Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Cyano-Substituted Oligo(p-phenylene vinylene) Single-crystal with balanced hole and electron injection and transport for Ambipolar Field-effect Transistor

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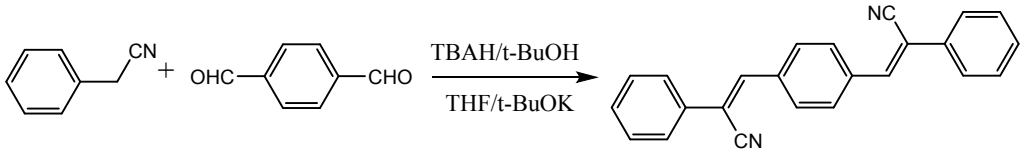
Supporting Information

1. Synthetic route of CNDSB



Scheme S1. Synthetic route of CNDSB.

CNDSB was synthesized according to the procedure shown in Scheme S1.[21] All chemicals were purchased commercially and used without further purification. The mixture of Benzylcyanide (201 mg, 1.5 mmol) and Terephthalaldehyde (0.345 mL, 3 mmol) in tert-butyl alcohol (10 mL) was stirred at 46 °C for 30 min. Then, potassium tert-butoxide (1 M solution in tetrahydrofuran, 0.25 mL) and Tetrabutylammonium hydroxide (TBAH, 1 M solution in methanol, 0.25 mL) were added, and then stirred for 20 minutes. The resulting precipitate was filtered and purified by column chromatography using dichloromethane. CNDSB powder (348 mg) was obtained in yield of 70% by evaporated the solvent.

2. Growth condition of CNDSB single crystal

Table S1. The growth condition of the CNDSB crystal.

No. of batches	Sublimation temperature/K	Growth temperature/K
1	523	433
2	518	433
3	513	433
4	513	436
5	513	438

3. Crystal facets determination.

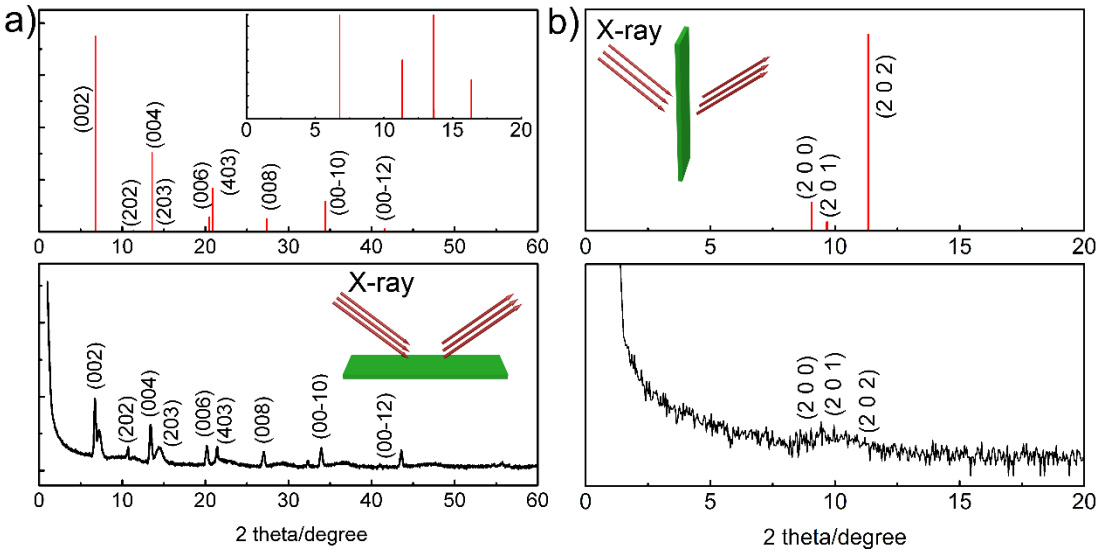


Figure S2. a) The predicting data based on single crystal (top) and experimental test (bottom), the insert shows the XRD test configuration. b) XRD pattern while the crystal was upright. The inset shows the schematic diagram of the XRD measurement setup.

