Electronic Supplementary Information for:

The Prediction of hole mobility in organic semiconductors and its calibration based on the grain-boundary effect

Jin Woo Park, Kyu Il Lee, Youn-Suk Choi,* Jung-Hwa Kim, Daun Jeong, Young-Nam Kwon, Jong-Bong Park, Ho Young Ahn, Jeong-Il Park, Hyo Sug Lee** and Jaikwang Shin

Samsung Advanced Institute of Technology, Samsung Electronics Co. Ltd., 130 Samsung-ro, Yeongtong-gu, Suwon-si, Gyeonggi-do 16678, Republic of Korea

Table S1 Grain size (G) and hole mobilities (μ in $cm^2\ V^{-1}\ s^{-1}$) of in-house OTFTs according to processing temperature (T_{sub} in ℃). These data were used in Fig. 5 to develop calibration model

Molecule	T_{sub}	N_{grain}[a]	G[b]	μ_{exp}	$\mu_{calculated}$	$\mu_{calibrated}$[c]
1 (DTBTT)	25	1540	0.13	2.82	18.9	2.81
	40	174	0.38	6.89		6.15
	60	22	1.07	13.87		10.04
	80	12	1.44	8.26		-
2 (C_1-DTBTT)	80	312	0.28	5.44	21.4	5.79
	100	66	0.62	7.86		9.06
	120	24	1.02	5.13		-
3 (DTNTT)	80	106	0.49	4.4	12.9	4.84
	120	25	1.00	6.0		6.70
	160	16	1.25	9.75		7.23
4 (C_{10}-DSeBTBT)	70	612	0.20	5.6	24.6	5.24
	90	195	0.36	7.3		7.73
	110	78	0.57	8.8		9.98

[a] Number of grains were counted from the AFM images. [b] Average grain size in μm.
[c] Calibrated using equation (3) in the manuscript. Mobilities beyond the maximum μ_{exp} were not calibrated.

Table S2 Averaged absolute value of transfer integrals ($\langle|J|\rangle$) between the neighboring pairs in the morphology, reorganization energy (λ), and their ratio for the organic molecules used in this work.

Molecule	$\langle\|J\|\rangle$ (eV)	λ (eV)	$\langle\|J\|\rangle$ / λ
1 (DTBTT)	0.01417	0.14425	0.09821
2 (C_1-DTBTT)	0.01387	0.14638	0.09476
3 (DTNTT)	0.01349	0.09040	0.14920
4 (C_{10}-DSeBTBT)	0.01349	0.08421	0.16017
5 (DNTT)	0.01744	0.13024	0.13387
6 (2,9-C_1-DNTT)	0.01041	0.13842	0.07518
7 (2,9-C_{10}-DNTT)	0.01814	0.14215	0.12763
8 (2,9-DPh-DNTT)	0.01605	0.14528	0.11046
9 (BBTNDT)	0.01254	0.12400	0.10110
10 (DBTTT)	0.00791	0.23875	0.03314
11 (DTTE3)	0.01388	0.33602	0.04130
12 (DTTE4)	0.01501	0.28635	0.05243
13 (DN-TTF)	0.01259	0.40191	0.03131
14 (BBBT)	0.00550	0.11578	0.04748
15 (DBTTB)	0.00773	0.17784	0.04348
16 (C_{12}-BTBT)	0.01548	0.24285	0.06373
17 (Hexacene)	0.02154	0.07679	0.28055
18 (TTTTT)	0.02031	0.30588	0.06639
19 (DTNN)	0.00929	0.20317	0.04572
20 (DTNQ)	0.02249	0.22740	0.09891
21 (BTAT)	0.01591	0.11420	0.13936

