

Supporting Information

New Organic Semiconductors and their Device Performance as a Function of Thiophene Orientation

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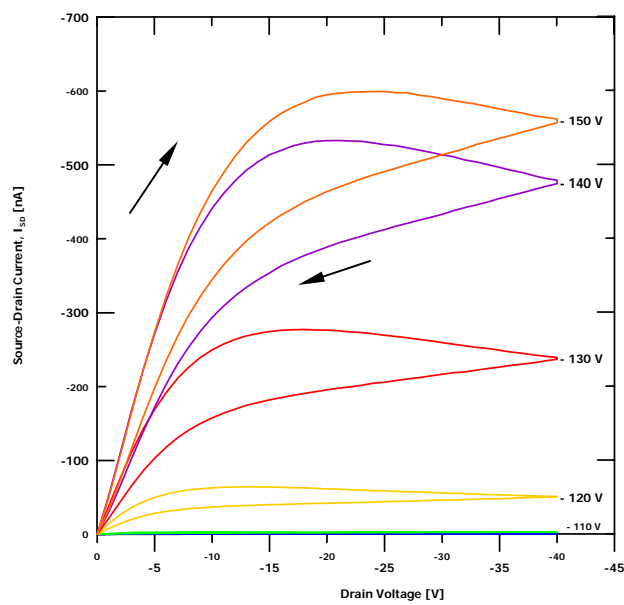


Figure S1. Output characteristic of **2** (180 nm, 75 °C) on OTS-treated p-Si/SiO₂ (300 nm).

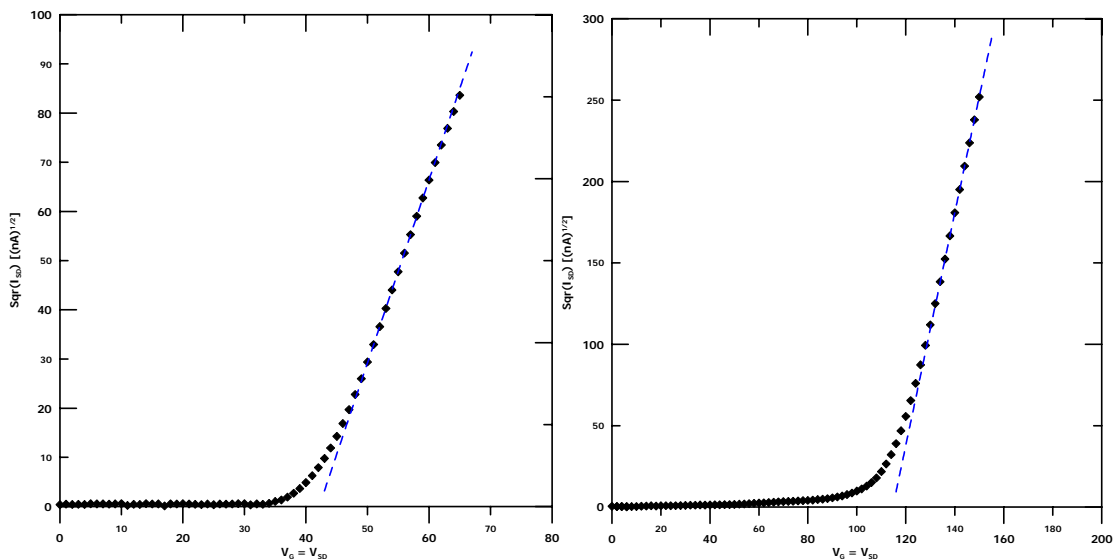


Figure S2. Mobility plot of **1** (left; $C_i = 32.1 \text{ nFcm}^{-2}$, $\mu = 0.011 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$ and **2** (right; $C_i = 11.3 \text{ nF/cm}^2$, $\mu = 0.12 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$).

Experimental Details and Data tables

Thin films of **1** (60 nm) and **2** (180 nm) were analyzed by X-ray diffractometry (XRD) using standard θ - 2θ scan with Cu $K\alpha$ radiation. The data were acquired on a PANalytical X'Pert Pro diffractometer in the Instrumentation Center, College of Arts and Sciences, University of Toledo, OH. The experimental parameters and results are summarized in Tables S1-S5.

