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RESONANT ENERGY TRANSFER FROM A DYE MOLECULE TO A CARBON NANOTUBE

In this paper, the features of the Förster resonance energy transfer from excited dye molecules to semiconducting single-walled carbon nanotubes are investigated, in particular, the dependence of the energy transfer rate on the distance between the dye molecule and the carbon nanotube itself. Analysis of the obtained results shows, in particular, that the energy band gap ε_g *within the limits* $\varepsilon_g \sim (0.5\text{–}5) \times 10^{-19}$ *J does not significantly affect the energy transfer rate* $\gamma(\hbar\Omega)$*, the value of which is determined by the induced dipole moment* μ_{eg}*, the amount of energy transferred in the resonant transfer process* $\hbar\Omega$*, and the effective mass of the electron in the semiconductor carbon nanotube* m^**. The proposed approach sheds a new light on the understanding of the physical process of resonant energy transfer in various types of low-dimensional physical and biological nanostructures.*

Keywords: graphene, dye molecule; density functional theory, Förster mechanism, rate of energy transfer, carbon-based hybrid nanostructure.

1. Introduction

The absorption of light (electromagnetic radiation) energy by nanoparticles, in particular metal nanoparticles, has always been in the focus of P.M. Tomchuk's interests. It is enough to recall his widely known works on this subject, in particular papers published in highly rated journals [1, 2]. Now, they have found their ideological continuation in the study of the energy transfer in various types of nanostructures, in particular in structures such as a dye molecule – carbon nanotube [3]. Recently, carbon nanotubes (CNTs) are one of the candidates for the next generation of semiconductor electronics [4], optoelectronics neighbor infrared range [5] and absorbers light or transparent conductors for solar elements [6]. In particular, with the use of semiconductors CNTs from controlled forbidden zone, are being prepared now mesoscale networks with tight intertwined bundles (films) [7, 8]. These structures (films) can be used in photovoltaic installations and photodetectors, in which semiconductor tubes are photoabsorbers, similar to electron-donating polymers in polymer solar elements [9]. Like polymers, CNTs have high optical absorption, which can be regulate, and them can process solution, but nanotubes demonstrate superfast charge and energy transfers onto large distances and more stable in air [10]. Although photophysics of individual nanotubes is a common topic of research [9, 11], the properties of these new mesoscale structures (films) mostly unknown. In addition, the possibility to control the composition of the prohibited substance zones films does their model system for studying various kinds of charge and energy transfer processes. The task of studying the features of the energy transfer in such structures is interesting and relevant. The energy transfer from a dye molecule to a carbon nanotube can be considered as the process of nonradiative energy transfer from an excited donor to an acceptor? It is known as Förster resonance energy transfer (FRET) [12]. In FRET, the interaction between the donor and the acceptor are

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Coulombic. The electronic transition dipoles of the donor and the acceptor interact electrostatically leading to an R^{-6} dependence of the rate of transfer onto the distance $\gamma(R)$ between the donor and the acceptor. Förster studied this process theoretically and obtained the analytic expression for the distance dependence of the rate of energy transfer [12]. The rate of FRET from a dipole to the bulk electronic excitation modes of a metal has a d^{-3} dependence (d is the distance from the dipole to the metal) [13, 14]. Previously, it was demonstrated in works that the energy transfer from fluorophore to graphene is dependent d^{-4} and is very efficient [15, 16]. Experiments have shown that graphene can quench the fluorescence of the fluorophores and the process can be used to visualize graphene on surfaces [17] and graphene flakes in solution [18] and to suppress the fluorescence in resonance Raman Spectroscopy [19]. More recently, Govorov et al [20] reported on the study of the process of excitation energy transfer from nanoparticles to nanowires. When the radius of the nanoparticle is small compared to the distance between the nanoparticle and the nanowire d, one can consider the excitations in the nanoparticles as localized and, therefore, dipolar. For large distances of nanoparticles to the wire, they find a d^{-5} dependence. Since the acceptor excitations are limited to dimension 1, the velocity has a d^{-5} dependence.

In this paper, we will study the features of the process of Förster resonance energy transfer from excited dye molecules (fluorophores) to semiconducting single-walled carbon nanotubes, in particular, the dependence of the energy transfer rate on the distance between the dye molecule and the carbon nanotube itself. We will show that the energy gap in the electron spectrum of a semiconductor nanotube does not significantly affect the energy transfer rate, the value of which is determined by the induced dipole moment, the amount of energy transferred in the resonant transfer process, and the effective mass of the electron in the nanotube.

