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SUPPORTING INFORMATION

Additive Induced Crystallization of a Twisted Perylene Diimide Dimer Within a Polymer Matrix

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MATERIALS AND METHODS

Optical Absorption Spectroscopy (UV/vis/near-IR): All absorption measurements were recorded using an Agilent Technologies Cary 60 UV-vis spectrometer at room temperature.

Atomic force microscopy (AFM): AFM measurements were performed by using a TT2-AFM (AFM Workshop, USA) in the tapping mode and WSxM software with a 0.01-0.025 Ohm/cm Sb (n) doped Si probe with a reflective back side aluminum coating.

X-Ray Diffraction: X-ray diffraction experiments were performed on a PROTO AXRD Benchtop Powder Diffractometer using θ-2θ scans and Cu K-α radiation.

Solar Cells Fabrication: Solar cells were fabricated following the initial procedure for cleaning, ZnO deposition and organic layer deposition reported above. The fabricated films were then moved to an N2 atmosphere glovebox for 24 h before evaporating MoOx and Ag. The evaporations of 10 nm of MoOx followed by 100 nm of Ag were thermally deposited under high vacuum (10-5 torr).

Solar Cells Testing: Current density-voltage (J-V) characteristics were measured using a Keithley 2420 Source Measure Unit. Solar cell performance used an Air Mass 1.5 Global (AM 1.5G) Solar Simulator (Newport, Model 92251A-1000) with an irradiation intensity of 100 mWcm-2, which was measured by a calibrated silicon solar cell and a readout meter (Newport, Model 91150V).

ADDITIONAL RESULTS

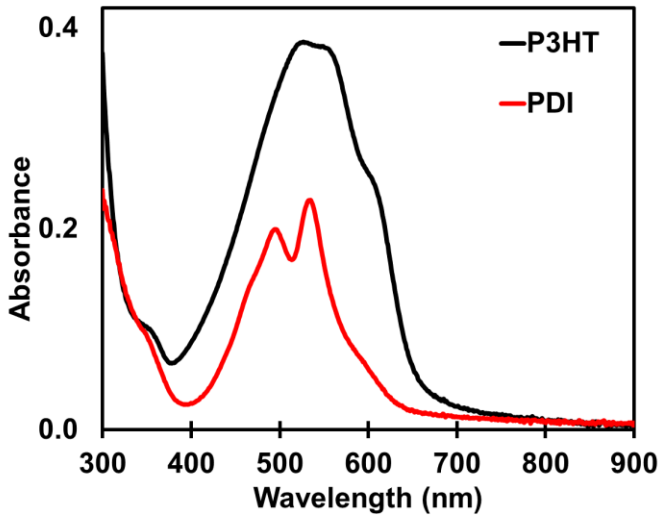

Figure S1. Raw data (not-normalized) UV-Vis spectra of P3HT and PDI films from toluene solution

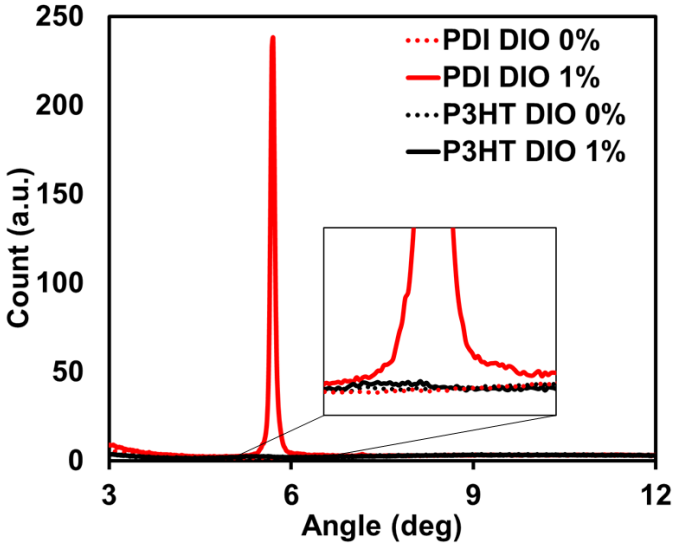

Figure S2. X-ray diffraction pattern of a neat film of P3HT (A) and PDI (B) processed from toluene with 0% or 1% (v/v) DIO.

