SUPPORTING INFORMATION

Dichotomy between band and hopping transport in organic semiconductors: insights from the experiments

I. Yavuz

Marmara University, Physics Dep. 34722, Ziverbey, Istanbul, Turkey.

e-mail: ilhan.yavuz@marmara.edu.tr

Table S1. Experimental and theoretical room-temperature hole (default) and electron (n) mobility data collected from the literature and predicted in this study where unavailable. Units are in cm^2/Vs

	name	**μ_{exp} (hole,p) (electron,n)**	**ref.**	**μ_{band} (hole,p) (electron,n)**	**ref.**	**μ_{hop} (hole,p) (electron,n)**	**ref.**
1	Naphtalene	~1.0, ~0.6 (n)	[1]	74.4, 39.8(n)	[50]	1.59,0.26(n)	[54,55]
2	Anthracene	2.93, 1.7 (n)	[2]	42.2, 245(n)	[50]	3.46,0.91.(n)	[54,55]
3	Tetracene	2.4	[3]	92.5	[50]	4.24	[57]
4	Pentacene	35	[4]	58	[51]	18.5	[56]
5	Hexacene	4.28	[5]	13[a]		1.461	[5]
6	Rubrene	40, 0.81(n)	[6,7]	242.6, 4.5[a](n)	[51]	20, 1 (n)	[55,56]
7	Picene	9	[8]	12[a]		6.87	[54]
8	DNTT	8.3	[9]	137.7	[51]	9.5	[51]
9	DATT	16	[10]	322.6	[51]	21.2	[51]
10	C_8-BTBT	31	[11]	609	[52]	7.5[b]	
11	C_{12}-BTBT (1)	0.2	[12]	62.5	[12]	1.7	[12]
12	C_{12}-BTBT (2)	170	[12]	140.5	[12]	3.7	[12]
13	C_{12}-BTBT (3)	0.1	[12]	8.1	[12]	1.6	[12]
14	C_{12}-BTBT (4)	0.5	[12]	43.9	[12]	9.4	[12]
15	iPr-BTBT	0.04	[13]	10[a]		0.68[b]	
16	tBu-BTBT	0.4	[13]	3.9[a]		0.22[b]	
17	ditBu-BTBT	7.1	[13]	10.9[a]		0.67[b]	
18	diTMS-BTBT	0.3	[13]	8.8[a]		0.23[b]	
19	HTP	0.27	[14]	5.5[a]		0.16	[59]
20	PDIF-CN2	6 (n)	[15]	132.8(n)	[51]	2.3(n)	[51]
21	4T/HT	0.23	[16]	5.3[a]		0.19	[54]
22	BB-PTA	0.5	[17]	34[a]		7.56	[54]
23	DT-TTF	1.4	[18]	2.2[a]		1.26	[54]
24	TTDM-TTF	0.4	[19]	5.5[a]		0.63	[54]

25	HM-TTF	7	[20]	138[a]		1.76	[54]
26	TTF	0.23	[21]	195[a]		0.06	[54]
27	DB-TTF	0.6	[22]	58[a]		0.24	[60]
28	PBBTZ	3.6	[23]	27[a]		1.64	[54]
29	DPA	3.7, 13 (n)	[24]	419[a], 14[a] (n)		8.6, 11.6 (n)	[54,55]
30	NTMTI	0.37	[25]	37[a]		0.92	[1]
31	TPBIQ	1	[26]	17.4[a]		1.96[b]	[61]
32	TIPSAntBt	0.23	[27]	41[a]		3.6	[27]
33	TIPSAntNa	3.7	[27]	67[a]		0.88	[27]
34	DBTDT	1.83	[28]	1.2[a]		1.8	[54]
35	DPNDF1	1.3	[29]	21[a]		0.4[b]	
36	DPNDF2	0.2	[29]	11.8[a]		2.08[b]	
37	DPNDF3	0.6	[29]	4.7[a]		0.52[b]	
38	DDQT-3	0.04	[30]	0.008[a]		0.038	[62]
39	Bist-tetracene(1)	6.1	[31]	36[a]		6.81[b]	
40	Bist-tetracene(2)	0.4	[31]	6.5[a]		1.61[b]	
41	PET	0.8	[32]	39[a]		5.34	[58]
42	THA1	0.26	[33]	5.3[a]		0.72[b]	
43	TFPT	1.83 (n)	[34]	3.4[a]		1.2	[55]
44	FRUB	4.2 (n)	[35]	11.6[a]		5.2	[55]
45	TCNQ	1.6 (n)	[36]	4.7[a]		0.75	[55]
46	TFTT	1.2 (n)	[37]	9.5[a]		0.22	[55]
47	TFDT	0.18 (n)	[37]	3.7[a]		0.14	[55]
48	PERY-a	5.5 (n)	[38]	2[a]		0.95	[55]
49	PERY-b	0.4 (n)	[39]	0.3[a]		0.4	[55]
50	FPTTF	0.1 (n)	[40]	1.8[a]		0.76	[55]
51	C60	11 (n)	[41]	15.4[a]		5.1	[55]
52	TFAPT	2.4 (n)	[42]	3.2[a]		0.68	[55]
53	TFPTP	3.1 (n)	[43]	1.8[a]		5.6	[55]
54	PTCDA-α	0.005 (n)	[44]	0.03[a]		0.017	[55]
55	PTCDA-β	0.005 (n)	[44]	1[a]		0.005	[55]
56	pMSB	0.1 (n)	[45]	1[a]		0.12	[55]
57	oMSB	0.009 (n)	[45]	0.08[a]		0.0066	[55]
58	BDTT	1.91	[46]	91[a]		16.4[b]	
59	BDTTE	0.58	[46]	1.3[a]		0.26[b]	
60	ditBu-BTBT	1.5	[47]	15.4[a]		3.0[b]	
61	CNT	7.9×10^4	[48]	1.2×10^5	[53]	n/a	
62	SL-Graphene	4.0×10^5	[49]	3.5×10^5	[52]	n/a	
63	BL-Graphene	3.0×10^5	[49]	4.2×10^5	[52]	~40	

