

Supporting information for:

Fullerene-derivative as Interlayer for High Performance Organic Thin-film Transistors

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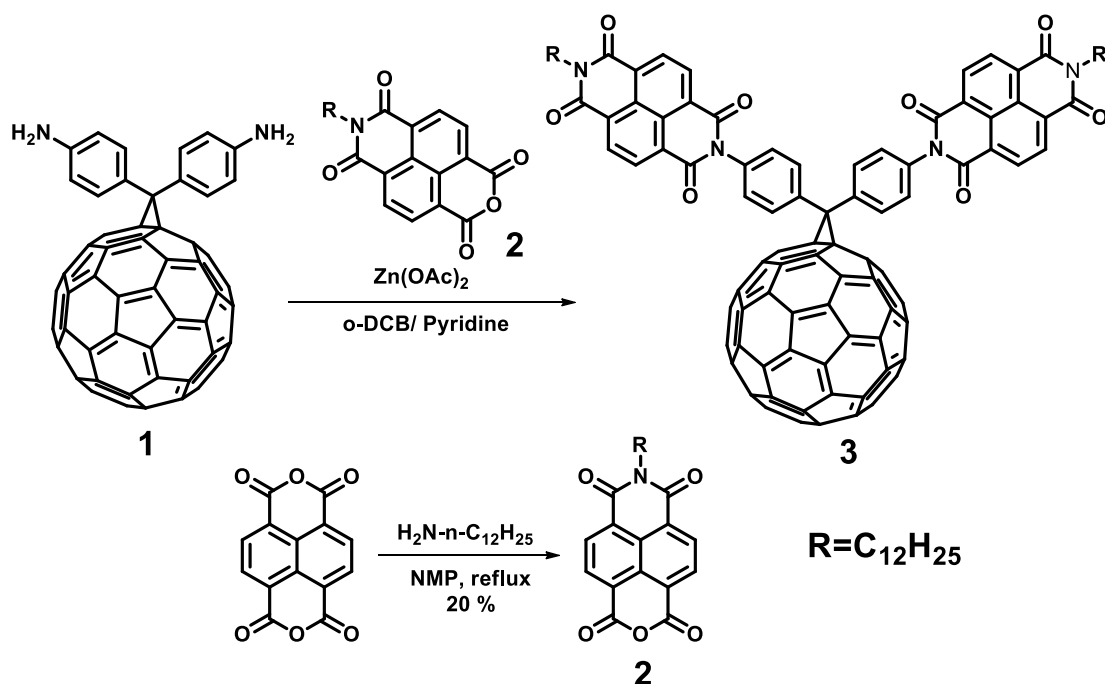
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Reference

Synthetic procedures



[6,6]-Bis-(4-aminophenyl)methanofullerene (**1**)

The synthesis route of compound **1** is similar to that described by Martín and coworkers¹.

N-Dodecyl-naphthalene-1,4,5,8-tetracarboxylic acid-1,4-anhydride-5,8-dicarboximide (**2**)

1,4,5,8-Naphthalenetetracarboxylic Bisanhydride, (5.00 g; 18.6 mmol) was added to NMP (50 mL) and the suspension was degassed (vacuum/argon) and heated to reflux under an atmosphere of argon. Dodecyl amine (3.46 g, 18.6 mmol) was added, and the brown solution was refluxed over night. After cooling to room temperature, the reaction mixture was filtered, the solids (crude bisimide) were washed with toluene and the combined filtrate was evaporated to dryness. The product was purified by column chromatography (SiO₂, CH₂Cl₂) to give compound **2** (1.63 g, 20%) as yellow crystal.

¹H-NMR (CDCl₃, 400 MHz) δ = 8.81 (4H), 4.18(t, J = 7.1 Hz, 2H), 1.72 (m, 2H), 1.40-1.25 (m, 18H), 0.85 (b, 3H)

¹³C-NMR (CDCl₃, 100 MHz) δ = 162.4, 159.0, 133.4, 131.4, 128.2, 123.0, 32.1, 30.2-29.5, 28.2, 27.3, 23.4, 22.9, 15.9, 14.3.