2. Energy Transfer Rate Model

Now, consider the process of FRET from the dye molecule to electrons confined by a very long nanotube with radius R and length $L \to \infty$ (see Fig. 1).

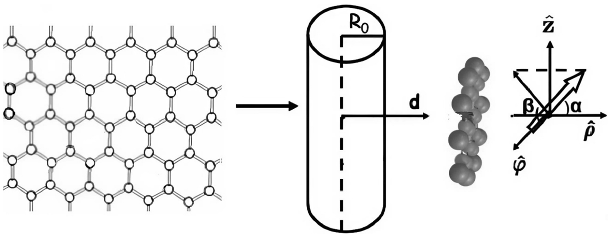

Fig. 1. A schematic of the transition dipole moment of the donor dye and the tube. Note that a nanotube is formed by folding a sheet of graphene. On the right, we show the transition dipole of the dye molecule angles that is makes with the coordinate axes

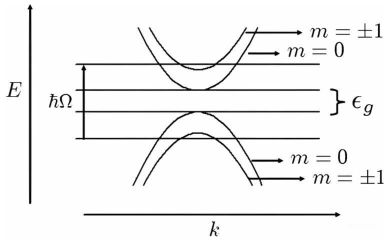

Fig. 2. A schematic of the one-dimensional energy bands of the nanotube showing the quantum numbers along the equatorial direction, the energy gap and the amount of energy transferred

We adopt the simplest possible description for the electrons in a nanotube. Let us have a semiconductor nanotube that has a structure similar to a boron nitride nanotube, with a band gap ε_g (see Fig. 2 [21]).

The states above and below the band gap ε_g can be characterized by a momentum parallel to the tube axis, which we will denote by k, and an angular momentum about the tube axis, which is (where $i = 0, \pm1, \pm2, ...$) [22, 23] as

$$\Psi^{\pm}_{k,m}(\rho,\phi,z) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} e^{ikz_i + im\varphi} \chi^{\pm}(c\,\mathbf{r} - \mathbf{R}_i), \quad (1)$$

The superscripts ± in the wave function $\Psi^{\pm}_{k,m}(\rho,\phi,z)$ denote states above (+) or below (–) the band gap ε_g. The functions $\chi^{+}(r - R_i)$ and $\chi^{-}(r - R_i)$ denote localized orbitals at the i-th site of the graphene lattice, contributing to the conduction band and valence band, respectively; N- the number of sites in the nanotube lattice. We will assume that the electron energy levels in the nanotube are described by the following relation:

$$\varepsilon^{\pm}_{k,m} = \pm\left(\frac{\varepsilon_g}{2} + \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 m^2}{2m^* R}\right), \quad (2)$$

where m^* is the effective mass of the electron in nanotube, R is the nanotube radius. In view of the above, the excitation of an electron from $\psi^-_{k_{i,m_s}}(\mathbf{r})$ to $\psi^+_{k_{f,m_f}}(\mathbf{r})$ leads to the appearance of a transient charge density on the nanotube, which is defined as

$$\sigma(\mathbf{r}) = -e\psi^{+*}_{k_f,m_f}(\mathbf{r})\,\psi^-_{k_i,m_i}(\mathbf{r}) = -e\frac{1}{N}\sum_{i=1}^{N} e^{-iqz_i}\times$$
$$\times\, e^{-im_q\varphi_i}\chi^-(\mathbf{r}-\mathbf{R}_i)\,\chi^{+*}(\mathbf{r}-\mathbf{R}_i), \tag{3}$$

where we have put $k_f = k_i + q$, $m_f = m_i + m_q$ and neglected the product of χ^s which belong to different sites of the lattice, (R,φ,z) are the cylindrical polar coordinates of $\mathbf{R}_i$. The electromagnetic potential due to such transition density is given by

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int d\mathbf{r}_2\frac{\sigma(\mathbf{r}_2)}{|\mathbf{r}-\mathbf{r}_2|}. \tag{4}$$

Since the density $\chi^-(\mathbf{r}_2-\mathbf{R}_i)\,\chi^{+*}(\mathbf{r}_2-\mathbf{R}_i)$ is localized near the i-th atom, one can write the potential as

