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Unification of trap-limited electron transport in semiconducting polymers

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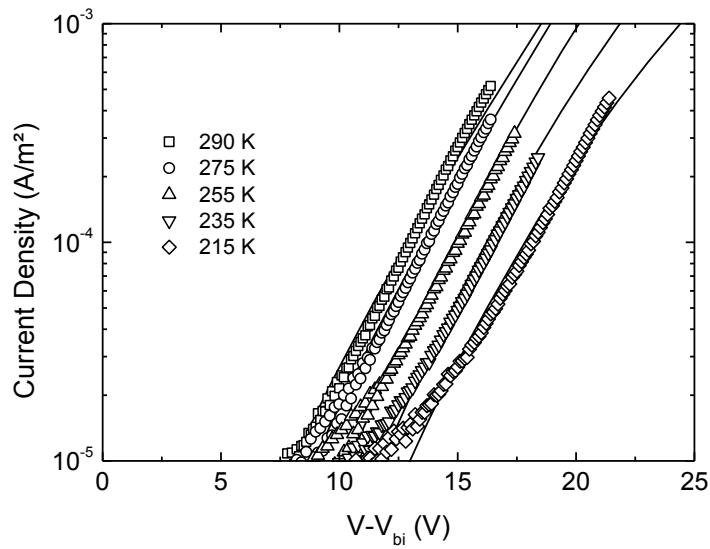


Figure S1. Temperature-dependent J - V curves of 320 nm NRS-PPV electron-only diodes and fits with a Gaussian trap at a trap depth of 0.76 eV.

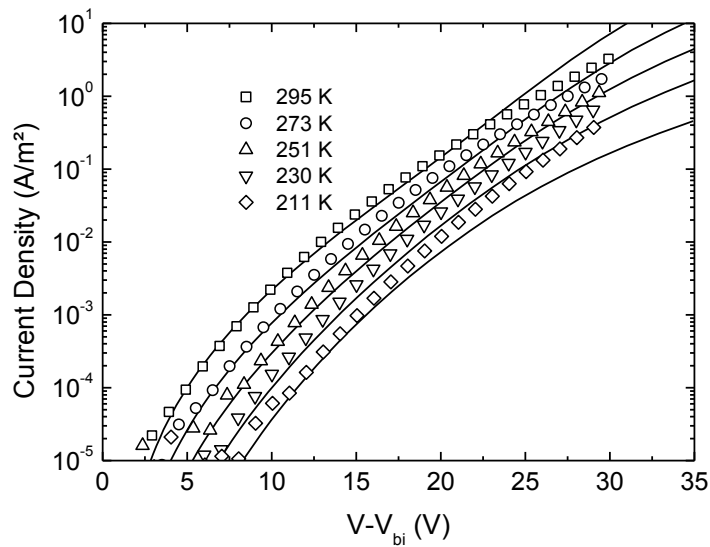


Figure S2. Temperature-dependent J - V curves of 300 nm OC₁C₁₀-PPV electron-only diodes and fits with a Gaussian trap at a trap depth of 0.70 eV.

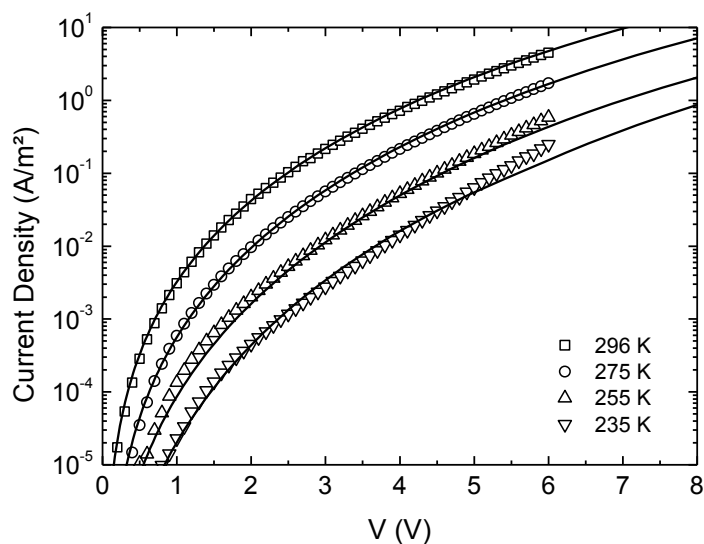


Figure S3. Temperature-dependent J - V curves of 173 nm F8BT electron-only diodes and fits with a Gaussian trap at a trap depth of 0.55 eV.

