

Supplemental Material to the article

“Spatially localized photoeffect in ambipolar organic field-effect phototransistors”

Phototransistor model. The bound electron-hole pair dissociation rate k_{diss} is determined by the following formula, which was used in the model of organic solar cells with a bulk heterojunction [12]:

$$k_{\text{diss}}(a, E) = \frac{3\alpha}{4\pi a^3} \exp\left\{-\frac{e^2}{\varepsilon\varepsilon_0 akT}\right\} \cdot \frac{J_1(2\sqrt{-2b})}{\sqrt{-2b}}, \quad b = \frac{e^3|E|}{8\pi\varepsilon\varepsilon_0 k^2 T^2}, \quad (\text{S1})$$

where a – separation distance of bound e/h-pair, α – Langevin bimolecular recombination constant (see below), e – electron charge, ε – active layer dielectric constant, ε_0 – electric constant, k – Boltzmann constant, T – temperature, J_1 – first order Bessel function. The probability of bound e/h-pair dissociation is determined by formula:

$$p(a, E) = \frac{k_{\text{diss}}(a, E)}{k_{\text{diss}}(a, E) + k_f}. \quad (\text{S2})$$

Because organic semiconductors tend to disorder, in model it is proposed that separation distances of bound e/h-pairs are not constant throughout the system, therefore expression for bound e/h-pair dissociation probability has form:

$$P(E) = \int_0^\infty p(a, E) f(a, a_0) da, \quad (\text{S3})$$

where $f(a, a_0)$ – is distribution function:

$$f(a, a_0) = \frac{4}{\sqrt{\pi}a_0^3} a^2 \exp\left(-\frac{a^2}{a_0^2}\right). \quad (\text{S4})$$

The main equations of model are Poisson equation for electric potential φ :

$$\frac{d^2\varphi}{dx^2} = \frac{e}{\varepsilon\varepsilon_0} [p(x) - n(x)] + \frac{C_s}{\varepsilon\varepsilon_0 d} [\varphi(x) - V_G], \quad (\text{S5})$$

continuity equations for electron and hole current densities j_n and j_p :

$$\frac{dj_p}{dx} = eP(E)G(x) - e(1 - P(E))R(x), \quad (\text{S6})$$

$$-\frac{dj_n}{dx} = eP(E)G(x) - e(1 - P(E))R(x), \quad (\text{S7})$$

relations describing drift and diffusion of electrons and holes:

$$j_p(x) = e\mu_p p(x) \frac{d\varphi}{dx} - \mu_p kT \frac{dp}{dx}, \quad (\text{S8})$$

$$j_n(x) = e\mu_n n(x) \frac{d\varphi}{dx} + \mu_n kT \frac{dn}{dx}, \quad (\text{S9})$$

where $p(x)$ and $n(x)$ are free holes and electrons concentrations, C_s is gate-dielectric-active layer electric capacitance per area, d is thickness of current conducting layer, V_G is gate voltage, μ_p is hole mobility, μ_n is electron mobility, $G(x)$ is bound e/h-pairs generation rate under incident radiation, $R(x)$ is charge carrier recombination rate. In this work the bimolecular Langevin recombination is considered:

$$R(n) = \alpha [n(x)p(x) - n_0 p_0]. \quad (\text{S10})$$

Charge carrier recombination constant is determined by Langevin formula:

$$\alpha = \frac{e(\mu_n + \mu_p)}{\varepsilon\varepsilon_0}. \quad (\text{S11})$$

System of equations (S5)–(S9) is complemented by boundary conditions at contacts with source and drain electrodes at $x = 0$ and $x = L$ for unknown functions $\varphi(x)$, $p(x)$ and $n(x)$. Solving this system at different values of source-drain voltage V_D , which is contained in boundary conditions for electric potential, and source-gate voltage V_G , it is possible to obtain output and transfer characteristics. For numerical solution of this problem the program on language *C* was written. Numerical values of input parameters are given in Table 1 and correspond to typical values for transistors based on organic semiconductors.

1. Input parameters of model

| Parameter | Symbol | Value | Units |
|--------------------------------------|---------------|----------------------|---|
| Channel length | L | 1 | μm |
| Permittivity | ε | 2 | |
| Temperature | T | 290 | K |
| Electron mobility | μ_n | 10^{-3} | $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ |
| Hole mobility | μ_p | 10^{-3} | $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ |
| Channel thickness | d | 3 | nm |
| Transistor capacitance per area | C_S | 1.8×10^{-3} | F/m^2 |
| Left electrode work function | A_1 | 5.05 | eV |
| Right electrode work function | A_2 | 4.05 | eV |
| Electron affinity | χ | 4.0 | eV |
| Band gap | E_g | 1.1 | eV |
| Separation distance of e/h pair | a_0 | 1.3 | nm |
| e/h-pair fission rate | k_f | 10^4 | s^{-1} |
| e/h-pair generation rate | G_0 | 10^{30} | $\text{m}^{-3} \text{s}^{-1}$ |
| Density of states in conduction band | N_c | 10^{26} | m^{-3} |
| Density of states in valence band | N_v | 10^{26} | m^{-3} |

