Supporting Information for

Effects of Temperature and Light Illumination on the Current-Voltage Characteristics of Molecular Self-Assembled Monolayer Junctions

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Contents:

1. Representative plots of the I-V temperature dependence based on the hopping conduction, P-F and thermionic emission models, respectively.

Figures S1a-S1d show the plots of I vs V and ln (I/V) vs 1/T, in both dark and light illuminations at given bias (-5 to + 5 V) and at temperature from 91 to 300 K for the DT junction. The plots of I vs V show preferable linear relation in both dark and light conditions at a low bias (- 1 to + 1 V), while the plots of ln (I/V) vs 1/T show nonlinearity both in the dark and under light conditions. So the hopping conduction is not the main charge transport mechanism. Generally, the hopping mechanism is used to explain the charge transport of inorganic or thick organic films. Okada et al. reported electrical stress-induced variable range hopping conduction in ultrathin silicon dioxides.[S1] Reghu et al. investigated the hopping transport of PPy-PF_6 films with thickness of 10 to 20 μm.[S2] In our case, the crossbar junctions are made of SAMs with thickness of about 10-20 Å.

Figures S2a-S2d show the analysis of ln (I/V) vs $V^{1/2}$ and ln (I) vs 1/T, respectively. Apparent nonlinear relationship exhibited both in the dark and under light conditions, suggesting that the P-F emission is not the charge transport mechanism. Moreover, Figures S3a-S3d plot the ln (I/T^2) vs 1/T and ln (I) vs $V^{1/2}$. It is evident to see the nonlinear dependences of the ln (I/T^2) vs 1/T in the dark and the ln (I) vs $V^{1/2}$ under light, respectively. We thus concluded that the thermionic emission may not be the dominant mechanism too.

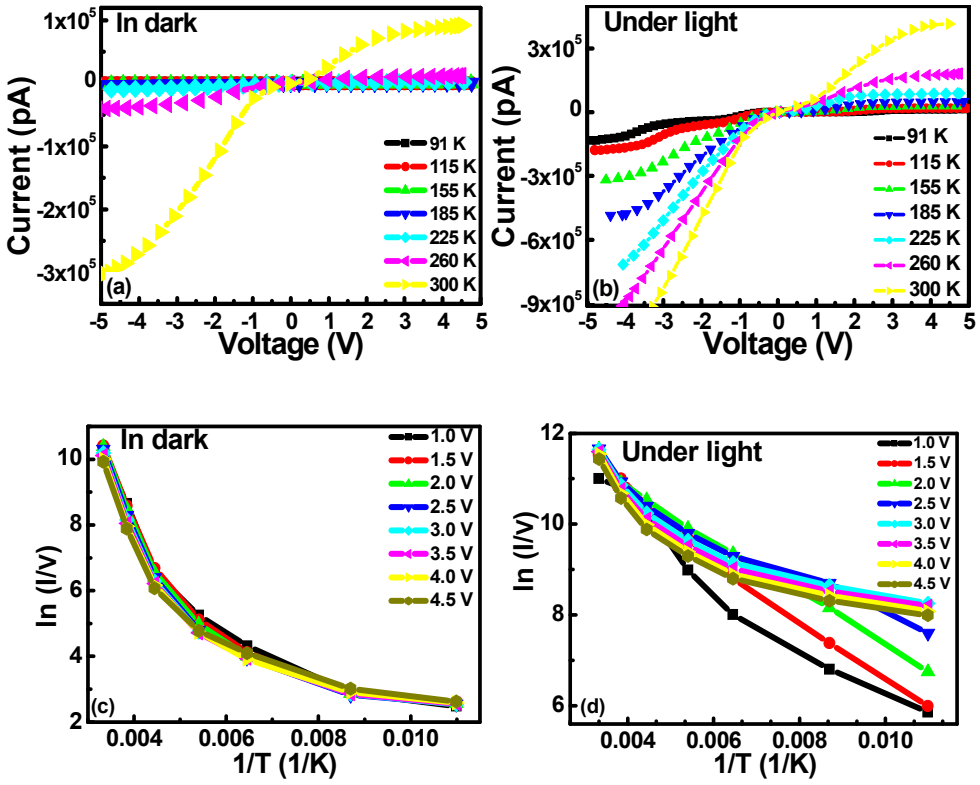

Figure S1. Plots of I vs V at different temperatures (a) in the dark and (b) under light, respectively. Plots of ln (I/V) vs 1/T in the positive bias at different temperatures (c) in the dark and (d) under light situations, respectively.

