Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Highlighting the processing versatility of a silicon phthalocyanine derivative for organic thin-film transistors

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Table S1. Relevant transfer integrals (J_e) and intermolecular vectors expressed in Cartesian (r_x, r_y, r_z) and cell coordinates (a, b, c) for polymorph 1.

#	J_e (eV)	r_x (Å)	r_y (Å)	r_z (Å)	$\|r\|$ (Å)	*a*	*b*	*c*
1	1.6	-10.23	0	0	10.23	-1	0	0
2	1.6	+10.23	0	0	10.23	+1	0	0
3	7.6	+2.38	-8.21	-6.92	11.00	0	-1/2	-1/2
4	7.6	+2.38	8.21	-6.92	11.00	0	+1/2	-1/2
5	7.6	-2.38	-8.21	+6.92	11.00	0	+1/2	-1/2
6	7.6	+2.38	8.21	+6.92	11.00	0	+1/2	+1/2

Table S2. Relevant transfer integrals (J_e) and intermolecular vectors expressed in Cartesian (r_x, r_y, r_z) and cell coordinates (a, b, c) for polymorph 2.

#	J_e (eV)	r_x (Å)	r_y (Å)	r_z (Å)	$\|r\|$ (Å)	*a*	*b*	*c*
1	11.4	-11.27	0	0	11.27	-1	0	0
2	11.4	+11.27	0	0	11.27	+1	0	0
3	0.7	-4.39	+8.66	-6.13	11.48	-1/2	+1/2	-1/2
4	0.7	+4.39	+8.66	+6.13	11.48	+1/2	+1/2	+1/2
5	0.7	-4.39	-8.66	-6.13	11.48	-1/2	-1/2	-1/2
6	0.7	4.39	-8.66	+6.13	11.48	+1/2	-1/2	1/2
7	10.1	+6.88	+8.66	-6.31	12.65	1/2	+1/2	-1/2
8	10.1	-6.88	+8.66	+6.31	12.65	-1/2	+1/2	+1/2
9	10.1	+6.88	-8.66	-6.31	12.65	+1/2	-1/2	-1/2
10	10.1	-6.88	-8.66	+6.31	12.65	-1/2	-1/2	+1/2

