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Molecular Engineering of Conjugated Polymers for Efficient Hole Transport and Defect Passivation in Perovskite Solar Cells

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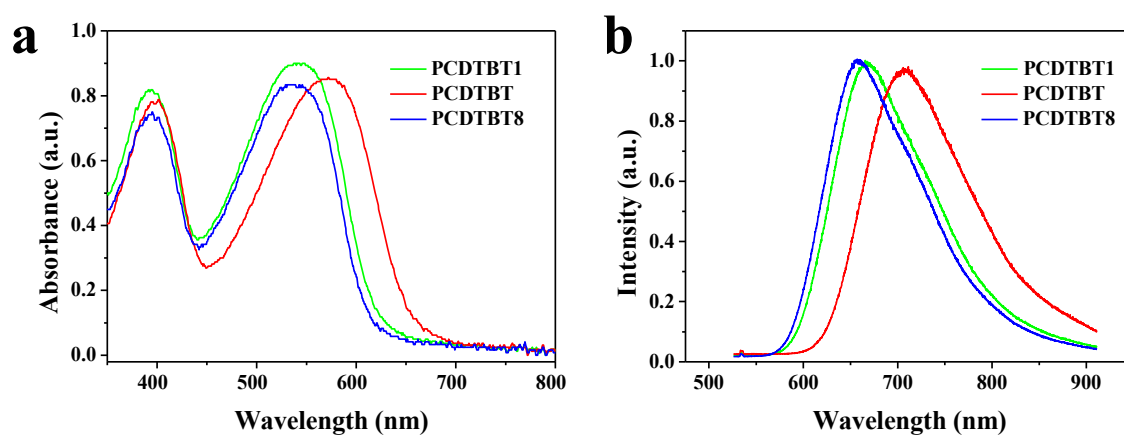


Figure S1. Optical properties of three conjugated polymers. (a) Absorption and (b) photoluminescence (PL) spectra of ITO/PCDTBT1, ITO/PCDTBT and ITO/PCDTBT8.