[a] calculated in this work from Eq. 8 and L is taken to be 10 meV if it is not reported in the reference. Some transport parameters are taken from the reference.

[b] calculated in this work using Eq. (12)-(13). λ_s and $\hbar\omega$ is taken to 100 and 200 meV, respectively. Some transport parameters are taken from the reference.

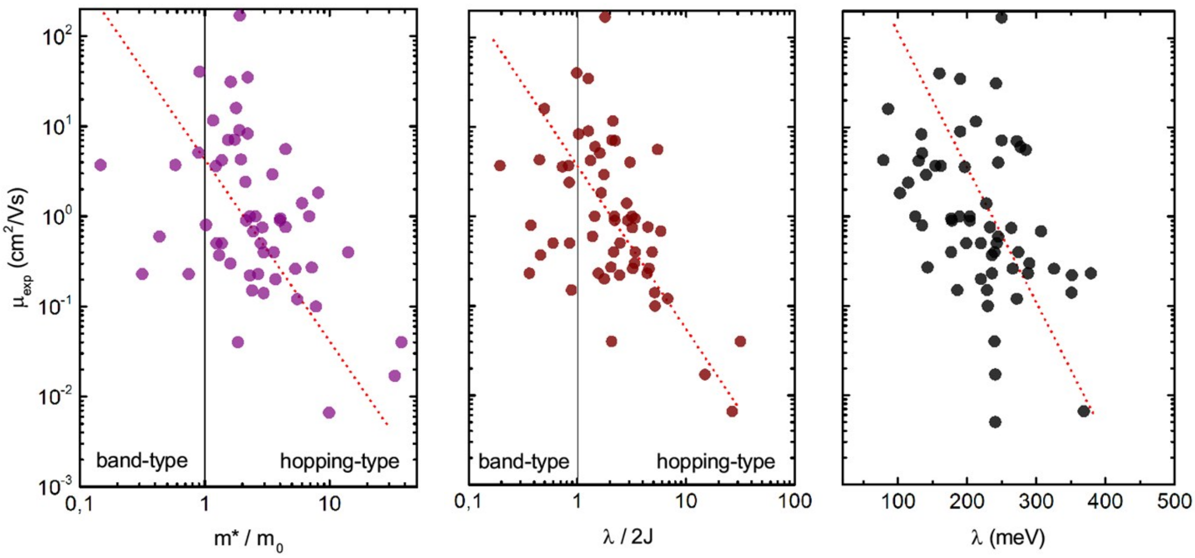

Figure S1: Plots showing the calculated experimental organic crystal mobilities versus the m^*/m_0, $\lambda/2J$ and λ parameters and red dotted lines are fitting. Each parameter weakly correlates with the experimental mobility.

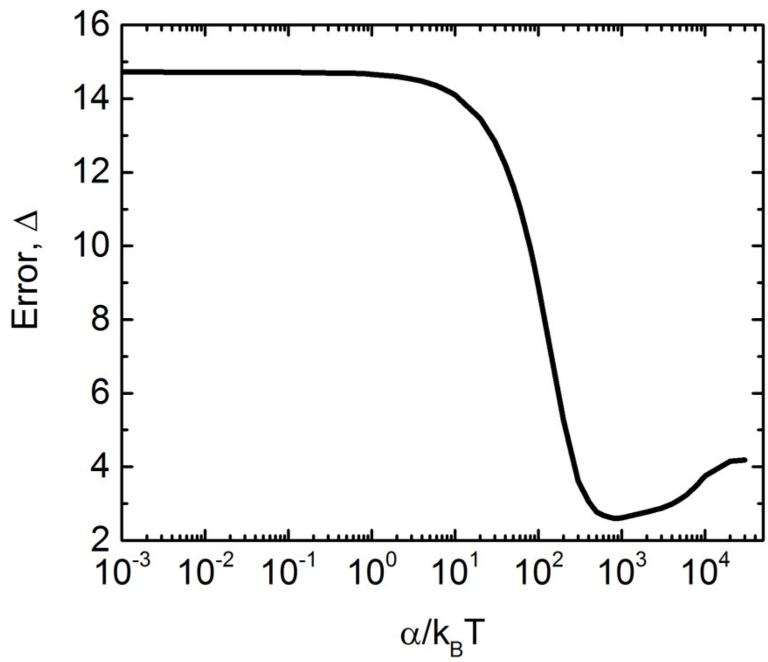

Figure S2: Error, $\Delta = \exp[N^{-1}\Sigma_{i=1}^{N} |\ln(\mu_{\exp}^{i} / \mu_{pred}^{i})|]$, [54] between the predicted mobility vs experimental mobility at room temperature using Eq. (19), in the main text, as a function of α parameter. Note that the error is optimized at around $\alpha=10^3$.

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