MS (MALDI-TOF): m/z = 435 (M₊)

Fullerene-bis(naphthalene) derivative (**3**)

The naphthalene monoimide monoanhydride, **2**, (71 mg, 0.16 mmol), compound **1** (50 mg, 0.055 mmol), and Zn(OAc)₂·2H₂O (24 mg, 0.11 mmol) was added to 1,2-dichlorobenzene (20 mL) and dry pyridine (5 mL). The mixture was stirred at reflux temperature for 18 h. The product was precipitated (MeOH), purified by column chromatography (6 % EtOAc, toluene), and precipitated again (MeOH) to yield a brown

powder (23 mg, 25 %).

$^1\text{H-NMR}$ (CDCl_3 , 500 MHz) δ = 8.83 (m, 8H), 8.38 (d, J = 8.4 Hz, 4H), 7.53 (d, J = 8.4 Hz, 4H), 4.22 (m, 4H), 1.77 (m, 4H), 1.50-1.19 (m, 36H), 0.88 (t, J = 7 Hz, 6H).

$^{13}\text{C-NMR}$ (CDCl_3 , 126 MHz) δ = 162.87, 162.74, 147.63, 145.22, 145.16, 144.77, 144.72, 144.33, 143.86, 142.99, 142.41, 142.17, 140.95, 139.16, 138.38, 134.40, 132.07, 131.46, 131.10, 129.15, 127.09, 127.06, 126.87, 126.64, 78.56, 56.77, 41.11, 31.93, 29.66, 29.64, 29.61(2 carbon), 29.55, 29.36, 28.11, 27.11, 22.70, 14.14.

MS (MALDI-TOF): m/z = 1753 (M^+)

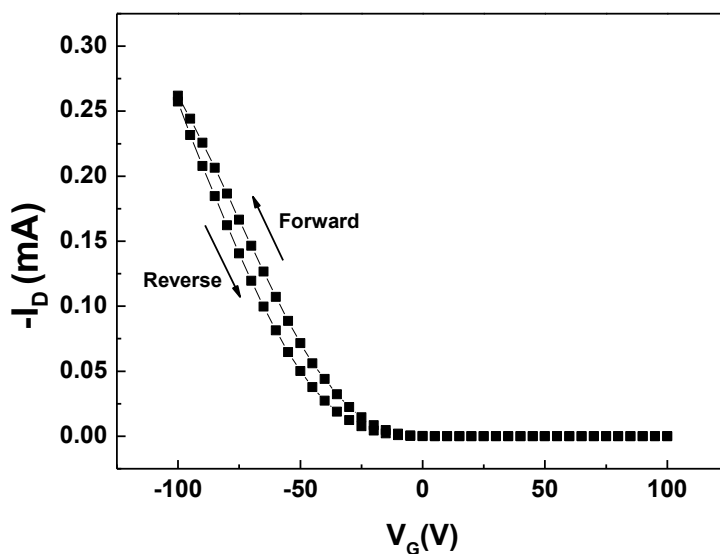


Figure S1 The cycle sweep characteristics of pentacene thin-film transistor with C_{60} -NDI interlayer ($V_{\text{DS}} = -100\text{V}$).

