Supporting Information for:

Self-Organization of Amine Based Cathode Interfacial Materials in Inverted Polymer Solar Cells

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Calculation of Surface Energy: The surface energies of different films were calculated based on the results of the contact angle measurement and equation from the "three-liquid procedure" developed by van Oss et al. was used. Water and ethylene glycol were selected as the polar pair, whereas the hexadecane was used in terms of the apolar liquid. Surface energy parameters are shown in **Table S1**.[S1-S2]

$$\gamma_{LV1}(1 + \cos\theta_1) = 2(\sqrt{\gamma_S^{LW}\gamma_{LV1}^{LW}} + \sqrt{\gamma_S^{+}\gamma_{LV1}^{-}} + \sqrt{\gamma_S^{-}\gamma_{LV1}^{+}})$$

$$\gamma_{LV2}(1 + \cos\theta_2) = 2(\sqrt{\gamma_S^{LW}\gamma_{LV2}^{LW}} + \sqrt{\gamma_S^{+}\gamma_{LV2}^{-}} + \sqrt{\gamma_S^{-}\gamma_{LV2}^{+}})$$

$$\gamma_{LV3}(1 + \cos\theta_3) = 2(\sqrt{\gamma_S^{LW}\gamma_{LV3}^{LW}} + \sqrt{\gamma_S^{+}\gamma_{LV3}^{-}} + \sqrt{\gamma_S^{-}\gamma_{LV3}^{+}})$$

$$\gamma = \gamma^{LW} + \gamma^{AB}$$

$$\gamma_i^{AB} = 2\sqrt{\gamma_i^{+}\gamma_i^{-}}$$

γ is the surface energy, γ^{LW} refers to the Lifshitz-van der Waals interaction and γ^{AB} refers to the acid-base interaction. γ^{+} and γ^{-} stand for the Lewis acid and base parameters of surface energy.

Table S1. Surface Energy Parameters (in mN/m) of Testing Liquids.

	γ	γ^{LW}	γ^{AB}	$\gamma+$	$\gamma-$
Water	72.8	21.8	51	25.5	25.5
Ethylene Glycol	48	29	19	1.92	47.0
Hexadecane	27.5	27.5	0	0	0

The calculation of the surface energy of ITO will be given as an example and all the results of the surface energy were obtained by the same method.

Table S2. Contact angle measured on the ITO surface with different testing liquids.

	Contact angle		
	Water	Ethylene Glycol	Hexadecane
ITO	14°±1°	27°±2°	15°±1°

The surface energy parameters of testing liquids used in this calculation is given in **Table S1**.

In terms of water as testing liquid:

$$72.8 * (1 + \cos 14°) = 2(\sqrt{\gamma_{ITO}^{LW} * 21.8} + \sqrt{\gamma_{ITO}^{+} * 25.5} + \sqrt{\gamma_{ITO}^{-} * 25.5}) \qquad (1)$$

In terms of ethylene glycol as testing liquid:

$$48 * (1 + \cos 27°) = 2(\sqrt{\gamma_{ITO}^{LW} * 29} + \sqrt{\gamma_{ITO}^{+} * 47} + \sqrt{\gamma_{ITO}^{-} * 1.92}) \qquad (2)$$

In terms of hexadecane as testing liquid:

$$27.5 * (1 + \cos 15°) = 2(\sqrt{\gamma_{ITO}^{LW} * 27.5} + \sqrt{\gamma_{ITO}^{+} * 0} + \sqrt{\gamma_{ITO}^{-} * 0}) \qquad (3)$$

Combine equation (1), (2) and (3) to make a three element linear equation group.

$$\begin{cases} 72.8 * (1 + \cos 14°) = 2(\sqrt{\gamma_{ITO}^{LW} * 21.8} + \sqrt{\gamma_{ITO}^{+} * 25.5} + \sqrt{\gamma_{ITO}^{-} * 25.5}) \\[2mm] 48 * (1 + \cos 27°) = 2(\sqrt{\gamma_{ITO}^{LW} * 29} + \sqrt{\gamma_{ITO}^{+} * 47} + \sqrt{\gamma_{ITO}^{-} * 1.92}) \\[2mm] 27.5 * (1 + \cos 15°) = 2(\sqrt{\gamma_{ITO}^{LW} * 27.5} + \sqrt{\gamma_{ITO}^{+} * 0} + \sqrt{\gamma_{ITO}^{-} * 0}) \end{cases}$$

The solution of the equation group is calculated to be:

$$\begin{cases} \gamma_{ITO}^{LW} = 26.4 \\[2mm] \gamma_{ITO}^{+} = 0.62 \\[2mm] \gamma_{ITO}^{-} = 75 \end{cases}$$

Equation (4) gives the way to get the value of γ_{ITO}^{AB}.

$$\gamma_{ITO}^{AB} = 2\sqrt{\gamma_{ITO}^{+}\gamma_{ITO}^{-}} \qquad (4)$$

$$\gamma_{ITO}^{AB} = 14$$

According to equation (5), the surface energy of ITO would be the sum of γ_{ITO}^{LW} and γ_{ITO}^{AB}.

$$\gamma_{ITO} = \gamma_{ITO}^{LW} + \gamma_{ITO}^{AB} \tag{5}$$

$$\gamma_{ITO} = 40$$

Table S2. Calculated surface energy component of ITO.

	Calculated surface energy component (mN m^{-1})				
	γ	γ^{LW}	γ^{AB}	γ^+	γ^-
ITO	40.0	26.4	14	0.62	75.0

Reference:

S1. Wang, X. J.; Ederth T.; Inganäs, O. *In Situ* Wilhelmy Balance Surface Energy Determination of Poly(3-hexylthiophene) and Poly(3,4-ethylenedioxythiophene) During Electrochemical Doping-Dedoping. *Langmuir* **2006**, *22*, 9287-9294.

S2. Jasper, J. The Surface Tension of Pure Liquid Compounds. *J. Phys. Chem. Ref. Data* **1972**, *1*, 841-948.