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0 N}\boldsymbol{\mu}_\pm\nabla_\mathbf{r}\sum_{i=1}^{N}\frac{e^{-iqz_i}e^{-im_q\varphi_i}}{|\mathbf{r}-\mathbf{R}_i|}, \tag{5}$$

where $\boldsymbol{\mu}_\pm = -e\int d\mathbf{r}_2\chi^-(\mathbf{r}_2-\mathbf{R}_i)\,\chi^{+*}(\mathbf{r}_2-\mathbf{R}_i)$ is the transition dipole for the $\chi^-\to\chi^+$ transition. For small values of q, the sum in the above equation may be replacement by an integral so that

$$\Phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0 A_u}\boldsymbol{\mu}_\pm\nabla_\mathbf{r}\int dR_i\frac{e^{-iqz_i}e^{-im_q\varphi_i}}{|\mathbf{r}-\mathbf{R}_i|}, \tag{6}$$

where A_u is the surface area of the unit cell of the cylindrical surface. We consider that the unit cell of the lattice contains one atom leading to $A = NA_u$, where $A$is the surface area of the long cylinder. We now use the following multipole expression for the $1/|\mathbf{r}-R_i|$ term in cylindrical coordinates [24]

$$\frac{1}{|\mathbf{r}-R_i|} = \frac{1}{\pi}\sum_{m'=-\infty}^{\infty}\int\limits_{-\infty}^{\infty}dk'e^{im'(\varphi-\varphi_i)}\times$$
$$\times\, e^{ik'(z-z_i)}I_m(|k'|R)\,K_{m'}(|k'|dR)\,. \tag{7}$$

Where we have used $\mathbf{r} = d\cos\varphi\mathbf{i} + d\sin\varphi\mathbf{j} + z\mathbf{k}$ and $R_i = a\cos\varphi_i\mathbf{i} + a\sin\varphi_i\mathbf{j} + z\mathbf{k}$. Where $I_m(x)$ and $K_m(x)$ are Bessel functions of the first and second kinds, respectively. On substitution this back into (7) and evaluation the subsequent integrals, we get

$$\Phi(r) = \frac{R}{\varepsilon A}I_{|m_q|}(|q|R)\,\boldsymbol{\mu}_z\cdot\nabla_r[e^{-iqz}e^{-im\phi}]K_{|q|}(|q|R). \tag{8}$$

We now use $\boldsymbol{\mu}_z = \mu^+_\rho\hat{p} + \mu^+_\varphi\hat{\varphi} + \mu^+_z\hat{z}$ to obtain

$$\Phi(r) = \frac{eR}{\varepsilon A}I_{|m_q|}(|q|R)\,e^{-im_q\varphi}e^{-iqz}\times$$
$$\times\left[\begin{array}{l} -\dfrac{\mu^\pm_\rho|q|}{2}\left(K_{|m_q|-1}(|q|d) + K_{|m_q|+1}(|q|d)\right) - \\ -i\left(\dfrac{m_q\mu^\pm_\varphi}{d} + q\mu^\pm_z\right)K_{|m_q|}(|q|d) \end{array}\right]. \tag{9}$$

We now evaluate the interaction, using the matrix element for the interaction becomes $U = \boldsymbol{\mu}^{D\cdot}_{eg}\cdot\nabla\Phi$ and it is given by

$$U = \frac{R}{\varepsilon A}\Phi(r) = \frac{eR}{\varepsilon A}I_{|m_q|}(|q|R)\,e^{-im_q\varphi}e^{-iqz}\times$$
$$\times\left[\begin{array}{l} -\dfrac{\partial^2K_{|m_q|}(|q|R)}{\partial d^2}\mu^\pm_\rho\mu^D_\rho - \dfrac{\partial K_{|q|}(|q|R)}{\partial d}\times \\ \times\left\{\begin{array}{l} \dfrac{m_q}{d}\left(\mu^\pm_\varphi\mu^D_\rho + \mu^D_\varphi\mu^\pm_\rho\right) + q\left(\mu^D_z\mu^\pm_\rho + \mu^\pm_z\mu^D_\rho\right) - \\ -\dfrac{qm_q}{d}\left(\mu^\pm_z\mu^D_\varphi + \mu^\pm_\varphi\mu^D_z\right) \end{array}\right\} \end{array}\right]. \tag{10}$$

The rate of energy transfer from the dye molecule to the nanotube $\gamma(\hbar\Omega)$ can be calculated using Fermi's golden rule, which, in our specific case, can be written in the following form

$$\gamma(\hbar\Omega) = \frac{2\pi}{\hbar}\sum_{q}^{|U(\mathbf{q})|}{}^2F(\mathbf{q}), \tag{11}$$

where we have used $\mu^D_{eg} = \mu^D_\rho\hat{\rho} + \mu^D_\varphi\hat{\varphi} + \mu^D_z\hat{z}$. Where $F(\mathbf{q}) = \sum_{\mathbf{k}_i}\delta(E_{\mathbf{k}_i+\mathbf{q}} - E_{\mathbf{k}_i} - \hbar\Omega)$.