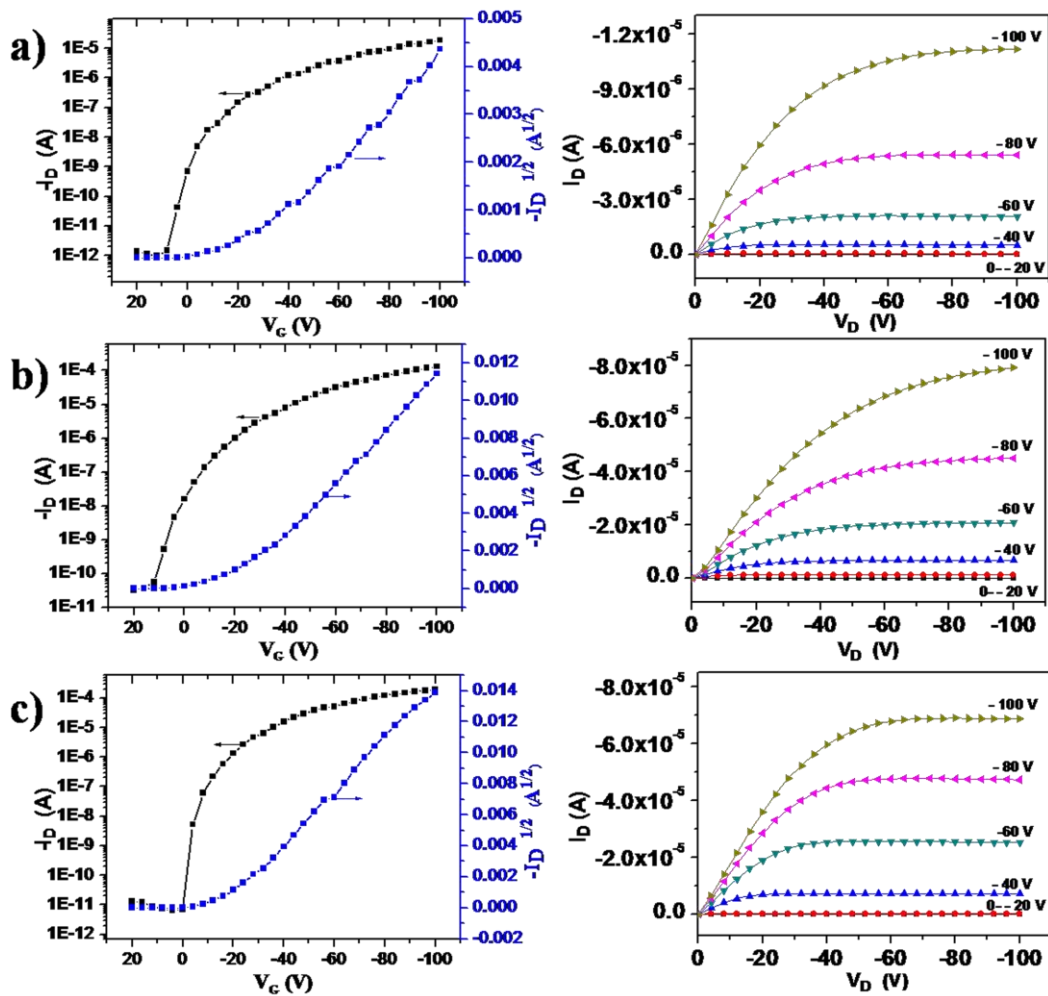


Figure S2 The typical transfer and output characteristics of pentacene thin-film devices based on (a) bare Si/SiO₂ (b) HMDS- and (c) OTS-treated substrates.

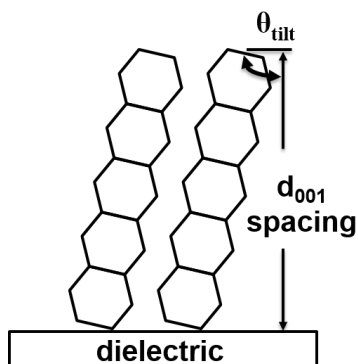
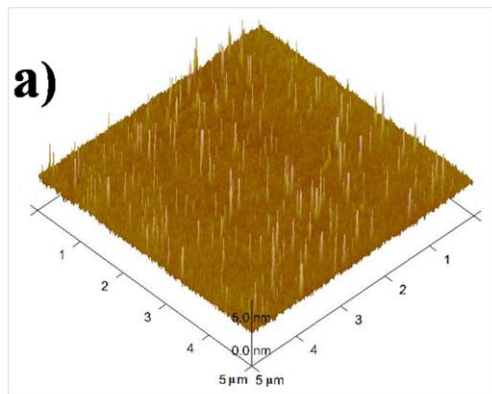
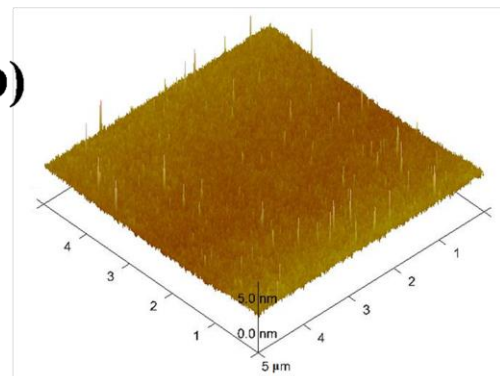


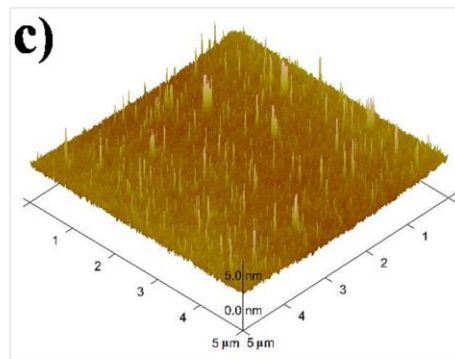
Figure S3 The diagram for the tilt θ evaluation



Surface RMS = 0.40 nm



Surface RMS = 0.38 nm



Surface RMS = 0.44 nm

Figure S4 AFM topographies for (a) bare Si/SiO₂ (b) HMDS- and (c) OTS-treated Si/SiO₂ substrate surfaces.