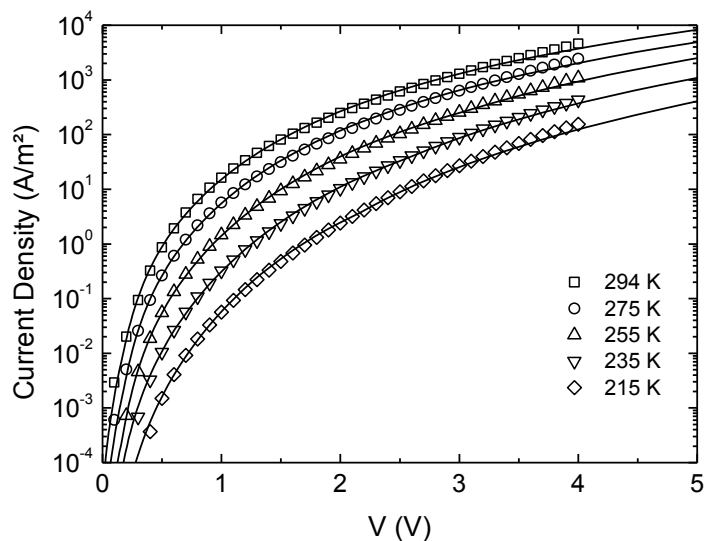


Figure S4. Temperature-dependent J - V curves of 85 nm PF10TBT electron-only diodes and fits with a Gaussian trap at a trap depth of 0.34 eV.

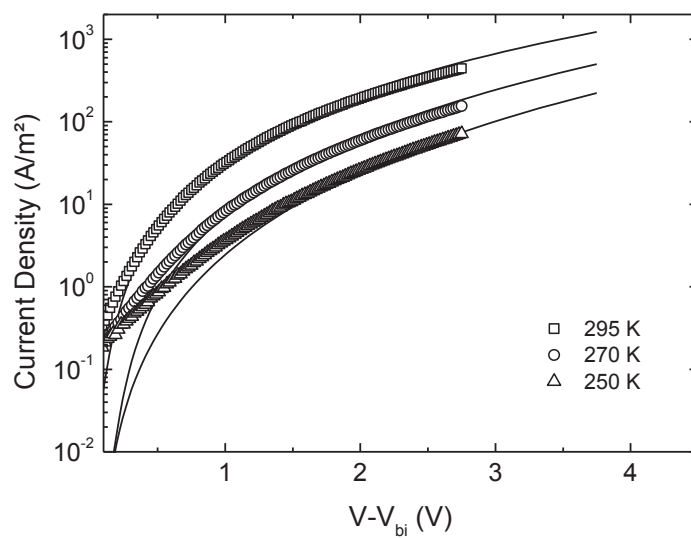
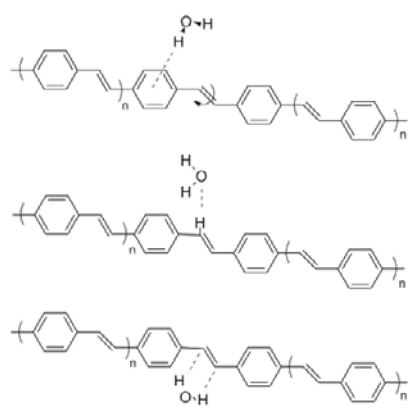


Figure S5. Temperature-dependent J - V curves of 148 nm PCPDTBT electron-only diodes and fits with a Gaussian trap at a trap depth of 0.21 eV.

Table S1. Frontier molecular orbital energies and vertical electron affinities for the H₂O-PPV complexes as determined at the B97D/6-311++G** level of theory with the CPCM dielectric model ($\epsilon = 3.0$).



	HOMO (eV)	LUMO (eV)	VEA (eV)
A2 A4 A6	-5.18	-2.42	-1.57
	-4.74	-2.91	-2.35
B2 B4 B6	-4.62	-3.05	-2.62
	-5.36	-2.57	-1.71
C2 C4 C6	-4.84	-3.01	-2.44
	-4.69	-3.12	-2.68
	-5.05	-2.30	-1.46
	-4.67	-2.84	-2.28
	-4.56	-3.00	-2.57
	-5.33	-2.58	-1.73
	-4.83	-3.01	-2.44
	-4.68	-3.13	-2.68

Table S2. Frontier molecular orbital energies and vertical electron affinities for select poly(paraphenylenevinylene) photooxidation products as determined at the B97D/6-311G**//AM1 level of theory with the CPCM dielectric model ($\epsilon = 3.0$).

