direction of a dipole moment $\vec d$ coincides with the direction towards the center of CNT (see Fig. 1*a*). The set (1)–(4) is to be completed with the material equations

$$n(\vec r\,') = n(\vec E(\vec r\,')). \qquad (5)$$

Here $n(\vec r\,')$ is the volume number density of the molecules. The effect of the charge-carrier field is the strongest in the case when the molecules possess an intrinsic electric-dipole moment $\vec d$. The electric-dipole moment in the organic molecules exists due to the presence of atomic groups that break the charge symmetry [7, 11].

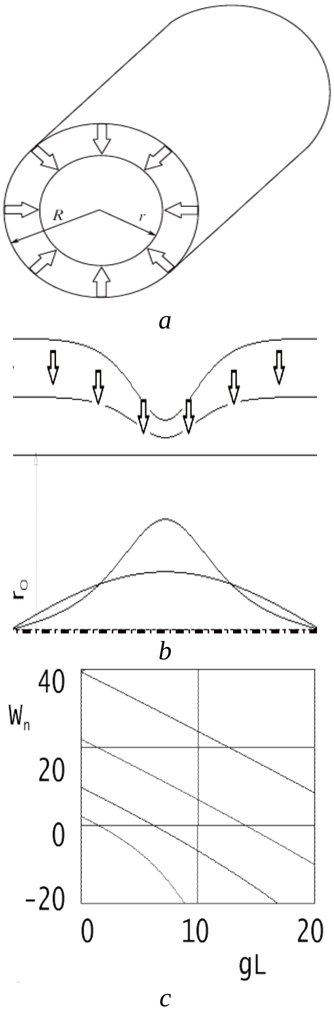

Fig. 1. (*a*) Cylindrical CNT with adsorbed polar molecules. Arrows indicate direction of electric polarization vector. (*b*) and (*c*) form of the carrier wave function, molecular layer and renormalized energy of levels W_n at different nonlinear interaction gL according to [8, 9]

With accounting of relations (4) and (3), Eq. (1) can be rewritten to describe the 1D motion of the charge carriers in the CNT as follows

$$-\frac{\hbar^2}{2m_{ef}}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x) = W_x\psi(x). \qquad (6)$$

SOFT RADIAL DEGREE OF FREEDOM

The soft molecular layer consisting of a liquid crystal or other adsorbed molecules with intrinsic electric dipole moment was considered in [8, 9]. The longitudinal quantization of a charge carrier is reduced to the spectral problem for nonlinear Schrodinger equation. The selfconsistent solution of the spectral problem is obtained in terms of elliptic functions. Features of behavior of the system are following: the higher interaction, the more nonlinearity; the lowest quantum levels feel the most nonlinearity; the effect should be more pronounced for heavier holes; under increasing of interaction the carriers are localized (see Fig. 1*b*,*c*).

MISFIT DISLOCATIONS

Hamiltonian of molecular chain on a substrate in continual approximation is [12]

$$U_s(\phi(x,t)) = U_0[1-\cos(\phi(x,t))]; \;\; \phi(x,t) = \frac{2\pi u(x,t)}{a_s}; \qquad (7)$$

where ϕ is effective phase, *u* is the displacement of a molecule from the equilibrium position in the layer. Then continual equation of motion has integral *E*

$$(\phi')^2 = \frac{2}{\lambda_0^2}(E-\cos\phi); \;\; \lambda_0 = \frac{a_m^2}{2\pi}\sqrt{\frac{2\kappa}{U_0}}. \qquad (8)$$

Here a_m is the molecular lattice constant, λ_0 is characteristic length and κ is elastic constant in the molecular layer. At $E>1$ continual equation has periodic solution

$$\cos(\frac{\phi(x)}{2}) = -\sigma\, sn(\xi, k_m)\; ; \;\; \xi = \frac{x-x_0}{k_m\lambda_0}\; . \qquad (9)$$

Here $sn(\xi,k_m)$ is Jakobi elliptic function with elliptic module k_m defined by relation [12]: $k_m^2 = 2/(E+1);\; 0 \le k_m \le 1.$ The period of $sn(\xi,k_m)$ in dependence on ξ is $4K(k_m)$. $K(k_m)$ is full elliptic integral of the first kind. The space period on *x* [12] in (9) is

$$l_x = 4k_m K(k_m)\lambda_0\; . \qquad (10)$$

The periodic misfit dislocations (9) arise in the molecular layer. Regions of local extension (kink, $\sigma = +1$) or constriction (antikink, $\sigma = -1$) exist. Then deviation of concentration and the potential U_{int}^{e0} (3) are

$$\delta n_S(x) = n_{S0}\frac{\partial u}{\partial x} = \frac{n_{S0}a_s}{\pi\lambda_0}\frac{\sigma}{k_m}dn(\frac{x}{k_m\lambda_0}, k_m); \qquad (11)$$

$$U_{int}^{e}(x) = U_{int}^{e0} + U_{int}^{e\delta}(x); \;\; U_{int}^{e\delta}(x) = -4\pi d e\,\delta n_S(x). \quad (12)$$

Accounting to relatively large size and complicated construction of organic molecules, creating of partial dislocations is very probable.