Thus, as follows from (11) the distance dependence of the energy transfer rate is thus determined by the functional forms of the interaction energy, $U(q)$ and $F(q)$. We will use the general formalism given above and developed in [15, 16, 25, 26] to understand the process of energy transfer from a localized donor in the case of a semiconducting graphene sheet folded to form a nanotube. Note that the law of carrier energy dispersion in a graphene nanotube has the following form

$$E^{\pm}_{\mathbf{k},m} = \pm\left(\frac{\varepsilon_g}{2} + \frac{\hbar^2 k^2}{2m^*} + \frac{\hbar^2 m^2}{2m^* R^2}\right), \tag{12}$$

where m^* is effective mass of the electron in a graphene nanotube.

Now, we evaluate the $F(\mathbf{q})$. In our specific case, this value will have the following form:

$$F(\mathbf{q}) = \frac{Lm}{\pi\hbar^2}\sum_{m_i}\int\limits_{-\infty}^{\infty} dk_i \delta\Bigg[(k_i+q)^2 + k_i^2 + \\ + \frac{(m_i+m_g)^2}{R^2} - \frac{2m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2}\Bigg]. \tag{13}$$

by evaluating the integral for k_i, we obtain

$$F(\mathbf{q}) = \frac{Lm}{\pi\hbar^2}\times \\ \times \sum_{\{m_i\}} \frac{1}{\left|\sqrt{\frac{4m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2} - \frac{2}{R^2}\left\{(m_i+m_g)^2+m_i^2\right\} - q^2}\right|}. \tag{14}$$

For small values of momentum transfer, we can neglected the q^2 term in comparison this

$$\frac{4m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2} - \frac{2}{R^2}\left\{(m_i+m_g)^2+m_i^2\right\}. \tag{15}$$

Now, substituting expression (15) into the expression for the energy transfer rate (11), we get:

$$\gamma(\hbar\Omega) = \frac{L^2 m^*}{\pi\hbar^2}\times \\ \times \sum_{\{m_s\},m_q} \frac{1}{\left|\sqrt{\frac{4m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2} - \frac{2}{R^2}\left\{(m_i+m_g)^2+m_i^2\right\}}\right|}\times \\ \times \int\limits_{-\infty}^{\infty} |U(q)|^2 d\bar{q}, \tag{16}$$

Where $U(\mathbf{q})$ is given by (10). To evaluate the integral over q, we change the variable of integration to $t = qd$ and subsequently use the asymptotic form of $I_{|m_q|}\left(\frac{|t|R}{d}\right)$ given by

$$I_{|m_q|}\left(\frac{|t|\,R}{d}\right) \simeq \left(\frac{|tR|}{2d}\right)^{|m_q|}\frac{1}{\Gamma(|m_q|+1)}. \tag{17}$$

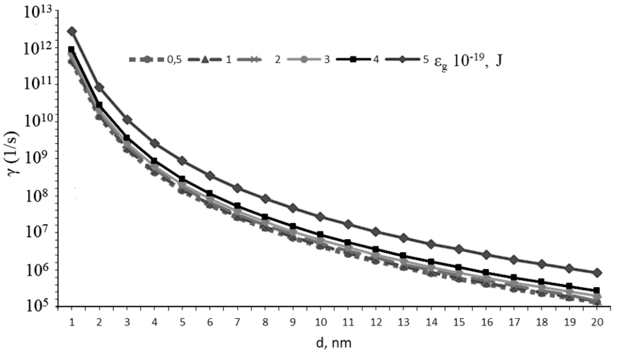

Fig. 3. Dependence of the rate of energy transfer from the dye to the semiconductor nanotube on the distance between them d

The integral over t can now be easily for various of $m_q = 0$. We evaluate the integral over all possible orientation of the donor transition dipole moment to get the following expression for the rate:

$$\gamma(\hbar\Omega) = \frac{3m^*\left(33\mu_z^{\pm^2} + 71\mu_\rho^{\pm^2}\right)}{8192\pi\hbar^3\varepsilon_0^2 d^5}\times \\ \times \sum_{|m_1|} \frac{\mu_{eg}^2}{\left|\sqrt{\frac{m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2} - \frac{m_i^2}{R^2}}\right|}, \tag{18}$$

where we have $\left|\mu_{eg}^D\right| = \mu_{eg}$. Therefore, the leading order term in the expression or the rate as d^{-5}.