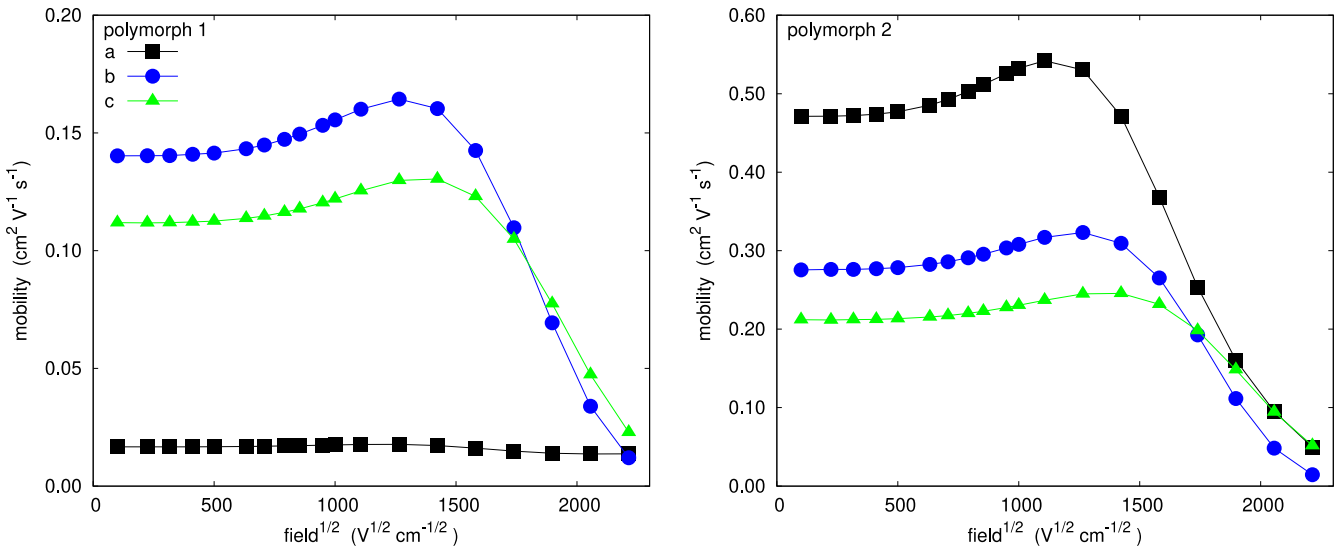

Figure S1. Electron mobility as a function of the magnitude of the electric field, set to be parallel to one of the crystallographic axes *a*, *b*, *c*, calculated in absence of external reorganization energy and of diagonal disorder (E = 1000 V cm^{-1}, λ = 0.21 eV, T = 300 K, σ = 0 eV).

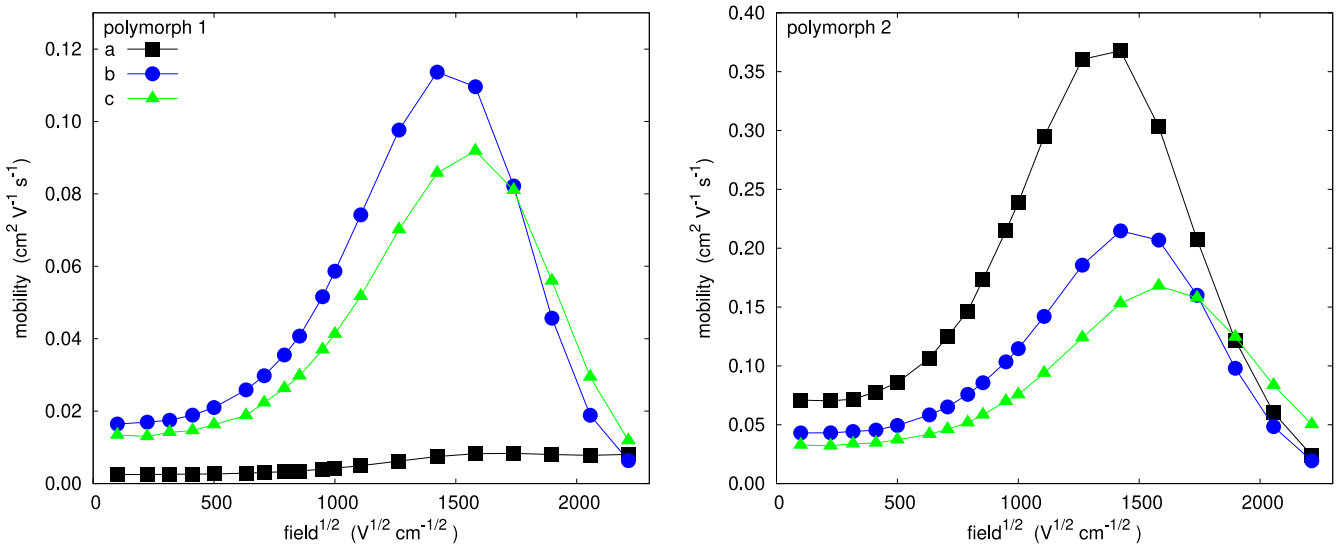

Figure S2. Electron mobility as a function of the magnitude of the electric field, set to be parallel to one of the crystallographic axes *a*, *b*, *c*, calculated without external reorganization energy and with diagonal disorder (E = 1000 V cm^{-1}, λ = 0.21 eV, T = 300 K, σ = 0.052 eV).