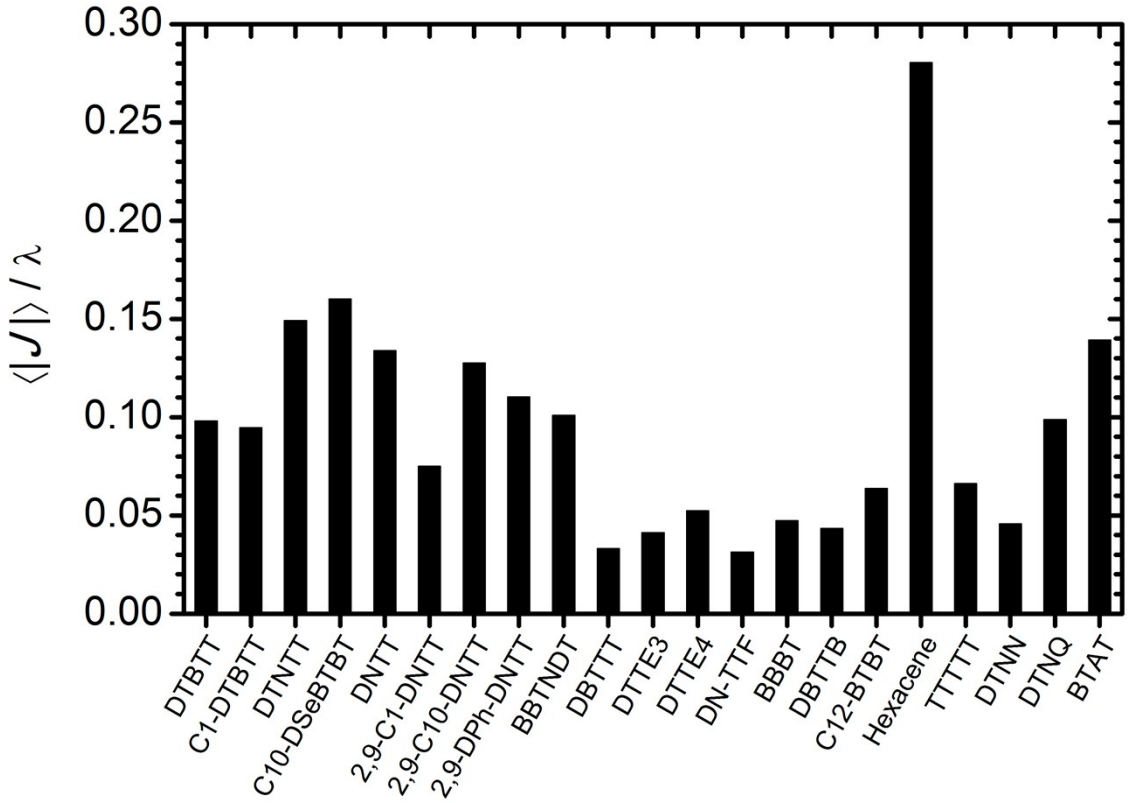

Fig. S1 Ratio of averaged absolute value of transfer integrals ($\langle|J|\rangle$) between the neighboring pairs in the morphology to reorganization energy (λ) for the organic molecules used in this work.

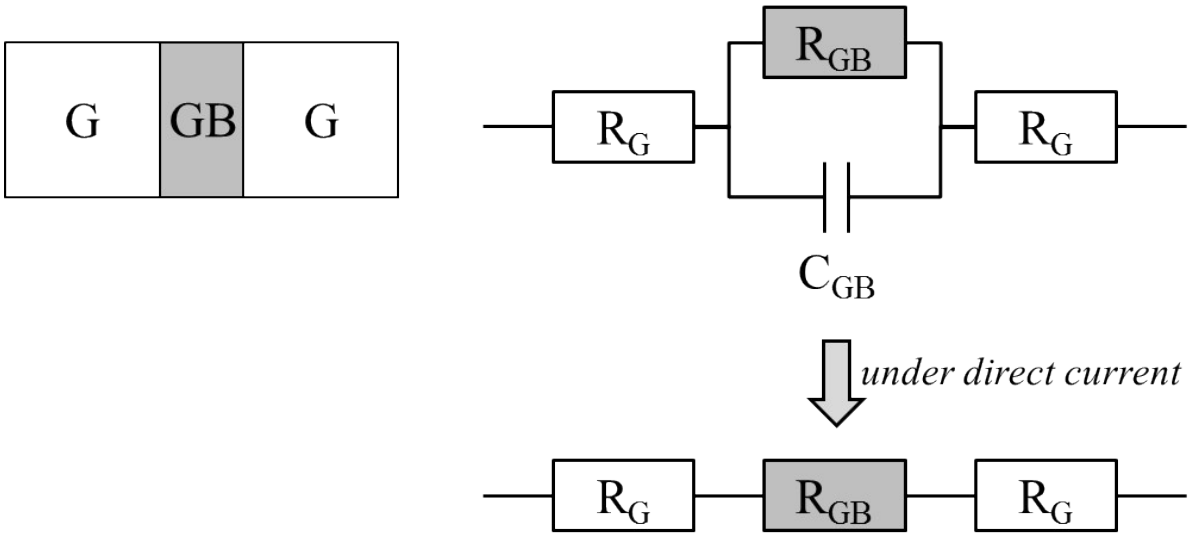

Fig. S2 Simple model containing grain (G) and grain boundary (GB), and corresponding equivalent circuits to represent electrical properties of organic semiconducting thin-film. R_G, R_{GB}, and C_{GB} denote the electrical resistances of grain and grain boundary, and capacitance of grain boundary, respectively.

The full citation for reference 31 is:

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