Electronic Supplementary Material (ESI) for Materials Horizons.

Supplementary Information

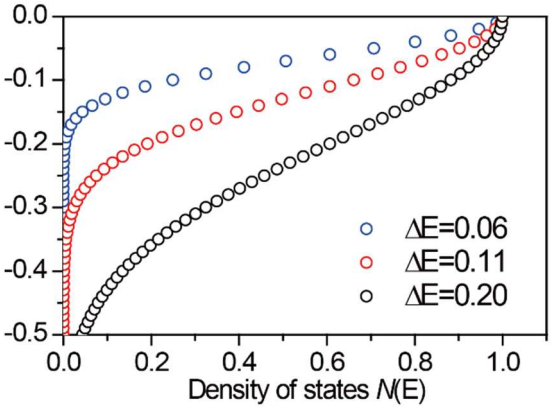

Figure S1 Normalized density of states $N(E)$ for different variances in density of states (DOS) (i.e., ΔE).

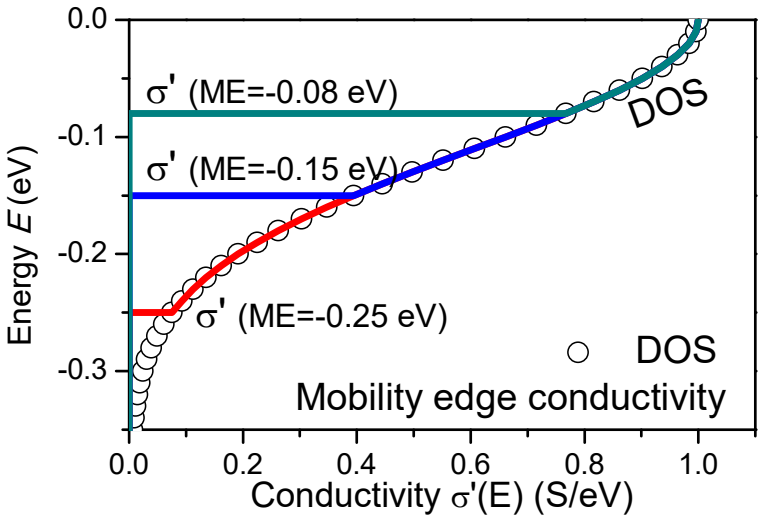

Figure S2 Normalized microscopic conductivity $\sigma'(E)$ for different mobility edge levels MB (ΔE is fixed at 0.11). The states are divided into the delocalized states ($\mu = \mu_0$) when $E \geq ME$ and the localized tail states ($\mu = 0$) when $E < ME$. Hence, diffusivity is constant above ME and the microscopic conductivity is only determined by DOS, which is different from the GER, as described in the main text.

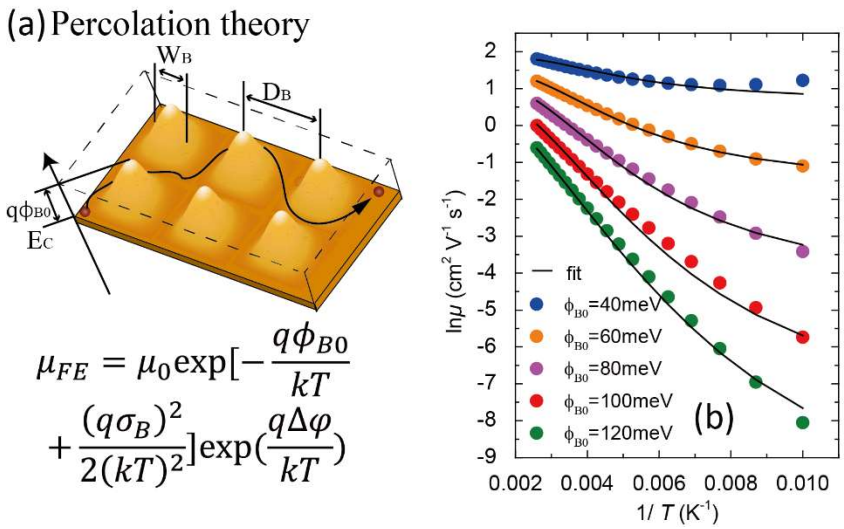

Figure S3 (a) The percolation model (PER, sketched by referencing [1]. (b) The PER model with varying the average potential barrier height ϕ_{B0}.