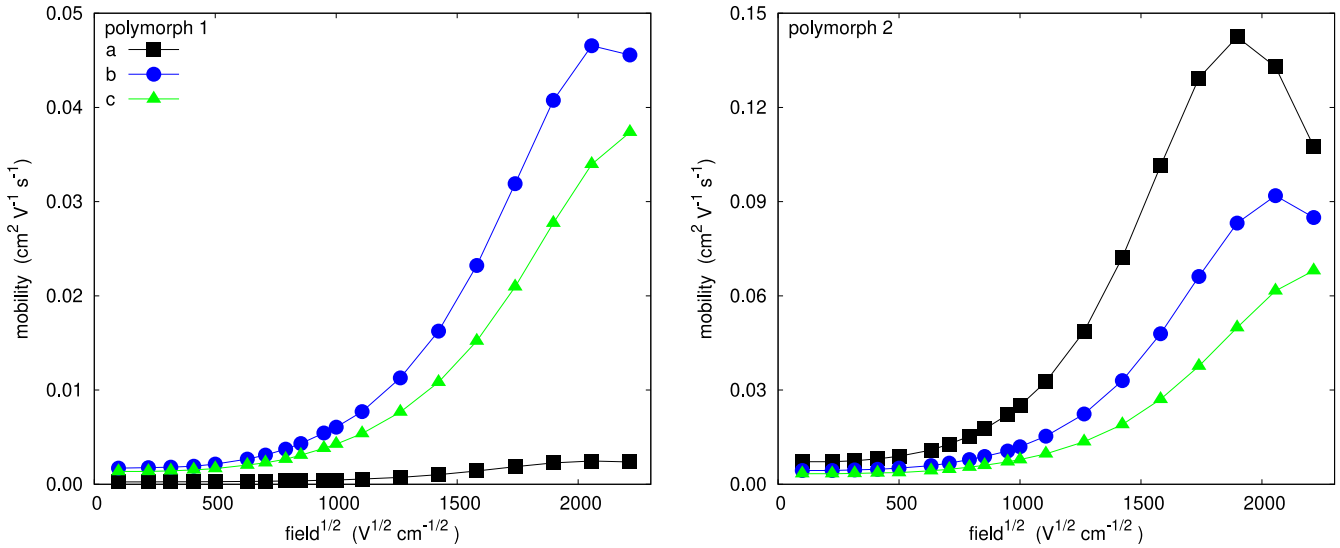

Figure S3. Electron mobility as a function of the magnitude of the electric field, set to be parallel to one of the crystallographic axes *a*, *b*, *c*, calculated assuming an external reorganization energy of 0.2 eV and diagonal disorder (E = 1000 V cm^{-1}, λ = 0.41 eV, T = 300 K, σ = 0.052 eV).

Table S3. Computed electron mobilities at zero field along the crystal axes and average mobility ($\mu_{e,\,avg}$ = (μ_a + μ_b + μ_c) / 3) of polymorph 1 and polymorph 2 determined by at zero field, using the expression:

$$\mu_i = \frac{q}{h}\left(\frac{\pi}{kT}\right)^{3/2}\frac{1}{\sqrt{\lambda_i}}exp\left(-\frac{\lambda_i}{4kT}\right)\sum_m J_m^2(\vec{r}_m\cdot\vec{e}_i)^2 \qquad (4)$$

Where the sum runs over all pairs of molecular neighbours separated by the distance vector $\vec{r}_m$, $\vec{e}_i$ is a unit vector representing the direction. Variables q, h and k are respectively the elementary charge, the Planck and Boltzmann constants, and T = 300 K. These mobilities are compared with Kinetic Monte Carlo mobilities extrapolated at zero field and without energetic disorder (**Figure S1**).

Polymorph	μ_a (x 10^{-2} cm^2 V^{-1} s^{-1})	μ_b (x 10^{-2} cm^2 V^{-1} s^{-1})	μ_c (x 10^{-2} cm^2 V^{-1} s^{-1})	$\mu_{e,\,avg}$ (x 10^{-2} cm^2 V^{-1} s^{-1})
1-Equation	1.7	14.2	11.6	8.9
2-Equation	50.8	14.3	33.9	33.0
1-KMC	1.7	14.0	11.1	8.9
2-KMC	47.1	27.6	21.2	32.0