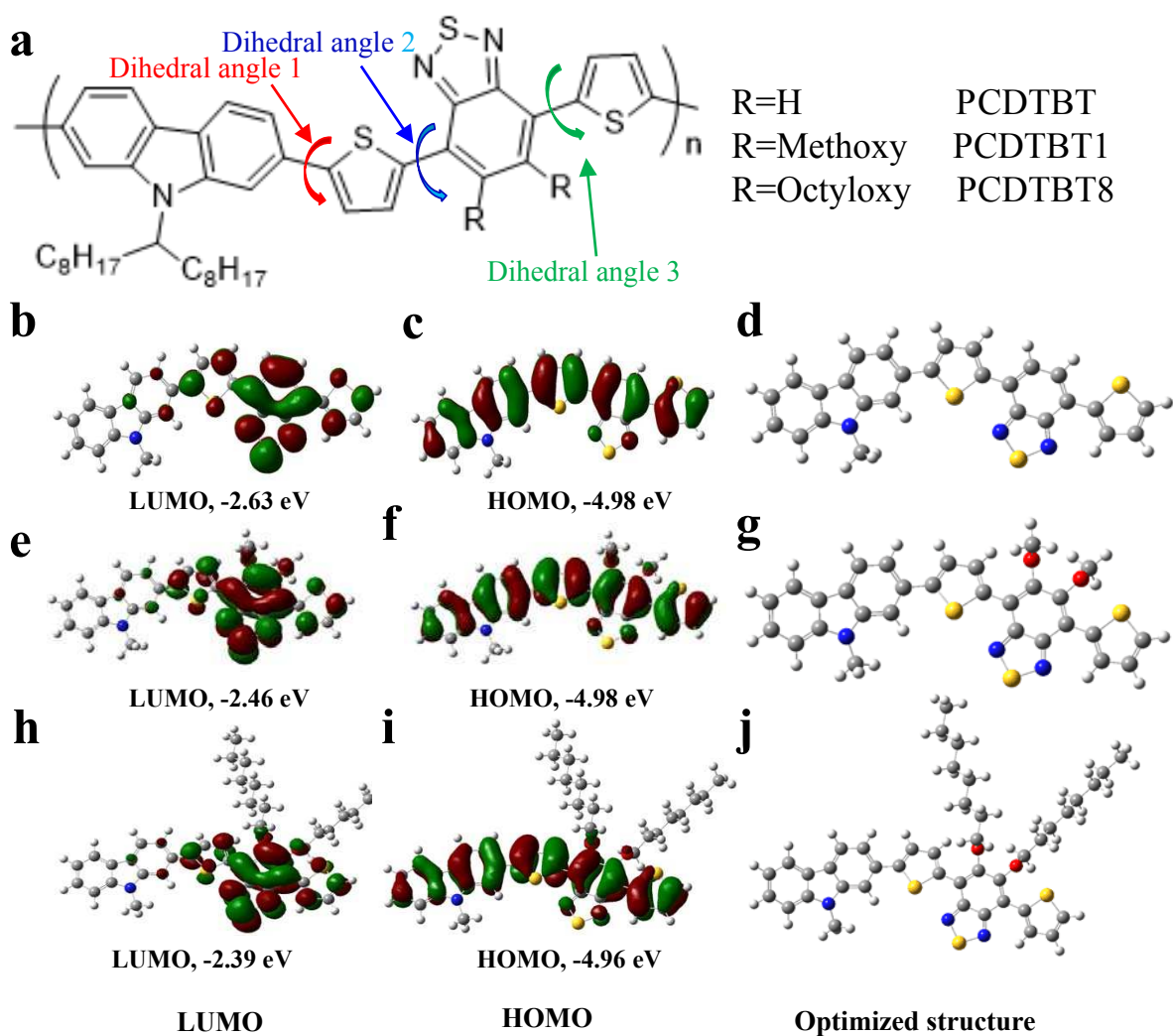


Figure S2. Geometry-optimized structures and frontier molecular orbitals of three conjugated polymers. (a) Chemical structures of conjugated polymers with three dihedral angles. (b-d), (e-g), (h-j) are the electron density distributions of frontier molecular orbitals obtained from DFT calculations and their geometry-optimized structures of the PCDTBT, PCDTBT1 and PCDTBT8, respectively.

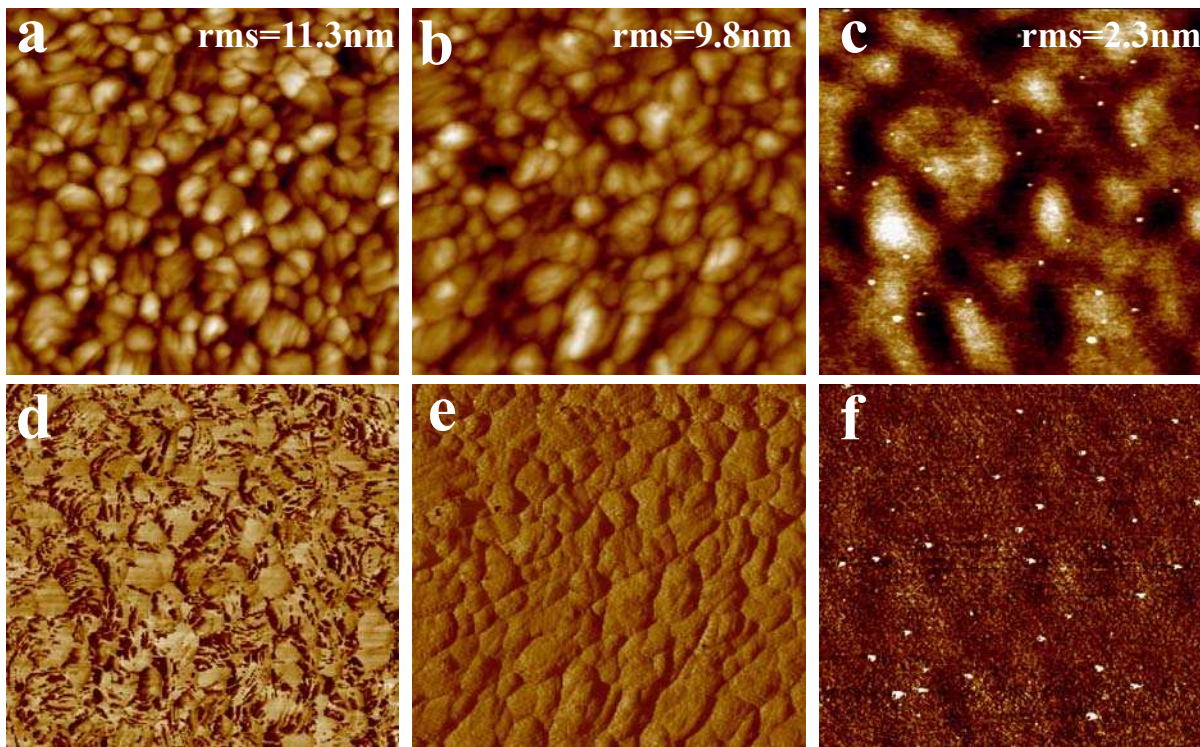


Figure S3. Surface morphology characterization. SPM surface height images from films made of (a) perovskite, (b) perovskite/PCDTBT1 (c) perovskite/Spiro-OMeTAD and (d-f) are the corresponding phase images respectively. Image size is $5\ \mu\text{m} \times 5\ \mu\text{m}$.