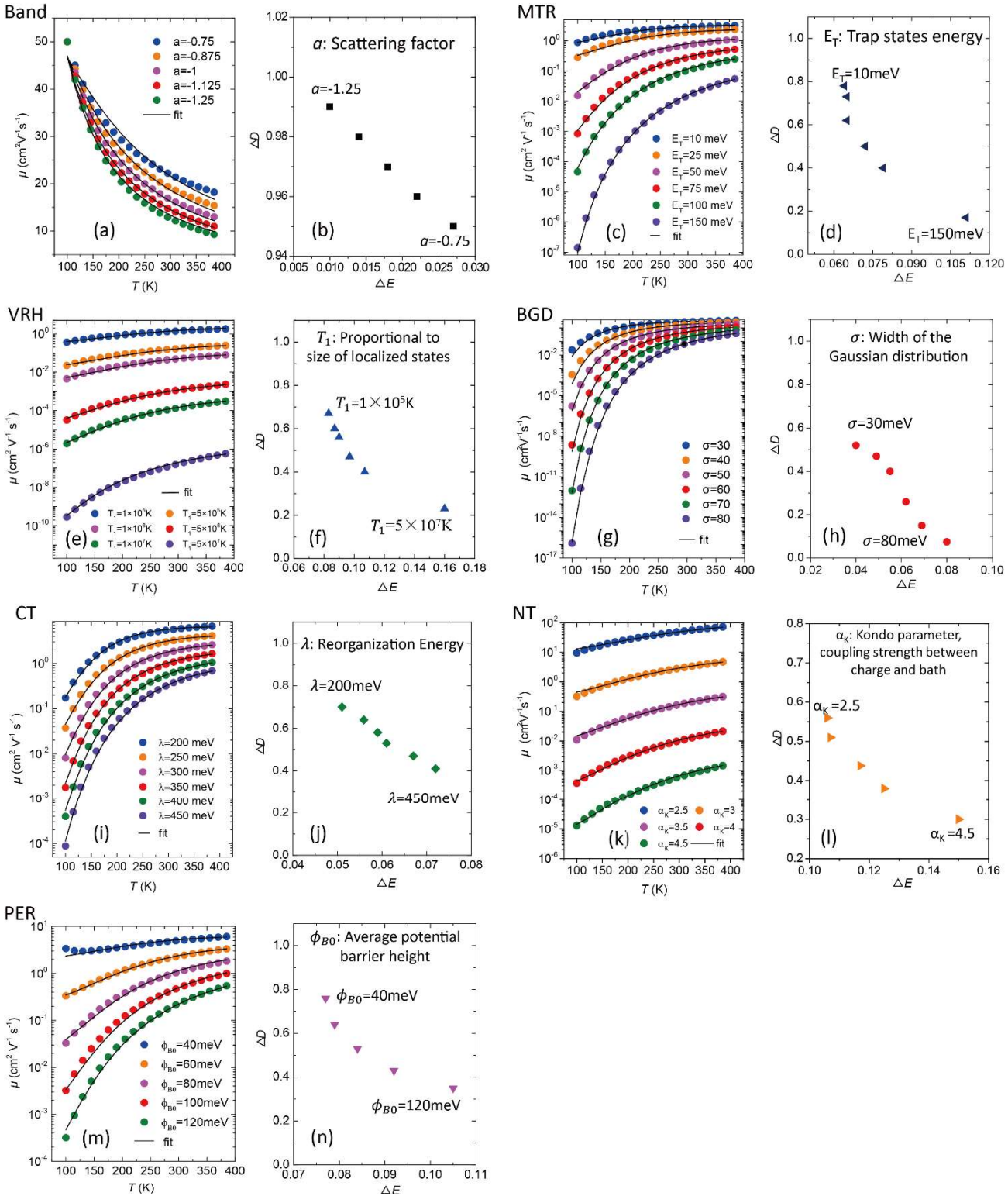

Figure S4. Mobility–temperature dependence predicted by different models and fittings by the GER: (a) band-like transport, (c) multiple trap and release (MTR) model, (e) variable range hopping (VRH) model, (g) Bassler's Gaussian disorder (BGD) model, (i) Marcus charge transfer (CT) model, (k) nuclear tunneling (NT) model and (m) percolation (PER) model. The limiting factor in each model for plotting the data is shown in the coordinate of DOS variance Δ*E* and delocalization degree Δ*D*: (b) band-like transport, (d) MTR model, (f) VRH model, (h) BGD model,

(j) CT model, (l) NT model, and (n) PER model.