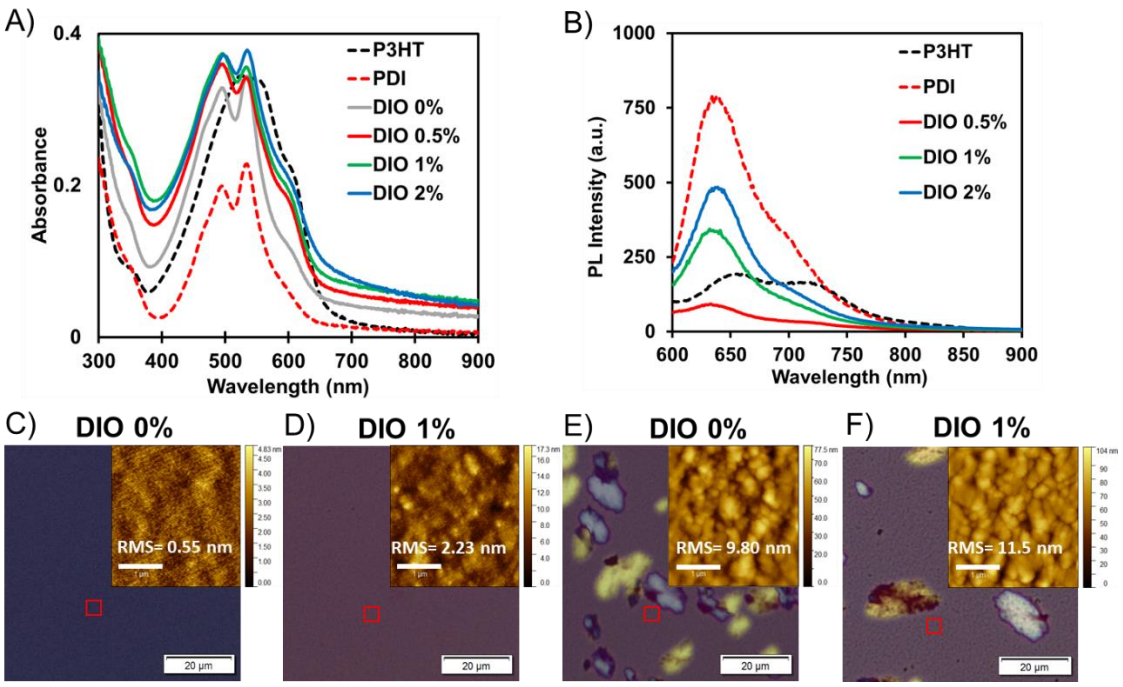

Figure S3. A) UV-vis spectra, B) PL spectra, and C-F) POM and AFM height images of 1:1 P3HT:PDI films processed from 0-2% (v/v) DIO and thermally annealed at 150°C for 10 min, 24 h after casting. Scale bars of the AFM images correspond to 1 µm.