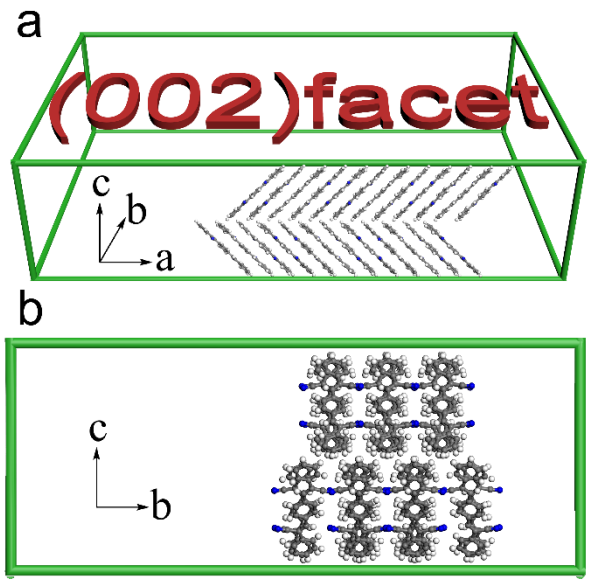


Figure S3. a) The molecule arrangement within the long side facet. b) The molecule arrangement within the short side facet.

4. OFETs characteristic.

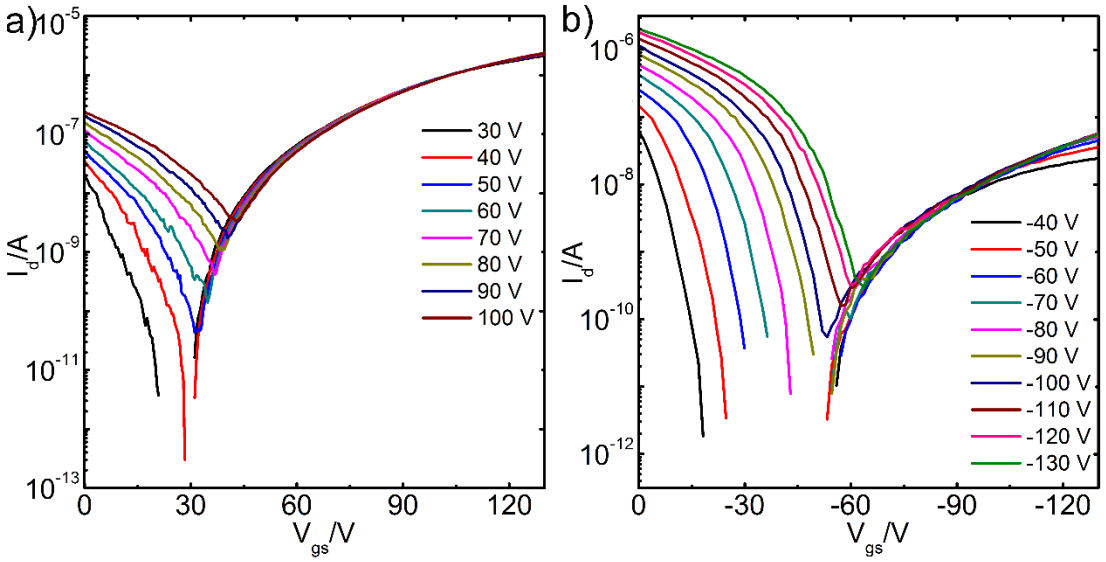


Figure S4. Transfer characters of CNDSB single crystal OFETs at various V_{ds}. In the figures, the $|V_{ds}|$ vary from 30 V to 100 V (N-channel) or 40 to 130 V (P-channel) with step =10 V. a) Transfer characters of N-channel, and b) P-channel.