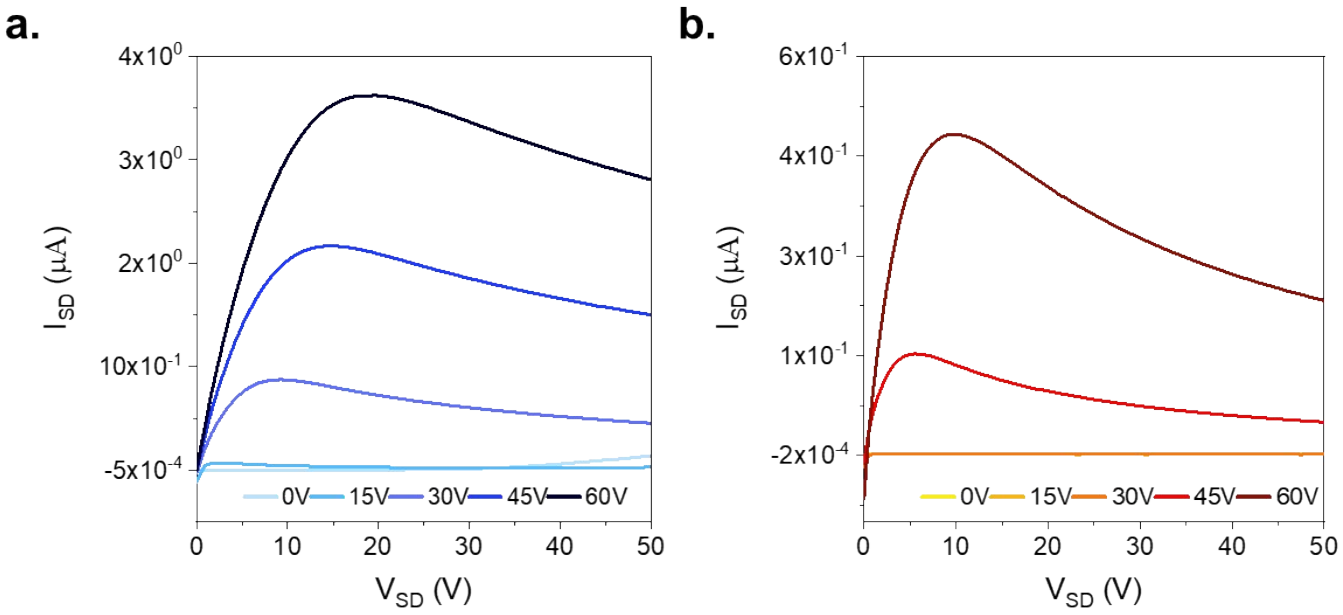

Figure S4. Characteristic output curves of (a) PVD and (b) solution fabricated $(3PS)_2$-SiPc OTFTs annealed at 25˚C for 1 hr and characterized at room temperature in a nitrogen environment.