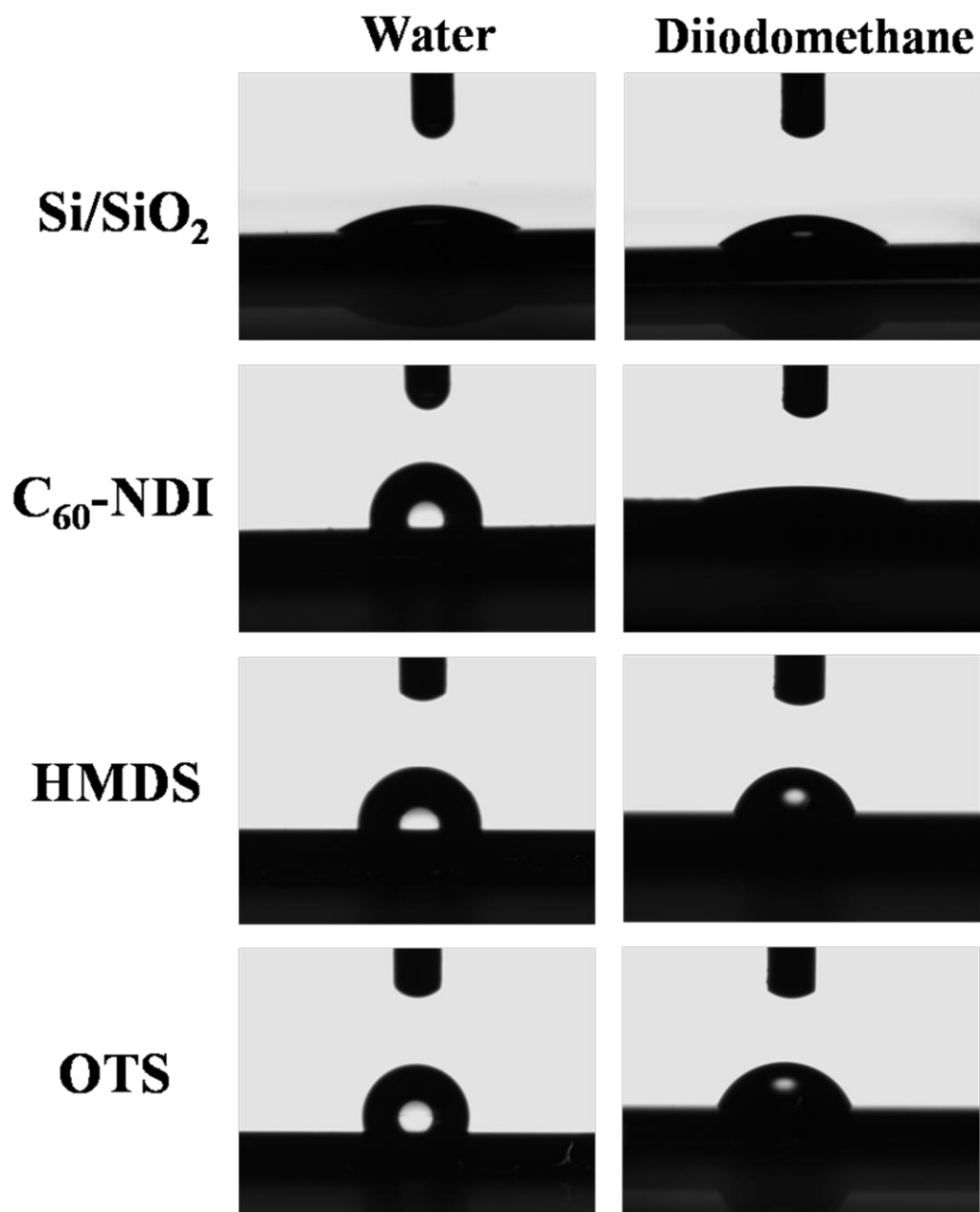


Figure S5. Contact angle of water and diiodomethane on the different substrates.