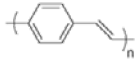
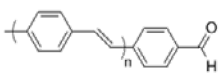
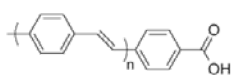
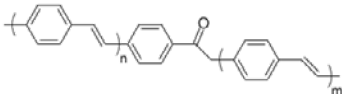
	HOMO (eV)	LUMO (eV)	VEA (eV)
 PPV4 n=4 PPV8 n=8 PPV16 n=16	-4.72	-2.97	-2.44
 CHO4 n=3 CHO8 n=7 CHO16 n=15	-4.57	-3.12	-2.78
 COOH4 n=3 COOH8 n=7 COOH16 n=15	-5.07	-3.08	-2.38
 OPPV4 n=1, m=2 OPPV8 n=3, m=4 OPPV16 n=7, m=8	-4.69	-3.19	-2.74
	-4.55	-3.23	-2.97
	-4.88	-3.25	-2.68
	-4.61	-3.28	-2.91
	-4.52	-3.28	-3.04
	-4.85	-3.13	-2.59
	-4.60	-3.20	-2.85
	-4.52	-3.22	-3.01

Table S3. Frontier molecular orbital energies and vertical electron affinities for bromine-terminated poly(thiophene) and select poly(thiophene) photooxidation products and bromine termination as determined at the B97D/6-311G**//AM1 level of theory with the CPCM dielectric model ($\epsilon = 3.0$).

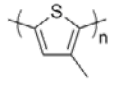
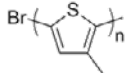
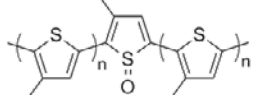
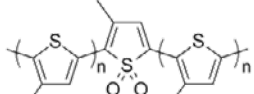
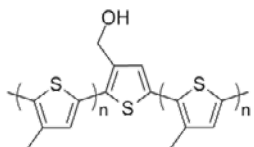
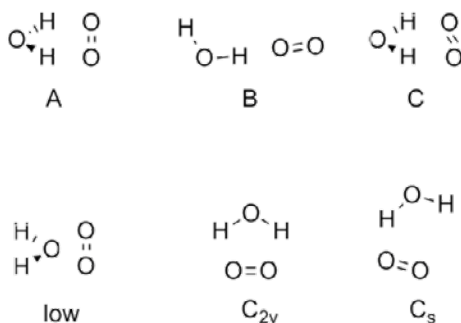
		HOMO (eV)	LUMO (eV)	VEA (eV)
	thio7 n=7 thio13 n=13 thio25 n=25			
	Br7 n=7 Br13 n=13 Br25 n=25			
	SO7 n=3 SO13 n=6 SO25 n=12			
	SOO7 n=3 SOO13 n=6 SOO25 n=12			
	SOH7 n=3 SOH13 n=6 SOH25 n=12			
Thiophene7		-4.04	-2.40	-1.88
Thiophene13		-3.92	-2.52	-2.16
Thiophene25		-3.88	-2.57	-2.34
Br7		-4.06	-2.45	-1.94
Br13		-3.93	-2.54	-2.19
Br25		-3.88	-2.58	-2.36
SO7		-4.22	-2.87	-2.27
SO13		-4.03	-2.88	-2.41
SO25		-3.92	-2.88	-2.50
SOO7		-4.28	-3.05	-2.43
SOO13		-4.06	-3.04	-2.53
SOO25		-3.93	-3.04	-2.59
SOH7		-4.05	-2.41	-1.89
SOH13		-3.93	-2.52	-2.17
SOH25		-3.88	-2.57	-2.35

Table S4. Frontier molecular orbital energies and vertical electron affinities for select hydrated oxygen complexes as determined at the B97D/6-311++G** and MP2/6-311++G** levels of theory with the CPCM dielectric model. The complex geometries were taken from Bell, A. J. & Wright, T. G., *Phys. Chem. Chem. Phys.* **6**, 4385-4390 (2004) and Gomes, J. A. G. *et al.*, *Spectrochim. Acta, Part A* **61**, 3082-3086 (2005).



	$\epsilon = 1.0$			$\epsilon = 3.0$		
	HOMO (eV)	LUMO (eV)	VEA (eV)	HOMO (eV)	LUMO (eV)	VEA (eV)
<i>B97D/6-311++G**</i>						
A	-7.20	-0.74	-0.49	-7.21	-0.60	-2.13
B	-7.20	-0.74	-0.53	-7.22	-0.60	-2.15
C	-7.20	-0.73	-0.48	-7.20	-0.59	-2.12
low	-7.20	-0.74	-0.49	-7.21	-0.60	-2.13
C _{2v}	-7.24	-0.77	-0.51	-7.24	-0.61	-2.14
C _s	-7.19	-0.76	-0.57	-7.24	-0.60	-2.17
<i>MP2/6-311++G**</i>						
A	-13.84	1.44	1.43	-13.95	1.52	0.18
B	-13.80	1.35	1.28	-13.93	1.44	0.02
C	-13.84	1.44	1.43	-13.95	1.52	0.18
low	-13.88	1.19	1.15	-13.91	1.35	-0.03
C _{2v}	-13.87	1.49	0.14	-13.95	1.54	-1.54
C _s	-13.59	1.49	-0.80	-13.75	1.58	-2.77