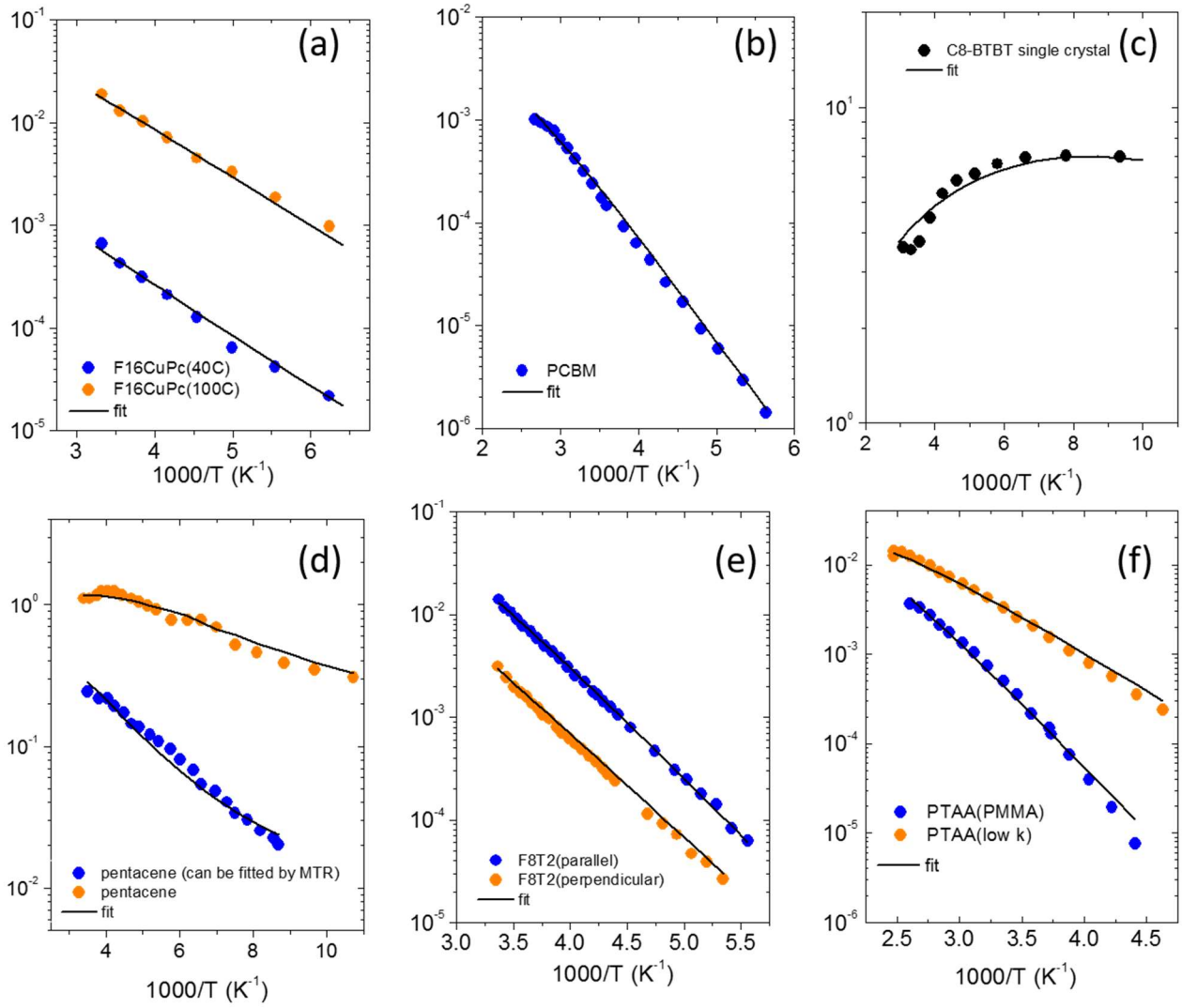

Figure S5. Mobility-temperature dependence for small molecules: (a) copper hexadecafluorophthalocyanine ($F_{16}CuPc$)[2]; (b) phenyl-C61-butyric acid methyl ester (PCBM)[3] (c) C8-BTBT[4]; (d) pentacene[5]; and for polymers: (e) poly (9, 9'-dioctylfluorene-co-bithiophene) (F8T2)[6]; (f) polytriarylamines (PTAA)[7].