Renormalization of substrate interaction. Material equation for renormalized interaction of the molecular layer with substrate has to account simultaneously the effect of the substrate U_s and carrier charge field U_{int}^{d} (4) potentials. The amplitude of the substrate potential can be found as $U_0(r) = [U_{si}(r) - U_{sc}(r)]/2$ through the interaction potentials in incommensurate fragments $U_{si}(r_0,x)$ and commensurate ones $U_{sc}(r_0,x)$

$$U_0 \to U_{0E}(r_0,x) = U_0 - \delta G_{4s}\,|\psi(x)|^4 < U_0;$$

$$\delta G_{4s} = [\frac{1}{k_{si}(r_0)} - \frac{1}{k_{sc}(r_0)}]\times[\frac{deF_\perp}{\varepsilon r_0'^2}]^2; \qquad (13)$$

The potential near the equilibrium radius r_0 depends on the rigidity $k_s(r) = \partial^2 U_{0s}(r)/\partial r^2$. Commensurate fragments are more rigid $k_{sc}(r_0) > k_{si}(r_0)$. Substitution of (13) into (7) gives the Frenkel-Kontorova potential renormalized by a carrier electric field. The terms $\sim|\psi(x)|^2$ are compensated. According to (10, 8) $l_{xE} \sim \lambda_{0E} \sim 1/\sqrt{U_{0E}}; U_{0E} < U_0; l_{xE} > l_x$. Due to nonlinearity of a molecule-substrate interaction, one has more rigid repulsion and more soft attraction.

Superlattice potential of the misfit dislocations. Let us consider an action of the functionalizing layer on a carrier inside CNT. In this case the Schrodinger equation (6) can be rewritten with the potential $U(x) = U_0(x) + U_{int}^{e0}(x) + U_{int}^{e\delta}(x)$. The initial potential equals inside $U_0(x) = 0$ and outside $U_0(x) = \infty$ of interval $-L < x < +L$. The potential U_{int}^{e0} is given by relation (3) and is responsible for a homogeneous shift of the quantum well bottom. The potential $U_{int}^{e\delta}(x)$ is given by relations (11, 12) and is responsible for creation of a superlattice structure in the case of a periodic dislocation arrangement. The inequalities $\lambda_0 << l_x << L$ have to be satisfied. Band structure modulation of semiconducting CNT at $E>0$ and $\sigma d > 0$ is shown in Fig. 2. The valence band top has narrow peaks.

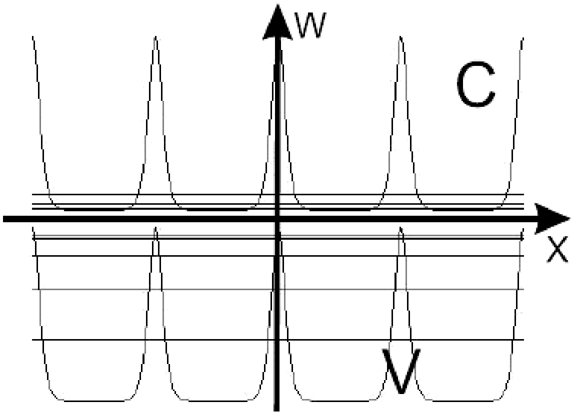

Fig. 2. The band structure of semiconducting CNT modulated according to (12) at $E>0$ and $\sigma d›0$. Quantum levels of electrons in conductivity band (C) and holes in a valent band (V) are shown. The molecular layer creates opposite conditions for localization or tunneling of the carrier on a superlattice of misfit dislocations

Selfconsistence. Misfit dislocation rearrangement. Let's consider a turn action of a carrier in CNT on the molecular layer. After substitution of (13) into (7) we obtain the renormalized Frenkel-Kontorova potential. A carrier attracts (repulses) the molecular layer that leads to the coherent regions widening and the characteristic length (8) takes form

$$\lambda_{0E}(x)=\frac{a^2}{2\pi}\sqrt{\frac{2\kappa}{U_{0E}(x)}}\approx\lambda_0[1+\frac{\delta G_{4s}\,|\psi(x)|^4}{2U_0}]. \quad (14)$$