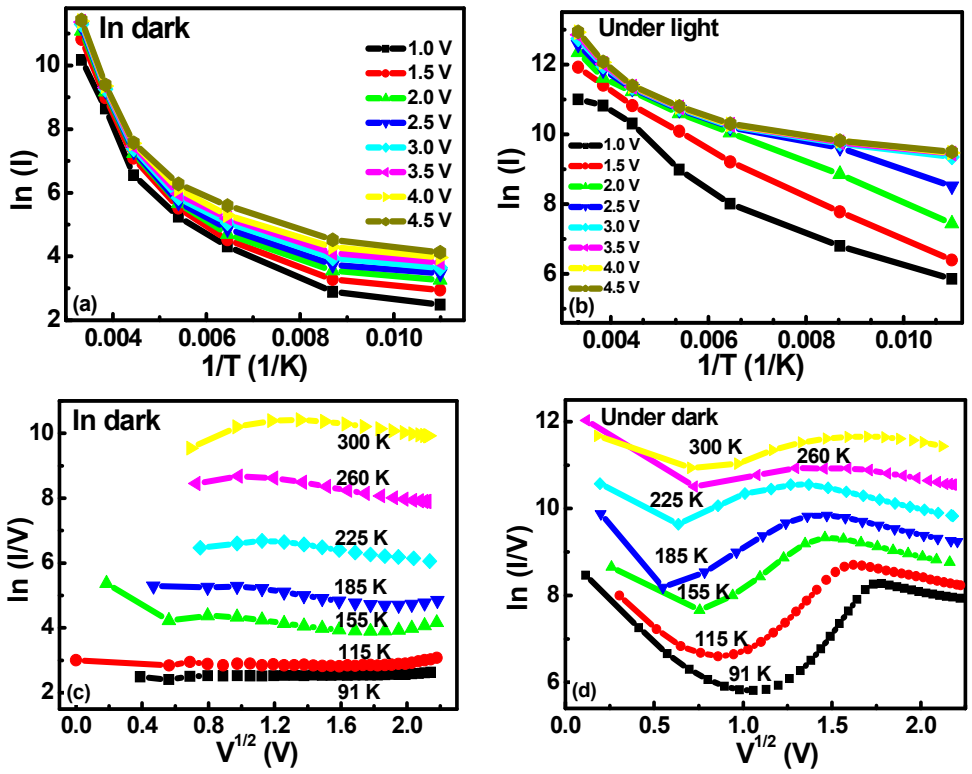

Figure S2. Plots of the ln (I) vs 1/T at different temperatures (a) in the dark and (b) under light, respectively. Plots of the ln (I/V^2) vs $1/V^{1/2}$ in the positive bias at different temperatures (c) in the dark and (d) under light situations, respectively.