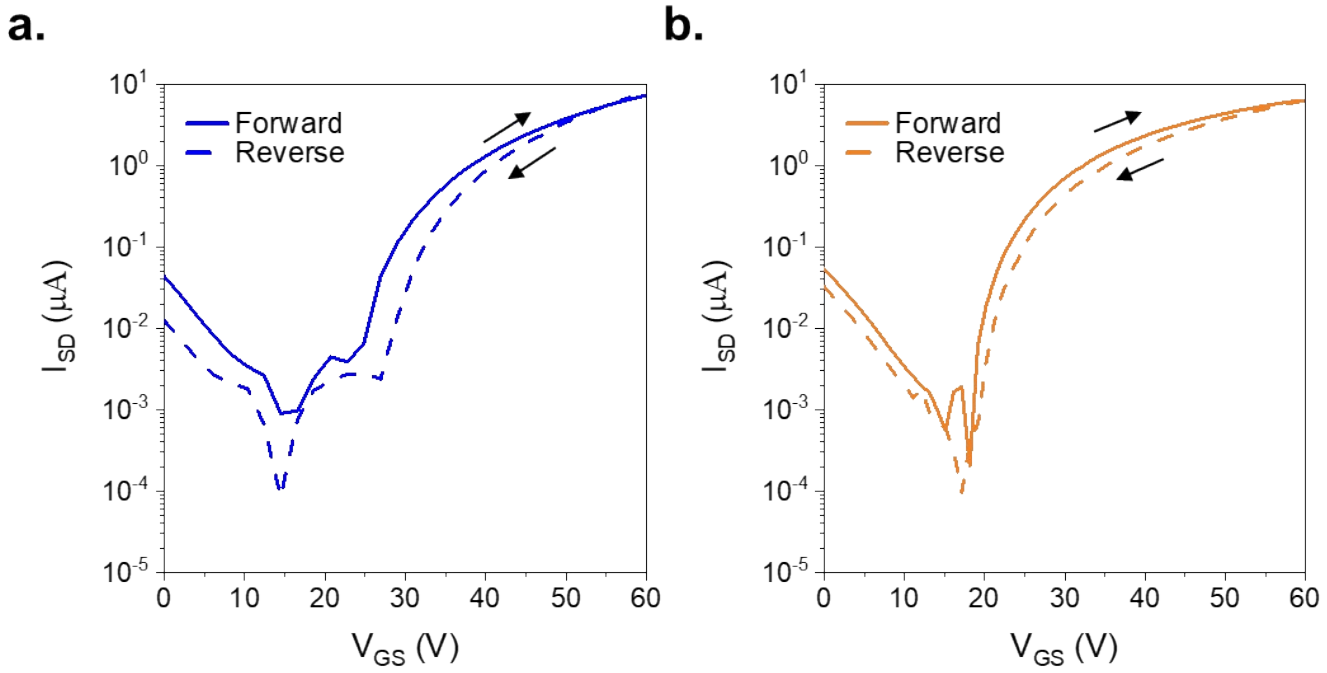

Figure S5. Characteristic forward and reverse transfer curves of (a) PVD and (b) solution fabricated $(3PS)_2$-SiPc OTFTs annealed at 25˚C for 1 hr and characterized at room temperature in a nitrogen environment.

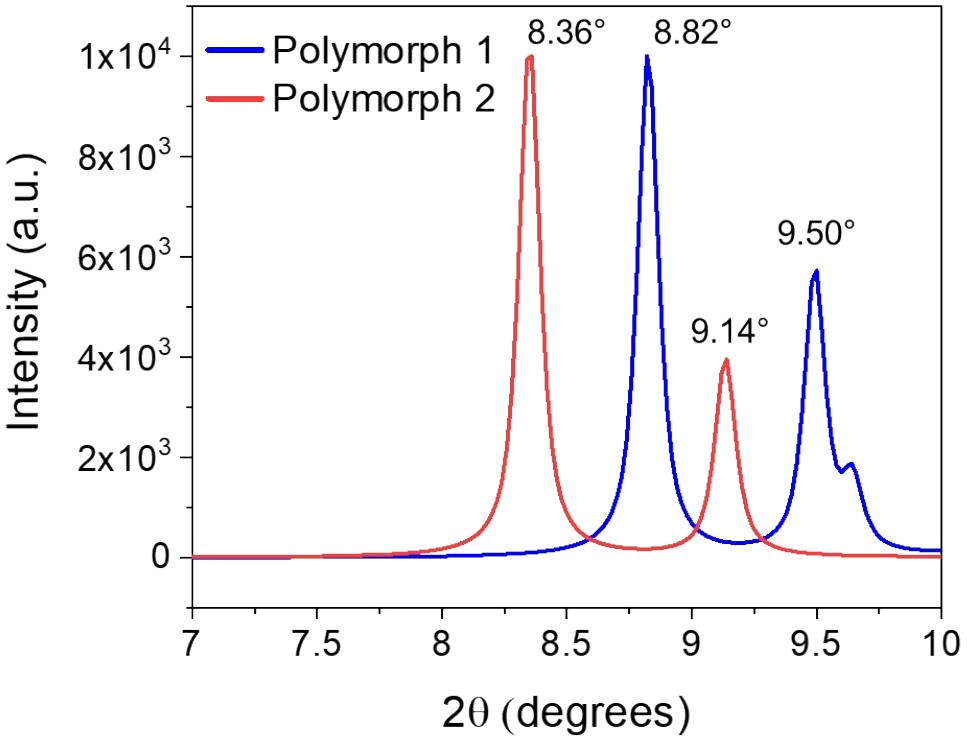

Figure S6. XRD pattern of polymorph 1 and polymorph 2 predicated from single crystal data using Mercury: visualization and analysis of crystal structures, from the Cambridge Crystallographic Data Centre.