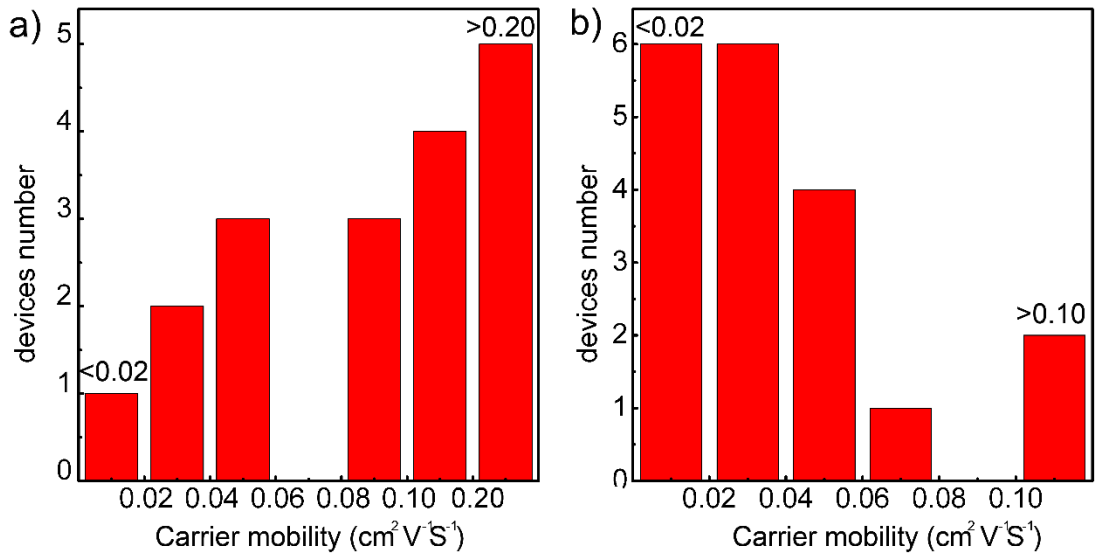


Figure S5. Histogram of electron (a) and hole (b) mobility calculated from 18 devices based on the CNDSB single-crystal OFETs.

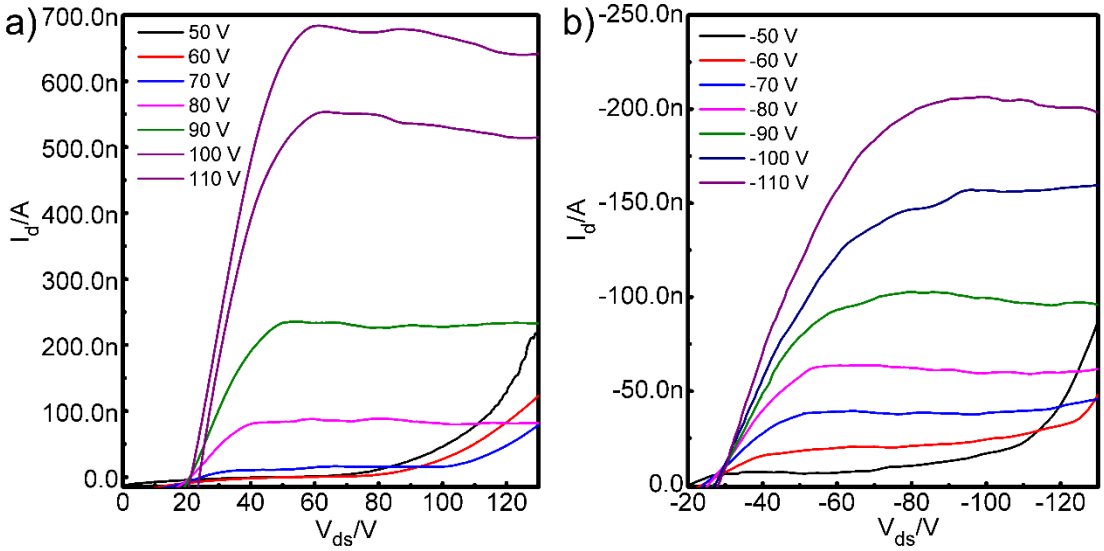


Figure S6. Out-put characters of the highest current density. Channel Width, 76 μm. (a) N-channel, (b) P-channel.

Table S2. Carrier mobility and structure information in the crystal of trans-DSB, CNDPDSB and CNDSB

Single Crystal	Method to measure the mobility	μ [$cm^2V^{-1}s^{-1}$]		Structure information in crystal	
		hole	electron	Lattice parameter (Å)	Distance of π-π planes(Å)
trans-DSB	Au-Ca OFETs	0.12	0.013	a = 5.873, b = 7.697, c = 34.866	
CNDPDSB	TOF	0.055	0.013	a = 6.645, b = 27.561, c = 7.653	3.574
CNDSB	Au symmetric OFETs	0.239	0.745	a = 19.5, b = 6.929, c = 26.031	3.394