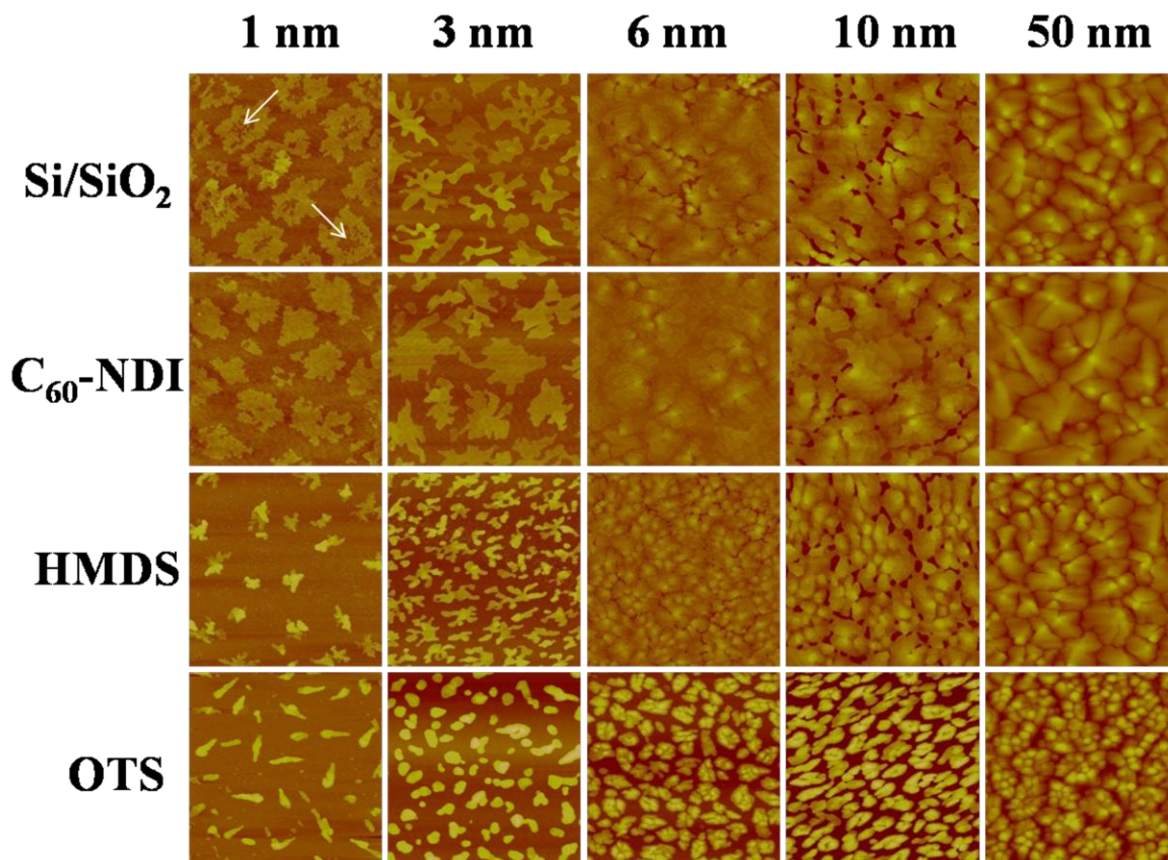


Figure S6 AFM images ($3 \mu\text{m} \times 3 \mu\text{m}$) for pentacene films of varying thickness deposited on different substrates.

Table S1 Summary of pentacene OFET performance on different substrates

Substrate	$\mu_{\text{FET}} [\text{cm}^2\text{V}^{-1}\text{s}^{-1}]$	$V_{\text{th}} [\text{V}]$	$I_{\text{on}}/I_{\text{off}}$
Si/SiO ₂	0.14 (± 0.02)	-28.4 (± 3.0)	5.3×10^7
C ₆₀ -NDI	1.65 (± 0.11)	-29.6 (± 5.1)	7.2×10^7
HMDS	0.66 (± 0.05)	-19.6 (± 2.2)	6.8×10^6
OTS	0.75 (± 0.06)	-16.1 (± 2.7)	1.9×10^7

Table S2 Summary of XRD spectrum and tilt angle

Substrate	$2\theta_{(001)}$ (degree)	d_{001} spacing (Å)	θ_{tilt} (degree)
Si/SiO ₂	5.58	15.84	12.1
C60-NDI	5.6	15.78	13.1
HMDS	5.76	15.34	18.7
OTS	5.74	15.40	18.1

Reference

1. Rafael Gómez, José L. Segura, and Nazario Martín. *Org. Lett.*, 2005, **7**, 717.