Table S1. Experimental parameters for thin film XRD acquisition.

Stage	Flat stage
Configuration	Flat stage
Goniometer	PW3050/60 (Theta/Theta)
Minimum step size 2Theta	0.001
Minimum step size Omega	0.001
Sample stage	PW3071/xx Bracket
Diffractometer system	XPERT-PRO
Measurement program	pbBB004Xflat
Scan Axis	Gonio
Start (End) Position [$^{\circ}2\theta$.]	3.0084 (64.9904)
Step Size [$^{\circ}2\theta$.]	0.0170
Scan Step Time [s]	10.3355
Scan Type	Continuous
PSD Mode	Scanning
PSD Length [$^{\circ}2\theta$.]	2.12
Offset [$^{\circ}2\theta$.]	0.0000
Divergence Slit Type	Fixed
Divergence Slit Size [$^{\circ}$]	0.1196
Specimen Length [mm]	10.00
Measurement Temperature [$^{\circ}\text{C}$]	25.00
Anode Material	Cu
K-Alpha1 [\AA]	1.54060
K-Alpha2 [\AA]	1.54443
K-Beta [\AA]	1.39225
K-A2 / K-A1 Ratio	0.50000
Generator Settings	40 mA, 45 kV
Diffractometer Type	0000000000030813
Diffractometer Number	0
Goniometer Radius [mm]	240.00
Dist. Focus-Diverg. Slit [mm]	91.00
Incident Beam Monochromator	No
Spinning	No
Dist. focus to div. slit	91.00000
Irradiated length	10.00000
Spinner used	No
Receiving slit size	0.10000
Step axis value	0.00000
Offset	0.00000
Sample length	10.00000

Table S2. Thin film XRD data and calculated d-spacings of **1**.

Pos. /°2Th.	Height /cts	FWHM /°2Th.	d-spacing/Å	Rel. Int. /%
6.8433	420.25	0.0727	12.90646	100.00
13.6589	84.36	0.1006	6.47777	20.07
20.5205	249.40	0.1080	4.32462	59.35

Pos. = peak position; Rel. Int. = relative intensity.

Table S3. Powder pattern simulated from **1** single-crystal data (CCDC254385.cif) with Cu K-alpha1 radiation (1.5406 Å).

#	h	k	l	m	2-theta (c)/°	2-theta (o)/°	d-sp(c)/Å	Intensity	F
1	2	0	0	2	6.878	6.84	12.8407	215482	20
2	4	0	0	2	13.782	13.66	6.4204	36597	16
3	0	1	0	2	14.563		6.0774	703.41	2.41
4	1	1	0	4	14.968		5.9141	344738.92	38.73
5	2	1	0	4	16.122		5.4932	398113.24	44.89
6	3	1	0	4	17.885		4.9556	280981.07	41.95
7	4	1	0	4	20.102		4.4136	88060.67	26.49
8	6	0	0	2	20.736	20.52	4.2802	182494.63	55.69
9	5	1	0	4	22.648		3.9229	133.86	1.17
10	1	0	1	4	23.100		3.8472	548942.65	76.42
11	3	0	1	4	25.119		3.5423	570052.68	85.02
12	6	1	0	4	25.432		3.4994	49800.82	25.46
13	0	1	1	4	27.191		3.2770	601759.11	94.98
14	1	1	1	8	27.416		3.2506	1005864.74	87.59
15	8	0	0	2	27.768		3.2102	1234.97	6.22
16	2	1	1	8	28.080		3.1752	20875.38	12.94
17	7	1	0	4	28.394		3.1408	73368.98	34.73
18	5	0	1	4	28.761		3.1016	15355.70	16.11
19	3	1	1	8	29.156		3.0604	209888.26	42.72
20	0	2	0	2	29.369		3.0387	46587.65	40.57
21	1	2	0	4	29.579		3.0176	44385.79	28.21
22	2	2	0	4	30.199		2.9570	13763.43	16.06
23	4	1	1	8	30.605		2.9188	35407.86	18.48
24	3	2	0	4	31.209		2.8636	49282.50	31.49
25	8	1	0	4	31.492		2.8385	56895.77	34.17
26	5	1	1	8	32.381		2.7626	36193.01	19.86
27	4	2	0	4	32.575		2.7466	88584.67	44.22