In the case of a fast carrier tunneling the dislocations have no time to move, so the undisturbed superlattice in Fig. 3*a* is kept. In relations (10) the space period of misfit dislocation depends on the carrier electric field $l_{xE}(x)\sim\lambda_{0E}(x)$. The higher carrier density inside CNT creates regions with larger space period of misfit dislocation. Direct inserting of (14) with $\psi\sim\cos(\pi x/2L)$ into (11) yields the picture of the dislocation rearrangement and band modulation shown in Fig. 3*b* The superlattice tunneling is destroyed and the electron turns to be locked in one period of the deformed dislocation structure. The periodic quantum wells for a hole in CNT are relatively narrow. They are divided by wide commensurate regions. This can lead to the carrier localization at a dislocation Fig. 3*c*.

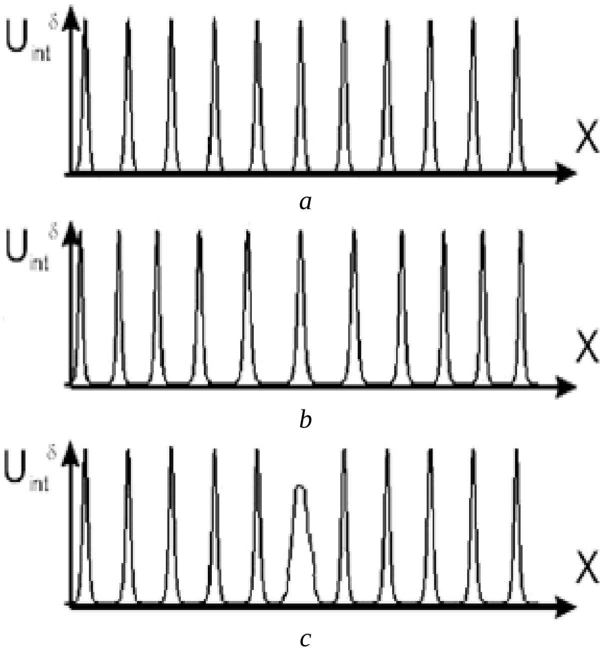

Fig. 3. Form of the conducting band bottom. (*a*) Homogeneous misfit dislocation distribution along CNT as in Fig. 2. (*b*) The first stage of the misfit dislocation rearrangement in the electron field. (*c*) Hole localization about a peak of valence band top

To estimate a carrier potential change due to the molecules we use parameters from [9, 11, 12]. From (3) the bottom level of the quantum well in CNT with functionalizing molecular layer is $|U_{int}^{e0}|\sim(1\div10)$ eV and the barrier height is $|U_{int}^{e\Delta}(x)|\sim|U_{int}^{e0}|\,a/\lambda_0\sim(01\div1)$ eV.

CONFORMATION TRANSITION

The conformation of a molecule means that two or more molecular configurations exist. The conformation transition (CT) means change of the configuration. In the general case an asymmetric molecule have different energies of conformation configurations [14] (the energy difference W_c). Let's denote the molecular electric dipole moment d_0 in the initial stable conformation and d_1 in the unstable one, the electric dipole moment change is $\Delta d=d_1-d_0$. CT is possible if the carrier electric field intensity exceeds the critical value E_c defined by relation that leads (4) to the critical values of the linear charge density τ_c and wave function density $|\psi_c|^2$ in CNT:

$$E_c=\frac{W_c}{\Delta d_r};\quad \tau_c=\frac{W_c\varepsilon r'}{2\Delta d_r};\quad |\psi_c|^2=\frac{\tau_c}{eF_\perp}. \quad (15)$$

Here d_r is the radial projection. CT is possible only for one mutual orientation of the vectors. A carrier with another sign of charge does not create CT. The CT goes as order-disorder phase transition in the carrier electric field. After CT the carrier decreases its energy on the value

$$\Delta U \equiv \Delta U^{e}_{int} = -4\pi n_s e \Delta d. \qquad (16)$$

The most probable scenario: a carrier tunnels into CNT on a high level and jumps to the basic state then conformation transition goes (the phonon relaxation is faster then conformation one). The basic state wave function must exceed the critical value (15) $\psi_1(x) \geq \psi_c$. As the result, the wave function has only one maximum and conformation domain takes symmetric position. The potential well of infinite depth with width $2l$ arises, it includes symmetrically a potential well of the finite depth ΔU (16) with width $2a(a<l)$. So the carrier potential inside CNT is

$$U(x) = \begin{cases} \infty; & |x| > l; \\ 0; & a \leq |x| \leq l; \\ -\Delta U; & |x| \leq a. \end{cases} \qquad (17)$$