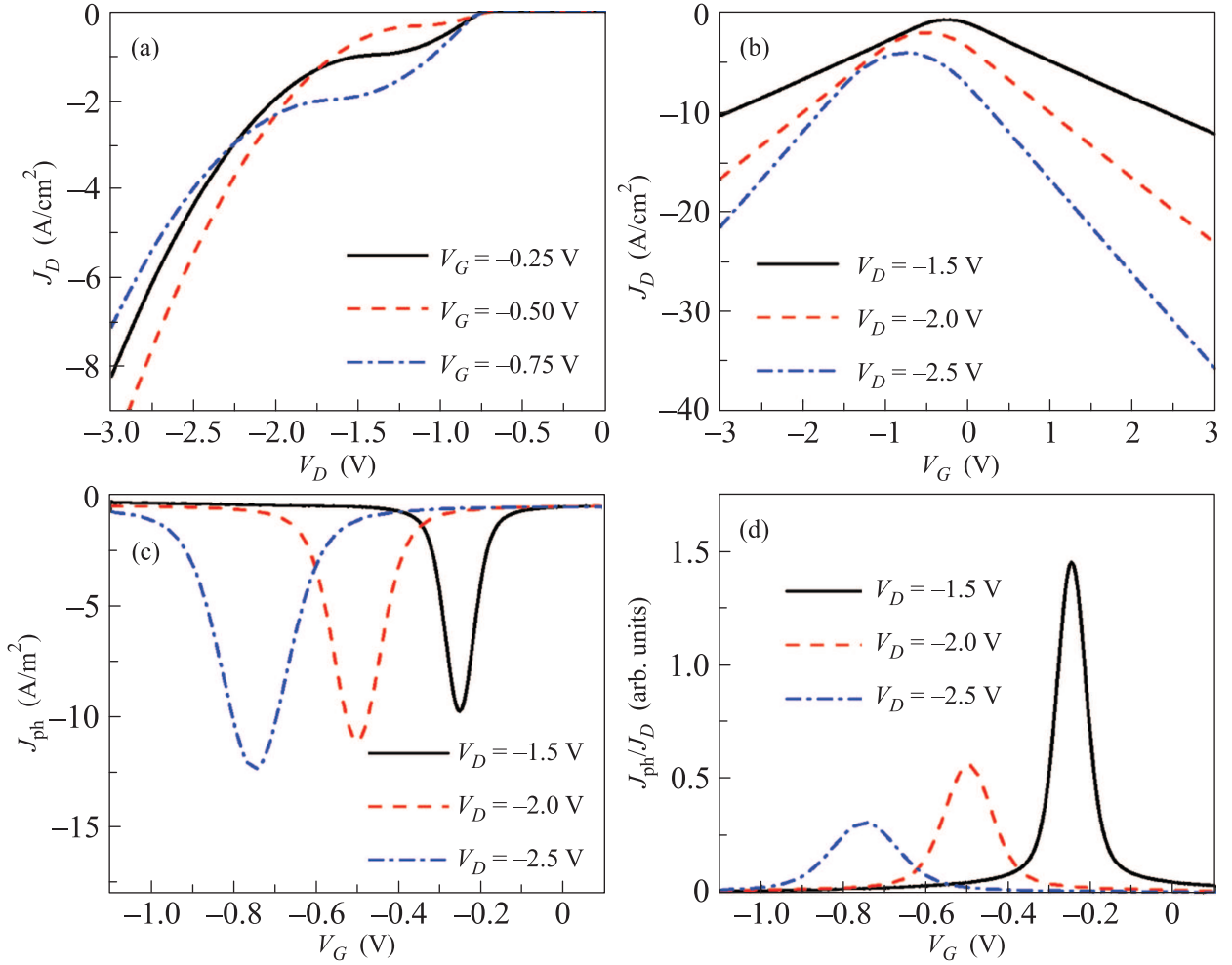


Fig. S1. Output (a) and transfer (b) characteristics of organic field-effect phototransistor. Photocurrent density (difference between current densities under illumination and in dark) (c), and photocurrent to dark current ratio (d) depending on V_G for three different V_D values

Current-voltage characteristics in dark and under illumination. Figure S1 presents output and transfer characteristics, and also photocurrent and photocurrent/dark current ratio dependences on gate voltage V_G under illumination with Gauss-distributed intensity along x axis according to Eq. (4) with full width at half-maximum $w_G = 200$ nm and peak position $x_0 = 500$ nm, i.e. in the middle of channel. Output characteristics are calculated for three different values of V_D , and transfer characteristics are calculated for three different values of V_D .