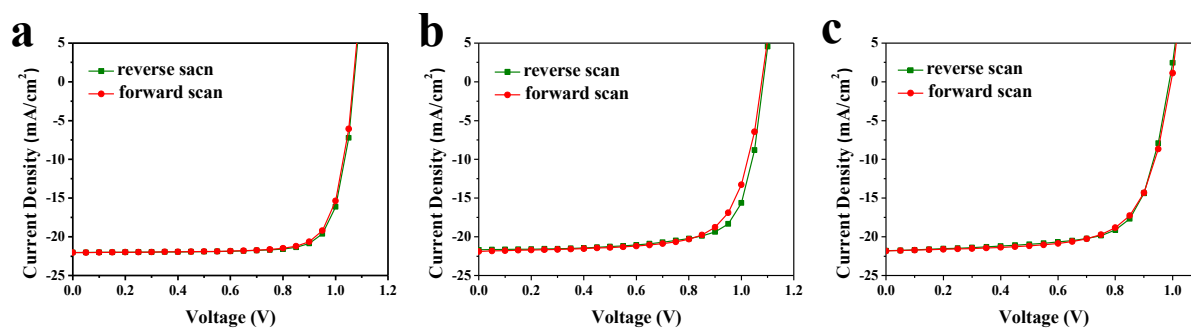


Figure S4. Hysteresis of devices having different HTMs. J - V curves of devices using (a) PCDTBT1, (b) PCDTBT and (c) PCDTBT8 as HTMs.

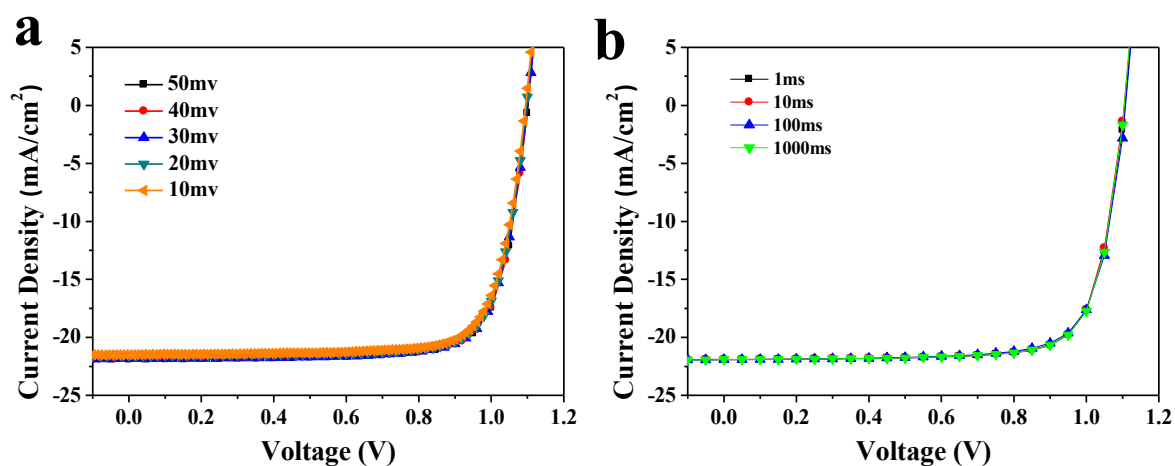


Figure S5. Photovoltaic performance measured under different scan rates and delay times. J - V curves of the same device measured with different (a) scan delay times and (b) voltage step sizes.

Table S1. Device metrics parameters of perovskite solar cells employing different HTMs. The active area is 4 mm^2 for each device.

HTMs	Scan direction	V_{oc} (V)	FF	J_{sc} (mA cm^{-2})	PCE_{ave} (PCE_{max})
PCDTBT	RS	1.04 ± 0.01	71.64 ± 1.15	-21.52 ± 0.24	$16.13 \pm 0.39(16.8)$
	FS	1.04 ± 0.01	71.32 ± 1.35	-21.34 ± 0.36	$16.02 \pm 0.34(16.7)$
PCDTBT1	RS	1.09 ± 0.01	77.12 ± 1.26	-21.65 ± 0.45	$18.42 \pm 0.35(18.9)$
	FS	1.09 ± 0.01	76.98 ± 1.12	-21.52 ± 0.38	$18.32 \pm 0.29(18.6)$
PCDTBT8	RS	1.01 ± 0.01	66.91 ± 1.02	-21.12 ± 0.39	$14.41 \pm 0.37(15.1)$
	FS	1.01 ± 0.01	66.25 ± 0.98	-21.06 ± 0.46	$14.36 \pm 0.46(14.8)$

V_{oc} , open circuit voltage; FF, fill factor; J_{sc} , short-circuit current density; PCE, power conversion efficiency.

Average performance parameters and their S.D. were obtained based on 20 cells for each set.