Following to [13] let us introduce the wave numbers k_0 (the conformation transition well depth), k (the basic energy level height), and κ (the basic energy level depth):

$$\Delta U = \frac{\hbar^2}{2m_{ef}} k_0^2; \quad W_x = \frac{\hbar^2}{2m_{ef}} k^2; \quad \kappa^2 = k_0^2 - k^2; \qquad (18)$$

Let us write the selfconsistent system of equations

$$\begin{cases} \kappa^2 = k_0^2 - k^2; \\ \tan ka = \dfrac{\kappa}{k} \dfrac{1}{\tanh \kappa(l-a)}; \\ \dfrac{1}{A^2} = a + \dfrac{1}{\kappa} \tanh \kappa(l-a) + \dfrac{\cos^2 ka}{\kappa} \left[\dfrac{2}{\mathrm{sh}\, 2\kappa(l-a)} - \dfrac{\kappa(l-a)}{\mathrm{sh}^2 \kappa(l-a)}\right]; \\ A \cos ka = \psi_c. \end{cases} \qquad (19)$$

The first equation of the system (19) defines the wave number κ, the second one is the first derivation the continuity condition in point $x=a$. The third equation is the normalization condition, A is the wave function amplitude. The fourth equation: the wave function on the boundary of the conformation domain takes the critical value $\psi(a)=\psi_c$. The last equation directly defines the selfconsistency of all sizes and energies of the problem.

The first and the last equations in (19) allow exclude the variables A and κ. After introducing the dimensionless variables C, D and parameters L, Φ the rest of the system can be transformed to the following selfconsistent form

$$\begin{cases} D \tan D = \sqrt{C^2 - D^2} \dfrac{1}{\tanh[\sqrt{C^2 - D^2}(\frac{L}{C} - 1)]}; \\ 1 + \dfrac{1}{D \tan D} + \\ \dfrac{1}{1 + \tan^2 D} \left\{ \dfrac{D \tan D}{C^2 - D^2} - \dfrac{1}{D \tan D} - \left(\dfrac{L}{C} - 1\right)\left(\dfrac{D^2 \tan^2 D}{C^2 - D^2} - 1\right) - \dfrac{1}{\Phi C} \right\} = 0 \end{cases} \qquad (20)$$

$$C = k_0 a; \quad D = ka; \quad L = k_0 l; \quad \Phi = \frac{|\psi_c|^2}{k_0}; \qquad (21)$$

The system of equations (20) is nonlinear and transcendental with two unknown variables. The first equation is generalization of the one unknown variable equation for the finite depth quantum well in [13] (there tanh(x) is absent, parameter C is fixed and ka is unknown). In [13] the equation is solved by graphic method on a plane. Here we use the graphic method. However, for two unknown variables graphic must operate with 3D space. The system's solution for the base quantum state can be ambiguous. We take the minimum energy solution. For dimensionless parameters values L=10; Φ=0.2 graphic solution of the system (20) gives the relative width and depth of the arising quantum well and position of the basic quantum level (see Fig. 4)

$$\frac{a}{l} = \frac{C_c}{L} \approx 0.11; \frac{k}{k_0} = \frac{D_c}{C_c} \approx 0.71; \frac{W}{W_0} = \frac{k^2}{k_0^2} \approx 0.50. \qquad (22)$$

ESTIMATIONS

The molecular electric dipole change is $\Delta d \sim d \sim |er_0| \sim 10^{-28}\ Cl \cdot m$. The carrier energy decreasing after conformation transition (16) is $\Delta U \sim (10^{+1}\text{–}10^{-1})\ eV$. The linear charge density (15) and the energy difference between the conformations are $\tau_c \sim e/2l \sim 10^{-13}\ Cl/m$; $W_c \sim 10^{-3}\ eV$. The shorter is CNT the more W_c can be overcame by a carrier.