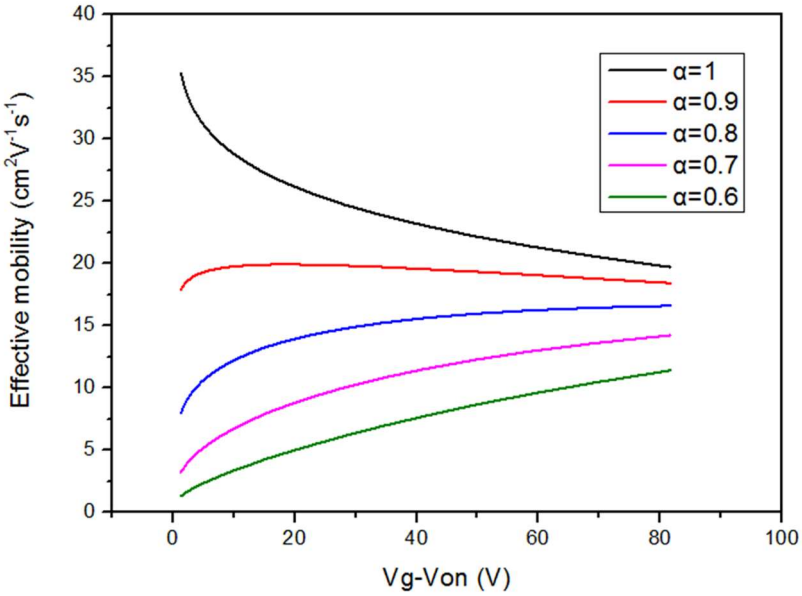

Figure S6. Mobility dependence on gate voltage. The calculated parameters are ΔE = 0.1 eV, T = 300 K, μ_0 = 2.5 cm²/Vs and $C_i = 2\times10^{-8}$ F/cm².

Table S1 The values of the parameters used for fitting different charge transport theories. (E_F= -0.2 eV).

Theory of charge transport	Theory's parameters		ΔD	ΔE	μ_0 (cm²/(V·s))	r²
Band-like transport $\mu = \mu_0 T^a$	$\mu_0 = 50b^{-a}$ (b = 100 K)	a = -0.75	0.95	0.027	1.55 (E_F = -0.05 eV)	0.9900
		a = -0.875	0.96	0.022	1.05 (E_F = -0.095 eV)	0.9957
		a = -1	0.97	0.018	1.05 (E_F = -0.05 eV)	0.9974
		a = -1.125	0.98	0.014	0.9 (E_F= -0.051 eV)	0.9987
		a = -1.25	0.99	0.01	0.98 (E_F= -0.026 eV)	0.9991
Crystal boundary/Multiple-trap & release (MTR) $\mu = \mu_0 \alpha \exp(-\frac{E_T}{k_B T})$	μ_0 = 10 cm²/(V·s) α = 0.5	E_T = 10 meV	0.81	0.07	0.45	0.9915
		E_T = 25 meV	0.72	0.076	0.39	0.9956
		E_T = 50 meV	0.619	0.078	0.238	0.9996
		E_T = 75 meV	0.49	0.084	0.183	0.9998
		E_T = 100 meV	0.372	0.092	0.14	0.9999
		E_T = 150 meV	0.17	0.111	0.07	0.9995
Bässler's Gaussian disorder model	μ_0 = 5 cm²/(V·s)	σ = 30 meV	0.52	0.04	0.36	0.9913
		σ = 40 meV	0.47	0.049	0.38	0.9971
		σ = 50 meV	0.4	0.055	0.35	0.9964