28	7	0	1	4	33.545	2.6694	28568.93	25.92
29	5	2	0	4	34.260	2.6153	2745.55	8.22
30	6	1	1	8	34.441	2.6020	12263.31	12.36
31	9	1	0	4	34.702	2.5829	3383.15	9.26
32	10	0	0	2	34.909	2.5681	120.00	2.48
33	6	2	0	4	36.225	2.4778	11832.10	18.14
34	7	1	1	8	36.743	2.4440	16876.98	15.56
35	0	2	1	4	37.524	2.3949	5639.40	13.02
36	1	2	1	8	37.693	2.3846	11392.76	13.15
37	10	1	0	4	38.007	2.3656	86911.90	51.84
38	2	2	1	8	38.196	2.3543	29554.31	21.50
39	7	2	0	4	38.435	2.3402	246.13	2.79
40	3	2	1	8	39.022	2.3064	42054.89	26.26
41	9	0	1	4	39.116	2.3011	128462.94	65.07
42	8	1	1	8	39.255	2.2932	31856.75	23.00
43	4	2	1	8	40.154	2.2439	7183.60	11.20
44	8	2	0	4	40.859	2.2068	57472.69	45.68
45	11	1	0	4	41.397	2.1794	40552.74	38.94
46	5	2	1	8	41.573	2.1706	49944.03	30.70
47	9	1	1	8	41.949	2.1520	40697.88	28.00
48	12	0	0	2	42.192	2.1401	238.19	4.31
49	6	2	1	8	43.254	2.0900	88701.84	42.77
50	9	2	0	4	43.470	2.0801	37066.86	39.32
51	0	3	0	2	44.698	2.0258	12012.77	32.67
52	10	1	1	8	44.801	2.0214	32422.54	26.90
53	1	3	0	4	44.844	2.0195	68.29	1.75
54	12	1	0	4	44.865	2.0186	36693.98	40.54
55	7	2	1	8	45.176	2.0055	85478.46	44.10
56	11	0	1	4	45.259	2.0020	17520.76	28.29
57	2	3	0	4	45.281	2.0011	24.91	1.07
58	3	3	0	4	46.002	1.9714	1994.72	9.72

59	10	2	0	4	46.247	1.9615	28099.27	36.72
60	0	0	2	2	46.648	1.9455	18312.95	42.33
61	4	3	0	4	46.997	1.9319	326.67	4.03
62	2	0	2	4	47.212	1.9236	143.18	2.68
63	8	2	1	8	47.317	1.9196	17284.69	20.90
64	11	1	1	8	47.796	1.9015	7308.27	13.74
65	5	3	0	4	48.253	1.8845	1984.43	10.24
66	13	1	0	4	48.411	1.8787	22394.70	34.52
67	4	0	2	4	48.876	1.8619	4130.15	14.99
68	0	1	2	4	49.130	1.8529	55403.59	55.22
69	11	2	0	4	49.174	1.8513	4659.98	16.03
70	1	1	2	8	49.266	1.8481	51294.88	37.69
71	9	2	1	8	49.658	1.8344	65193.73	42.87
72	14	0	0	2	49.659	1.8344	756.26	9.24
73	2	1	2	8	49.673	1.8339	58355.51	40.57
74	6	3	0	4	49.755	1.8311	140636.43	89.25
75	3	1	2	8	50.346	1.8110	10748.17	17.68
76	0	3	1	4	50.769	1.7969	1683.60	9.99
77	1	3	1	8	50.902	1.7925	5940.93	13.31
78	12	1	1	8	50.921	1.7918	16113.45	21.93
79	4	1	2	8	51.277	1.7803	18835.06	23.90
80	2	3	1	8	51.299	1.7795	5134.61	12.49
81	7	3	0	4	51.489	1.7734	2822.13	13.15
82	6	0	2	4	51.559	1.7712	13852.89	29.17
83	13	0	1	4	51.864	1.7615	22848.82	37.71
84	3	3	1	8	51.957	1.7585	55612.74	41.69
85	14	1	0	4	52.034	1.7561	2506.80	12.54
86	10	2	1	8	52.181	1.7515	16195.87	22.61
87	12	2	0	4	52.239	1.7497	17109.86	32.90
88	5	1	2	8	52.456	1.7430	11193.75	18.91
89	4	3	1	8	52.868	1.7304	2644.53	9.27

