

# Supporting Information for “Charge transport in mixed organic disorder semiconductors: trapping, scattering, and effective energetic disorder”

## Derivation of equation 6:

Assume that two materials are in the mixed organic semiconductors: material A with a content of  $x$  (mol), a energy level of  $\varepsilon_A$ , a disorder (standard deviation) of  $\sigma_A$  and a density function of  $p(A)$ ; material B with a content of  $1-x$  (mol), a energy level of  $\varepsilon_B$ , a disorder (standard deviation) of  $\sigma_B$  and a density function of  $p(B)$ .

Then the equations below are obtained:

$$\int p(A) d\epsilon = 1, \int p(B) d\epsilon = 1$$

$$\int \epsilon \cdot p(A) d\epsilon = \varepsilon_A, \int \epsilon \cdot p(B) d\epsilon = \varepsilon_B$$

$$\int \epsilon^2 \cdot p(A) d\epsilon = \varepsilon_A^2 + \sigma_A^2, \int \epsilon^2 \cdot p(B) d\epsilon = \varepsilon_B^2 + \sigma_B^2$$

And the density function of the mixed system,  $p_m$ , and the average energy level of the mixed system,  $\varepsilon_m$ , will be

$$p_m = x \cdot p(A) + (1 - x) \cdot p(B) \text{ and } \varepsilon_m = x \cdot \varepsilon_A + (1 - x) \cdot \varepsilon_B.$$

The deviation of the mixed system,  $\sigma_m^2$ , will be

$$\sigma_m^2 = \int (\epsilon - \varepsilon_m)^2 \cdot p_m d\epsilon$$

$$= \int [\epsilon - (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)]^2 \cdot (x \cdot p(A) + (1-x) \cdot p(B)) d\epsilon = I_A + I_B$$

where  $I_A = \int [\epsilon - (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)]^2 \cdot x \cdot p(A) d\epsilon$  and

$$I_B = \int [\epsilon - (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)]^2 \cdot (1-x) \cdot p(B) d\epsilon.$$

$$I_A = \int [\epsilon - (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)]^2 \cdot x \cdot p(A) d\epsilon$$

$$= \int \epsilon^2 \cdot x \cdot p(A) d\epsilon + \int 2\epsilon \cdot (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B) \cdot x \cdot p(A) d\epsilon \\ + \int (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)^2 \cdot x \cdot p(A) d\epsilon$$

$$= x \cdot (\epsilon_A^2 + \sigma_A^2) + 2x \cdot (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B) \cdot \epsilon_A + x \cdot (x \cdot \epsilon_A + (1-x) \cdot \epsilon_B)^2$$

$$= x \cdot \sigma_A^2 + x \cdot (1-x)^2 \cdot (\epsilon_A - \epsilon_B)^2.$$

$$\text{Similarly, } I_B = (1-x) \cdot \sigma_B^2 + (1-x) \cdot x^2 \cdot (\epsilon_A - \epsilon_B)^2.$$

$$\text{So we get } \sigma_m^2 = I_A + I_B = x \cdot \sigma_A^2 + x \cdot (1-x) \cdot (\epsilon_A - \epsilon_B)^2 + (1-x) \cdot \sigma_B^2.$$

This equation is valid for any type of DOS.

**Generalization of our conclusion to the TPD hosted system and NPB hosted systems<sup>12,13</sup> reported by So *et al.***

**Table S1.** The critical  $\Delta E$  and the effects of traps and scatters on hole transport characters in TPD hosted system and NPB hosted system.

Host	$\mu_h$ (cm <sup>2</sup> /Vs)	$\Delta E_{\text{critical}}$ (eV)	$\sigma_{\text{exp}}$ (meV)	$\lambda$		$\Delta E$	$\mu_h$ (cm <sup>2</sup> /Vs)	$\sigma_{\text{exp}}$ (meV) <sup>c)</sup>	$\lambda$
TPD <sup>12</sup>	7.87×10 <sup>-2 a)</sup>	0.20	76	2.1	TPD: Rubrene	-0.1 (shallow trap)	3.21×10 <sup>-2</sup>	80 (79)	2.4
					TPD:DCM1	-0.2 (shallow trap)	4.29×10 <sup>-3</sup>	103 (88)	6
NPB <sup>13</sup>	6.6×10 <sup>-3 b)</sup>	0.23	75	1.3	NPB:DCM1	-0.2 (shallow trap)	1.0×10 <sup>-3</sup>	100 (88)	Dispersive
					NPB:DCM2	-0.2 (shallow trap)	1.5×10 <sup>-3</sup>	98 (88)	Dispersive
					NPB:TBu-TBD	0.4 (high scatter)	4.7×10 <sup>-3</sup>	74 (75)	1.5
					NPB:BCP	1.0 (high scatter)	6.2×10 <sup>-3</sup>	77 (75)	2.0
					NPB:CuPc	-0.3 (deep trap)	6.0×10 <sup>-3</sup>	— (75)	2.5

<sup>a)</sup> Hole mobilities of the TPD system are the zero field mobilities.

<sup>b)</sup> Hole mobilities of the NPB system are under the field of 0.29 MV/cm.

<sup>c)</sup> Data in the brackets are the effective energetic disorders calculated via **equation 6**.

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