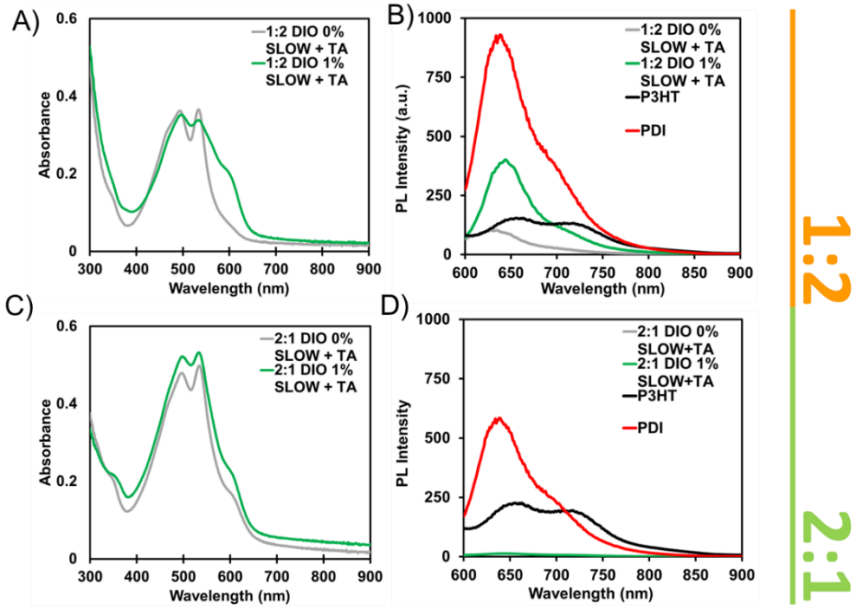

Figure S4. A-B) UV-vis spectra and C-D) PL spectra of 1:2 and 2:1 P3HT:PDI films processed from toluene with 0 or 1% (v/v) DIO processing additive and thermally annealed at 150 °C for 10 min, 24 h after casting (T-24h).

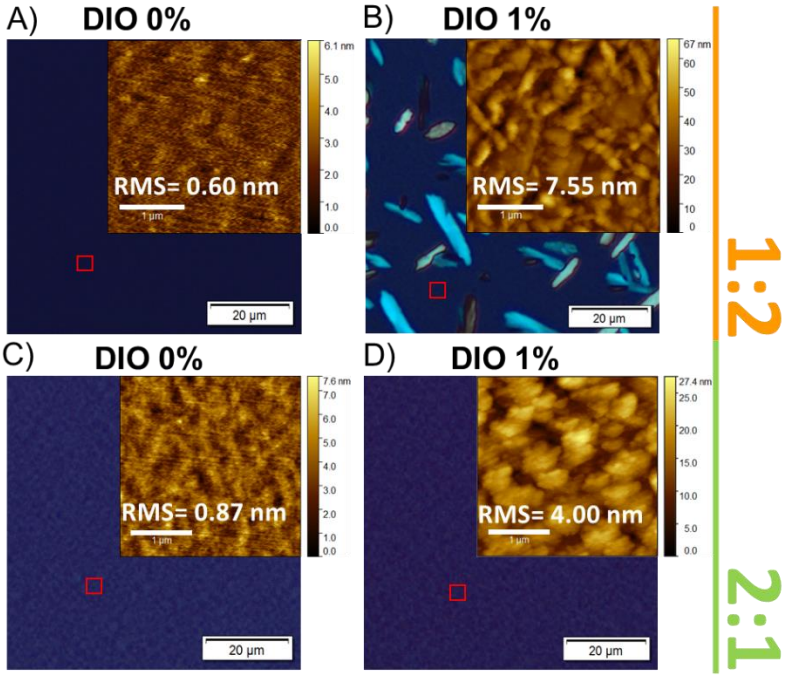

Figure S5. POM and AFM height images A-B) 1:2 and C-D) 2:1 P3HT:PDI films processed from toluene without or with 1% (v/v) DIO and thermally annealed at 150 °C for 10 min, 24 hours after casting. Scale bars in the AFM images correspond to 1 µm.

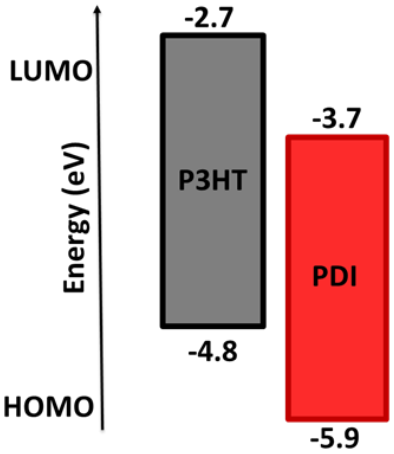

Figure S6. Energy levels diagram of P3HT and PDI. Values were calculated from cyclic voltammetry measurements as reported in previous publications.[1,2]

Table S1. Organic solar cell device parameters for P3HT:PDI BHJs.