For numerical calculations, we choose the following parameter values: the effective mass of the electron in a nanotube is $m^* = 0.25m_e$, Fermi velocity is $v_f = 0.9\times10^6$ m/c.

If we choose the simplest case where $m_i = 0$ then (18) can be written as

$$\gamma(\hbar\Omega) = \frac{3m^*}{8192\pi\hbar^3\varepsilon_0^2}\frac{\left(33\mu_z^{\pm^2} + 71\mu_\rho^{\pm^2}\right)}{d^5}\times \\ \times\frac{\mu_{eg}^2}{\sqrt{\left|\frac{m^*(\hbar\Omega-\varepsilon_g)}{\hbar^2}\right|}} = \frac{3\mu_{eg}^2\sqrt{m*}\left(33\mu_z^{\pm^2} + 71\mu_\rho^{\pm^2}\right)}{8192\pi\hbar^2\varepsilon_0^2\sqrt{(\hbar\Omega-\varepsilon_g)}d^5}. \tag{19}$$

The graphical dependence of the energy transfer rate from the dye $\gamma(\hbar\Omega)$ to the carbon semiconductor nanotube depending on the distance between them d is shown in Fig. 3. Analysis of the obtained results shows, in particular, that the energy gap ε_g within the limits $\varepsilon_g \sim (0.5\text{–}5)\times10^{-19}$J does not significantly affect the energy transfer rate $\gamma(\hbar\Omega)$, the value of which is determined by the induced dipole moment μ_{eg}, the amount of energy transferred $\hbar\Omega$ in the FRET and the effective mass of the electron in the nanotube m^*.

It also follows from Fig. 3 that the most efficient energy transfer occurs at distances of the order of a few nanometers and actually stops at $d \geq 20$ nanometers. This result, at least qualitatively, coincide with the results of paper [20], in which the spatial dependence of rates of energy transfer from a dye molecule to nanowires was calculated using a method different from our one.

3. Conclusions

We have investigated the dependence of the resonance energy transfer process from a localized donor, a dye molecule, to a semiconductor nanotube on the distance d between them. We have found that ,in the dye molecule-semiconductor carbon nanotube system, the energy transfer rate depends on the distance as d^{-5}. Analysis of the numerical simulation results shows, in particular, that the energy gap ε_g within the limits $\varepsilon_g \sim (0.5–5) \times 10^{-19}$J does not significantly affect the energy transfer rate $\gamma(\hbar\Omega)$, the value of which is determined by the induced dipole moment μ_{eg} of the dye molecule, the amount of energy transferred $\hbar\Omega$ in the FRET and the effective mass of the electron in the semiconductor nanotube m^*. We hope for that the simple analytic models of energy transfer, presented here, can lead to an interesting physical understanding of the resonance energy transfer process in various kinds of low-dimensional physical and biological nanostructures.

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РЕЗОНАНСНИЙ ПЕРЕНОС ЕНЕРГІЇ ВІД МОЛЕКУЛИ БАРВНИКА ДО ВУГЛЕЦЕВОЇ НАНОТРУБКИ

У цій роботі досліджено особливості процесу передачі енергії резонансу Ферстера від збуджених молекул барвника до напівпровідникових одностінних вуглецевих нанотрубок, зокрема, залежність швидкості передачі енергії від відстані між молекулою барвника та самою вуглецевою нанотрубкою. Аналіз отриманих результатів показує, зокрема, що ширина забороненої зони ε_g у межах $\varepsilon_g \sim (0{,}5\text{–}5)\cdot 10^{-19}$ Дж суттєво не впливає на швидкість передачі енергії $\gamma\,(\hbar\Omega)$, значення якої визначається індукованим дипольним моментом μ_{eg}, кількістю енергії, що передається в процесі резонансного переносу $\hbar\Omega$, та ефективною масою електрона в напівпровідниковій вуглецевій нанотрубці m^*. Запропонований підхід проливає нове світло на розуміння фізичного процесу резонансного переносу енергії в різних типах низьковимірних фізичних та біологічних наноструктурах.

Ключові слова: графен, молекула барвника, теорія функціонала густини, механізм Ферстера, швидкість передачі енергії, гібридна наноструктура на основі вуглецю.