(E_F= -0.6 eV) $\mu = \mu_0 \exp[-\left(\frac{2\sigma}{3k_BT}\right)^2]$		σ = 60 meV	0.26	0.062	0.38	0.9983
		σ = 70 meV	0.15	0.069	0.36	0.9984
		σ = 80 meV	0.075	0.08	0.45	0.9998
Variable range hopping (VRH) $\mu \propto \exp\left[\frac{-T_1}{T}\right]^{1/4}$	μ_0 = 100 cm²/(V·s)	T_1 = 1 × 10⁵ K	0.67	0.088	0.39	0.9974
		T_1 = 5 × 10⁵ K	0.615	0.088	0.063	0.9989
		T_1 = 1 × 10⁶ K	0.53	0.106	0.03	0.9994
		T_1 = 5 × 10⁶ K	0.449	0.1	1.16 × 10⁻³	0.9994
		T_1 = 1 × 10⁷ K	0.37	0.11	2.3 × 10⁻⁴	0.9994
		T_1 = 5 × 10⁷ K	0.16	0.16	1.42 × 10⁻⁶	0.9995
Percolation $\mu_{FE} = \mu_0 \exp[-\frac{q\phi_{B0}}{kT} + \frac{(q\sigma_B)^2}{2(kT)^2}]\exp(\frac{q\Delta\varphi}{kT})$	μ_0 = 15 cm²/(V·s) $\Delta\varphi$ = 4 meV σ_B = 20 meV	ϕ_{B0} = 40 meV	0.76	0.077	0.9	0.9716
		ϕ_{B0} = 60 meV	0.64	0.079	0.72	0.9994
		ϕ_{B0} = 80 meV	0.53	0.084	0.62	0.9994
		ϕ_{B0} = 100 meV	0.43	0.092	0.5	0.9996
		ϕ_{B0} = 120 meV	0.35	0.105	0.4	0.9999
Marcus charge transfer (CT) model $\mu = \frac{qa^2}{k_BT}k_{if}$ $k_{if} = \frac{2\pi}{\hbar}\lvert V_{if}\rvert^2\{\frac{1}{\sqrt{4\pi\lambda k_BT}}$ $\exp[\frac{-(\Delta G+\lambda)^2}{4\lambda k_BT}]$	a = 7×10⁻⁸ cm V_{if} = 0.1 ΔG = 30 meV	λ = 200 meV	0.63	0.048	0.8	0.9982
		λ = 250 meV	0.616	0.0559	0.6	0.9991
		λ = 300 meV	0.61	0.07	0.51	0.9999
		λ = 350 meV	0.553	0.075	0.42	0.9999
		λ = 400 meV	0.48	0.09	0.43	0.9998
		λ = 450 meV	0.426	0.097	0.365	0.9999
Nuclear tunneling (NT) model $\mu = v_0\exp(-2\alpha a - 0.5\sigma^2 + 0.8\sigma)\frac{\lvert\Gamma(\alpha_K)\rvert^2}{\lvert\Gamma(2\alpha_K)\rvert}$ $v_0 = \frac{1}{\hbar^2\omega_c}(\frac{\hbar\omega_c}{2\pi k_BT})^{1-\alpha_K}$	$\hbar\omega_c$ = 10 eV αa = 10 σ = 60 meV	α_K = 2.5	0.56	0.106	25	0.9987
		α_K = 3.0	0.51	0.107	2	0.9994
		α_K = 3.5	0.438	0.117	0.185	0.9995
		α_K = 4.0	0.38	0.125	0.017	0.9993
		α_K = 4.5	0.3	0.15	1.85 × 10⁻³	0.9991

Table S2 Values of the parameters used for fitting different semiconductor materials (**Figure** 3).

Semiconductor	Properties (e.g. crystallinity)	Dielectric	ΔD	ΔE (eV)	μ_0 ($cm^2/(V \cdot s)$)	E_F (eV)	r^2
Rubrene[8]	Single crystals	Parylene (2.9)	0.77	0.045	1.3	-0.13	0.9887
		SiO_2 (3.9)	0.65	0.047	0.80	-0.10	0.9290
		Si_3N_4 (7.5)	0.40	0.06	0.49	-0.10	0.9917
		Al_2O_3 (9.4)	0.58	0.05	0.56	-0.12	0.9917
		Ta_2O_5 (25)	0.32	0.09	0.38	-0.10	0.9918
C8-BTBT[4]	Single crystals	PMMA(3.6)	0.93	0.028		-0.15	0.9782
Pentacene 1[9]	Poly-crystalline (rough substrate, 70 ºC)	Silicon nitride	0.77	0.04	0.0025	-0.17	0.9993
	Poly-crystalline (smooth substrate, 70 ºC)		0.75	0.047	0.038	-0.21	0.9999
	Poly-crystalline (smooth substrate, room temperature)		0.6	0.054	0.065	-0.25	0.9984
Pentacene 2[5]	Poly-crystalline (low mobility, can be fitted by MTR)	SiO_2 (3.9)	0.61	0.07	0.085	-0.19	0.9846
	Poly-crystalline (high mobility, can't be fitted by MTR)		0.80	0.045	0.10	-0.17	0.9814
TIPS-pentacene[10]	Poly-crystalline (L = 20 μm)	CYTOP (2.1)	0.81	0.034	0.115	-0.15	0.9812
	Poly-crystalline (L = 40 μm)		0.758	0.037	0.075	-0.2	0.9891
F_{16}CuPC[2]	Poly-crystalline (40 ºC substrate)	SiO_2 (3.9)	0.17	0.14	0.001	-0.15	0.9923
	Poly-crystalline (100 ºC substrate)		0.18	0.12	0.02	-0.14	0.9951
PCBM[3]	Poly-crystalline	SiO_2 (3.9)	0.12	0.10	0.0023	-0.24	0.9940
PBTTT 1[7b]	Poly-crystalline	PMMA (3.6)	0.32	0.12	0.35	-0.21	0.9920
		PS (2.6)	0.41	0.093	0.10	-0.18	0.9936
P3HT[11]	Poly-crystalline (molecular weight 15 kD, in trichlorobenzene)	SiO_2 (3.9)	0.43	0.07	0.0018	-0.2	0.9964
	Poly-crystalline (molecular weight 37 kD, in trichlorobenzene)		0.66	0.058	0.012	-0.2	0.9975
	Poly-crystalline (molecular weight 270 kD, in trichlorobenzene)		0.7	0.05	0.012	-0.2	0.9922
F8T2[6]	Poly-crystalline (parallel to the channel)	PVP (4.1)	0.20	0.10	0.14	-0.27	0.9991
	Poly-crystalline (vertical to the channel)		0.1679	0.14	0.08	-0.25	0.9968