90	8	3	0	4	53.440	1.7132	409.02	5.22
91	6	1	2	8	53.873	1.7004	62807.56	46.17
92	5	3	1	8	54.023	1.6961	1840.76	7.93
93	13	1	1	8	54.169	1.6918	13120.97	21.23
94	11	2	1	8	54.874	1.6718	15319.47	23.28
95	8	0	2	4	55.157	1.6638	861.13	7.85
96	6	3	1	8	55.412	1.6568	1120.01	6.37
97	13	2	0	4	55.431	1.6563	5497.81	19.95
98	7	1	2	8	55.516	1.6539	28298.07	32.07
99	9	3	0	4	55.592	1.6519	2861.54	14.44
100	15	1	0	4	55.735	1.6479	6.91	0.71
101	0	2	2	4	56.085	1.6385	42914.97	56.50

#=No. of peak; m=multiplicity; c = calculated; o = observed;

Table S4. Thin film XRD data and calculated d-spacings of **2**.

Pos./°2Th.	Height/cts	FWHM/°2Th.	d-spacing/Å	Rel. Int./%
6.6462	4120.34	0.0780	13.28871	100.00
13.1660	252.04	0.0781	6.71913	6.12
19.7334	1634.62	0.0775	4.49530	39.67
26.3600	193.09	0.0779	3.37834	4.69
33.0891	476.75	0.0805	2.70507	11.57
39.9434	53.81	0.1098	2.25526	1.31
46.9351	21.41	0.1361	1.93431	0.52
54.1147	53.44	0.1098	1.69340	1.30

Pos. = peak position in the diffractogram; cts = counts; Rel. Int. = relative intensity.

Table S5. Indexed thin film diffraction data of **2**.

Thin film unit cell of **2** (indexing method: DICVOL91): $a=27.08(7)$, $b=6.8(3)$, $c=4.78(1)$, $\alpha=\beta=\gamma=90^\circ$; orthorhombic P; refined unit cell only and $h=20$, $k=0$, $l=0$; Snyder FOM 9.51.

#	h	k	l	Sin ² (c)	Sin ² (o)	Sin ² (d)	2Th(c)/°	2Th(o)/°	2Th(d)/°	d-sp(c)/Å	d-sp(o)/Å	d-sp (d)/Å
1	1	0	0	81			3.2601			27.07925 0		
2	2	0	0	324	336	-12	6.5229	6.6462	-0.1233	13.53963 0	13.288710	0.250917
3	3	0	0	728			9.7910			9.026417		
4	4	0	0	1295	1314	-19	13.0670	13.1660	-0.0990	6.769813	6.719129	0.050683
5	5	0	0	2023			16.3539			5.415850		
6	6	0	0	2913	2936	-23	19.6543	19.7334	-0.0791	4.513208	4.495301	0.017907
7	7	0	0	3965			22.9713			3.868464		
8	8	0	0	5179	5199	-20	26.3080	26.3600	-0.0521	3.384906	3.378340	0.006567
9	9	0	0	6554			29.6675			3.008806		
10	10	0	0	8092	8109	-17	33.0533	33.0891	-0.0359	2.707925	2.705072	0.002854
11	11	0	0	9791			36.4690			2.461750		
12	12	0	0	11652	11666	-14	39.9187	39.9434	-0.0247	2.256604	2.255265	0.001339
13	13	0	0	13675			43.4065			2.083019		
14	14	0	0	15860	15859	1	46.9371	46.9351	0.0020	1.934232	1.934308	-0.000076
15	15	0	0	18207			50.5155			1.805283		
16	16	0	0	20715	20692	23	54.1476	54.1147	0.0328	1.692453	1.693403	-0.000950
17	17	0	0	23385			57.8394			1.592897		

= peak number; (c)=calculated; (o)=observed; (d)=difference between calculated and observed; d-sp = d-spacing.