D/A ratio	Drying	DIO (v/v)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
1:1	Slow	0%	0.71	1.17	27.3	0.22
1:1	Fast	0%	0.71	2.47	35.0	0.61
1:1	Slow + TA	0%	0.71	2.59	29.5	0.55
1:1	Slow	0.5 %	0.62	4.98	42.6	1.30
1:1	Fast	0.5 %	0.61	4.31	47.2	1.23
1:1	Slow + TA	0.5 %	0.65	3.76	38.6	0.95
1:1	Slow	1%	0.58	4.16	49.6	1.20
1:1	Fast	1%	0.53	3.02	45.0	0.72
1:1	Slow + TA	1%	0.66	3.99	49.9	1.31
1:1	Slow	2%	0.52	2.76	48.4	0.69
1:1	Fast	2%	0.62	3.22	43.0	0.86
1:1	Slow + TA	2%	0.54	2.64	44.8	0.63
1:2	Slow	0%	0.88	0.78	24.3	0.17
1:2	Fast	0%	0.58	0.81	26.9	0.13
1:2	Slow + TA	0%	0.78	0.84	25.1	0.16
1:2	Slow	1%	0.55	3.61	38.0	0.78
1:2	Fast	1%	0.64	2.01	40.6	0.55
1:2	Slow + TA	1%	0.66	3.30	47.0	1.03
2:1	Slow	0%	0.72	1.78	27.4	0.35
2:1	Fast	0%	0.71	3.28	32.8	0.77
2:1	Slow + TA	0%	0.73	4.37	35.8	1.15
2:1	Slow	1%	0.67	4.26	54.5	1.55
2:1	Fast	1%	0.68	4.58	48.2	1.50
2:1	Slow + TA	1%	0.79	4.55	54.3	1.95

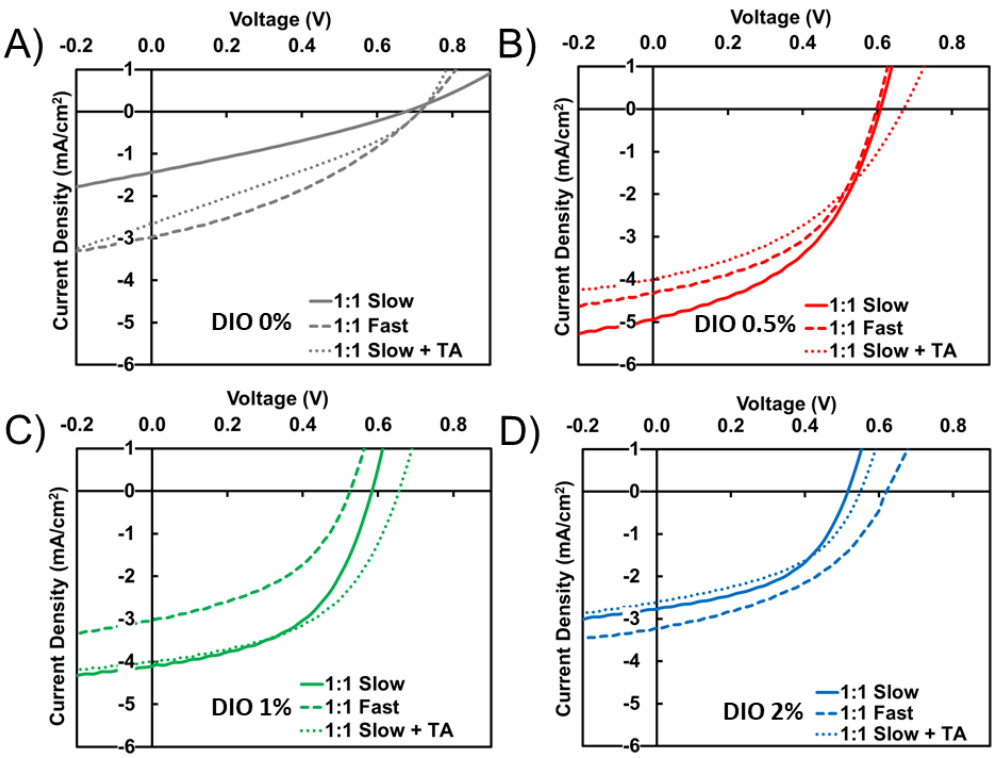

Figure S7. J-V curves of devices fabricated from 1:1 solutions of P3HT:PDI with various DIO loads (DIO % v/v), drying times and thermal treatments. Slow + TA refers to the thermally annealed films after 24 hours.