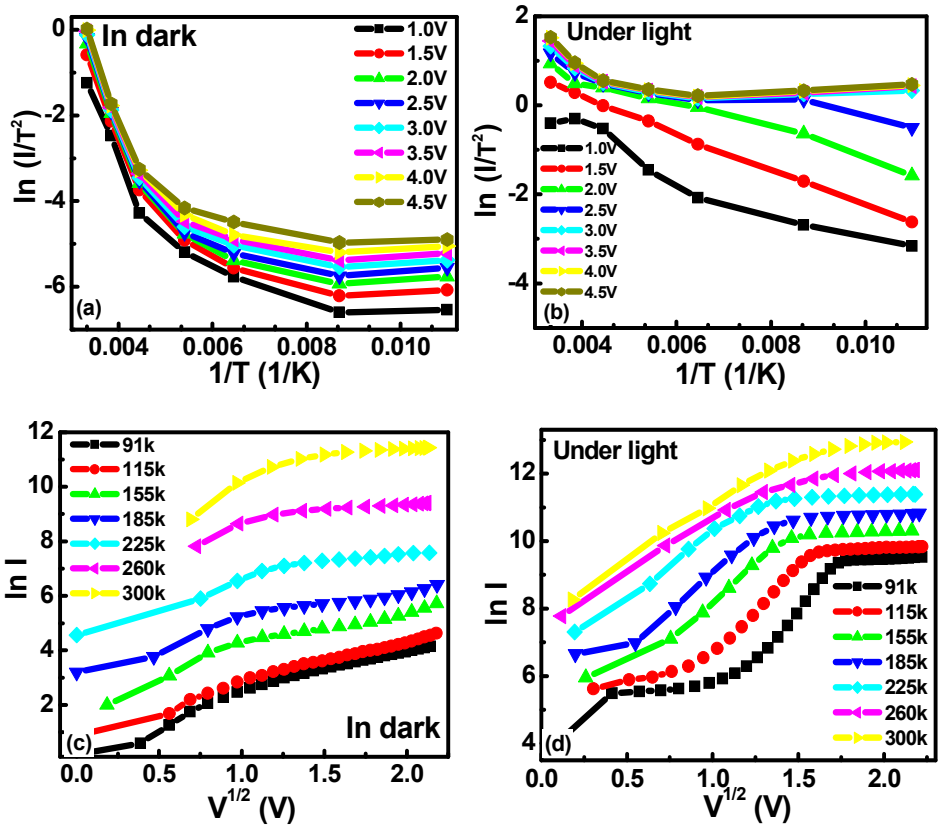

Figure S3. Plots of the ln I/T^2) vs 1/T at different temperatures (a) in the dark and (b) under light, respectively. Plots of the ln (I) vs $V^{1/2}$ in positive bias range at different temperatures (c) in the dark and (d) under light conditions, respectively.

2. Table summarized with the best fitting parameters (α, Φ, β) for the molecules of OT, NDT, DT, DDT, and M-1, respectively, as calculated from the Simmons model.

We simulated the fitting parameters for the molecules of OT, NDT, DT, DDT, and M-**1**, respectively. The Φ and β values for Simmons tunneling through alkanethiol and conjugated molecular junctions depend on the molecular length and/or structure, as shown in Table S1.

Table S1. Summary of the best Simmons fitting parameters for the alkanethiol and conjugated junctions studied at temperature range of 91 to 300 K with α=0.65.

Molecular	Condition	Bias（V）	ϕ (eV)	β($Å^{-1}$)
OT	Dark	0～+1.0	1.69～1.59	0.86±0.01
		-1.0～0	1.62～1.59	
	Light	0～+1.0	1.65～1.62	0.85±0.01
		-1.0～0	1.59～1.52	
NDT	Dark	0～+1.0	1.58～1.48	0.83±0.01
		-1.0～0	1.56～1.47	
	Light	0～+1.0	1.60～1.46	0.83±0.01
		-1.0～0	1.60～1.50	
DT	Dark	0～+1.0	1.50～1.39	0.81±0.01
		-1.0～0	1.47～1.42	
	Light	0～+1.0	1.49～1.39	0.81±0.01
		-1.0～0	1.46～1.33	
DDT	Dark	0～+1.0	1.44～1.38	0.80±0.01
		-1.0～0	1.46～1.41	
	Light	0～+1.0	1.43～1.41	0.80±0.01
		-1.0～0	1.43～1.41	
M-1	Dark	0～+1.0	0.72～0.30	0.56±0.06
		-1.0～0	0.78～1.38	
	Light	0～+1.0	0.46～0.43	0.37±0.02
		-1.0～0	0.59～0.56	

REFERENCES

S1. Okada, K.; Taniguchi, K. *Appl. Phys. Lett.* **1997**, *70*, 351-353.

S2. Yoon, C. O.; Reghu, M.; Heeger, A. J.; Cao, Y.; Chen, T.; Wu, X.; Rieke, R. D. *Synth. Met*. **1995**, *75*, 229-239.