PTAA[7]	Amorphous	PMMA(3.6)	0.2	0.12	0.4	-0.35	0.9945
		Poly(perfluoro-ethylene-co-butenyl vinyl ether (2.1)	0.45	0.09	0.01	-0.3	0.9942
P(NDI2OD-T2)[12]	Poly-crystalline	CYTOP (2.1)	0.15	0.17	0.15	-0.10	0.9987
		Polystyrene (2.6)	0.05	0.19	0.15	-0.10	0.9961
		PMMA (3.6)	0.07	0.18	0.12	-0.10	0.9931
CDT-BTZ-C20[13]	Poly-crystalline (gate field 0.5 MV/cm)	SiO_2 (3.9)	0.67	0.062	1.55	-0.20	0.9993
	Poly-crystalline (gate field 1.0 MV/cm)		0.74	0.05	1.11	-0.20	0.9901
	Poly-crystalline (gate field 1.5 MV/cm)		0.79	0.044	1	-0.20	0.9501
PSeDPPBT[14]	Poly-crystalline (hole mobility)	PMMA (3.6)	0.4	0.09	3	-0.39	0.9947
	Poly-crystalline (electron mobility)		0.5	0.085	0.51	-0.3	0.9993
N-alkyl perylene diimides (PTCDI)[15]	Poly-crystalline PTCDI-C_5	Polystyrene on SiO_2	0.52	0.065	0.015	-0.2	0.9976
	Poly-crystalline PTCDI-C_8		0.71	0.054	0.047	-0.2	0.9985
	Poly-crystalline PTCDI-C_{12}		0.76	0.051	0.01	-0.2	0.9980
PTDPPSe-Si[16]	Poly-crystalline PTDPPSe-SiC4 (n-channel)	SiO_2 (3.9)	0.64	0.058	0.052	-0.11	0.9881
	Poly-crystalline PTDPPSe-SiC4 (p-channel)				0.16	-0.11	0.9904
	Poly-crystalline PTDPPSe-SiC5 (n-channel)		0.56	0.062	0.083	-0.11	0.9962
	Poly-crystalline PTDPPSe-SiC5 (p-channel)				0.16	-0.11	0.9928

Table S3 The values of the parameters used for fitting different semiconducting materials with dependence on carrier concentration and temperature simultaneously in **Figure 4**.

Conducting layer	V_g or T	ΔD	ΔE	μ_0 (cm²/(V·s))	E_F (eV)
IDTBT[17]	240 K	0.9	0.08	0.078	——
	300 K			0.136	
PBTTT (PBTTT 2)[17]	240 K	0.61	0.13	0.006	——
	300 K			0.03	
DPPTTT	211.18K	0.4	0.12	1.15	——
	232.18K			1.30	
	253.58K			1.45	
	273.18K			1.65	
	294.17K			1.90	
P(NDI2OD-T2)	195.15K	0.5	0.1	0.17	——

(P(NDI2OD-T2-2)	213.85K			0.20	
	233.95K			0.25	
	249.35K			0.29	
	271.35K			0.35	
1L Pentacene (pentacene 3)[18]	V_g = -10 V	0.2	0.11	0.12	-0.102
	V_g = -20 V				-0.088
	V_g = -30 V				-0.079
2L Pentacene (pentacene 3)[18]	V_g = -35 V	0.88	0.027	0.18	-0.055
	V_g = -50 V				-0.014

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