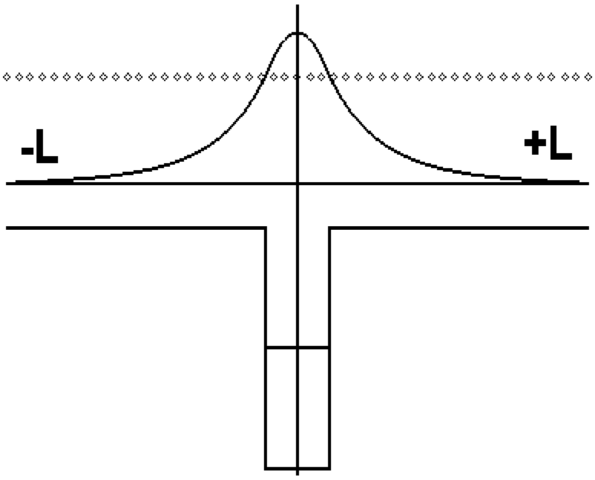

Fig. 4. The potential well, the basic state electron (or hole) wave function $\psi_1(x)$ shape, and position of basic energy level in CNT after conformation transition in the functionalizing molecular layer. Diamonds show level of the critical value ψ_c for a conformation transition

CONCLUSIONS

The energy spectrum of uncompensated charge carrier in a functionalized CNT is investigated. The physical mechanism responsible for this interaction is the molecular dipole moment interaction with the charge carrier electric field. A homogeneous distribution of the molecular dipoles creates homogeneous shift of electric potential along CNT. Following soft degrees of freedom in the functionalizing molecular system are considered: (i) radial elastic deformation of the molecules; (ii) the periodic system of misfit dislocations of the molecules along CNT; (iii) the molecules conformation.

The periodic misfit dislocations with extra or lack dipoles create a superlattice potential for a carrier inside a nanotube. The topological invariant $sign(\sigma d) = \pm 1$ defines creating the relatively narrow peaks or wells for electron (correspondingly the wells or peaks for hole). Considerable deviation of the bands edges relief from a sinusoidal function breaks symmetry of the spectra. The narrow peaks are easily penetrated by a carrier that causes the narrow gap or quasigap arising in corresponding band. In another band the narrow wells are divided by wide barriers; tunneling is rather difficult. It causes very narrow miniband. In its turn the charge carrier attracts the molecular layer that makes dislocation out of periodicity and coherent regions expand. It destroys miniband structure and can lead to carrier localization faster.

In CNT the spectra of holes and electrons are symmetric. The layer of the functionalizing molecules with the intrinsic electric dipoles breaks this symmetry in dependence on a charge sign, dipole orientation, and a kind of the dislocation or conformation. The conformation transition in the electric field and energy spectrum modification are possible for one sign of the carrier charge. The carrier with another sign of charge feels a homogeneous change of potential along CNT only. Thus, a functionalized CNT with a conformation transition can be used as a semiconductor rectifier.

The functionalized CNT and induced spectra are extremely sensitive to variation of the molecule-molecule and molecule-substrate interaction constants. It may be caused by temperature, phase transitions, filling of functionalizing layers and impurity containing. The charge-carrier energy spectrum depends on the rigidity of the functionalizing molecular system. The high rigidity of the functionalizing molecular system leads to suppression of localization. The CNT conductivity must grow significantly in these cases. Thus, a nanowire can be used as a sensor for the state of the molecular system. The processes considered should be taken into account in the design of chips based on CNT and layered organic surface structures [6, 7].

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Функціоналізовані напівпровідникові вуглецеві нанотрубки: три моделі для спектрів носія

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Теоретично досліджено електронні спектри функціоналізованої напівпровідникової вуглецевої нанотрубки (НТ). В молекулярній системі розглянуто наступні м'які ступені свободи: радіальна деформація, дислокації невідповідності і конформації. Для кожної моделі отримана самоузгоджена система рівнянь. Кожна система описує поздовжне квантування носія заряду в НТ, взаємодію носія в НТ з електричними диполями молекул, матеріальні рівняння для м'якого ступеня свободи і його реконструкції. Показано, що функціоналізація модифікує електронні спектри НТ і створює різні умови для локалізації або тунелювання дірок й електронів.

Функционализированные полупроводниковые углеродные нанотрубки: три модели для спектров носителя

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Теоретически исследованы электронные спектры функционализированной полупроводниковой углеродной нанотрубки (НТ). В молекулярной системе рассматриваются следующие мягкие степени свободы: радиальная деформация, дислокации несоответствия и конформации. Для каждой модели получена самосогласованная система уравнений. Каждая система описывает продольное квантование носителя в НТ, взаимодействие носителя в НТ с электрическими диполями молекул, материальные уравнения для мягкой степени свободы и ее реконструкции. Показано, что функционализация модифицирует электронные спектры НТ и создает различные условия для локализации или туннелирования дырок и электронов.