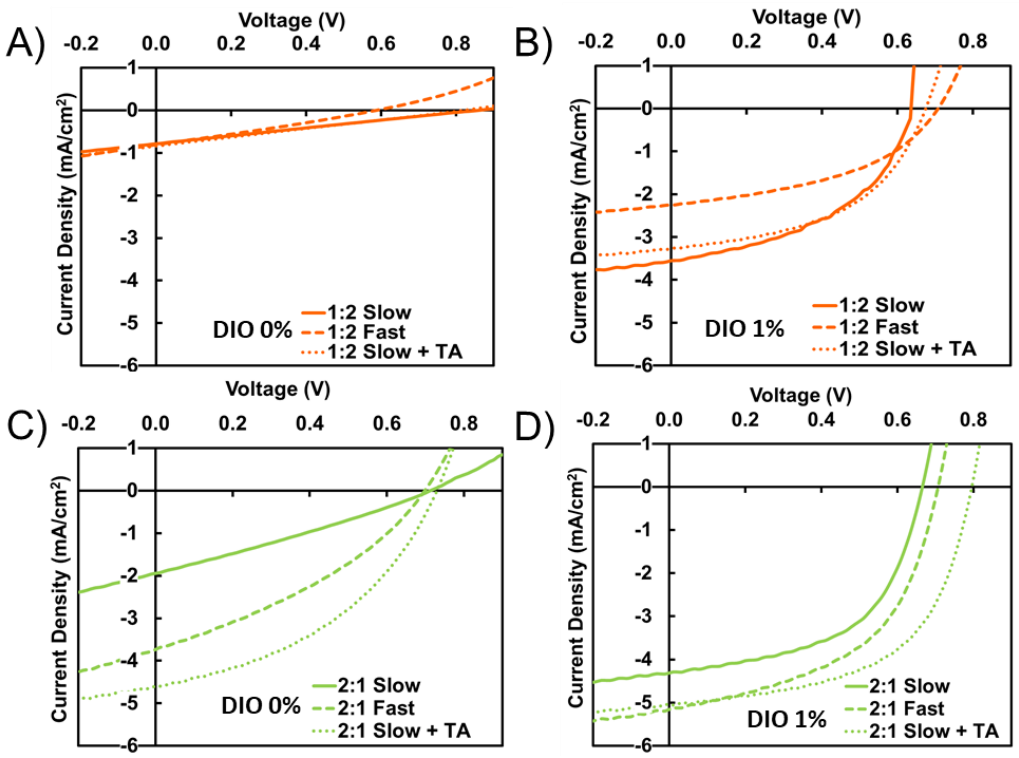

Figure S8. J-V curves of devices fabricated from 1:2 and 2:1 solutions of P3HT:PDI with various DIO loads (DIO % v/v), drying times and thermal treatments. Slow + TA refers to the thermally annealed films after 24 hours.

REFERENCES

(1) McAfee, S. M.; Payne, A.-J.; Dayneko, S. V.; Kini, G. P.; Song, C. E.; Lee, J.-C.; Welch, G. C. A Non-Fullerene Acceptor with a Diagnostic Morphological Handle for Streamlined Screening of Donor Materials in Organic Solar Cells. *J. Mater. Chem. A* **2017**, *5* (32), 16907–16913. https://doi.org/10.1039/C7TA05282K.

(2) Dayneko, S. V.; Hendsbee, A. D.; Welch, G. C. Combining Facile Synthetic Methods with Greener Processing for Efficient Polymer-Perylene Diimide Based Organic Solar Cells. *Small Methods* **2018**, 1800081. https://doi.org/10.1002/smtd.201800081.