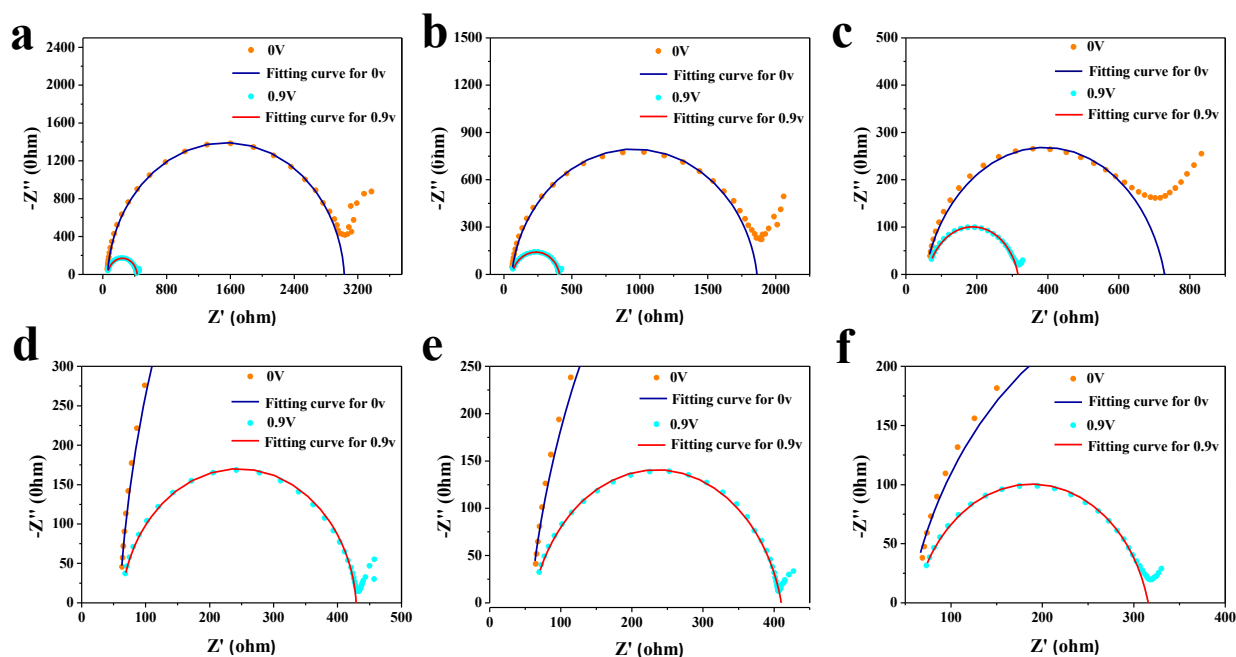


Figure S6. Nyquist plots of devices with different HTMs. (a), (b) and (c) correspond to EIS measurements under 1-sun illumination incorporating PCDTBT1, PCDTBT and PCDTBT8 as the HTMs, respectively. (d), (e) and (f) are zoomed-in on the low impedance region for (a), (b) and (c) respectively to show the results at 0.9 V applied bias clearly.

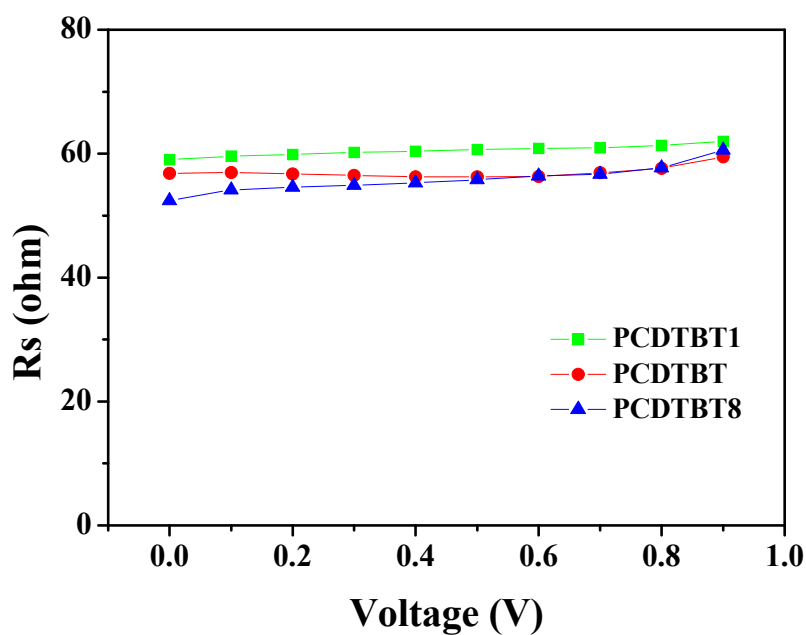


Figure S7. The R_s values of devices employing different HTMs obtained from fitting the

results through the equivalent circuit.

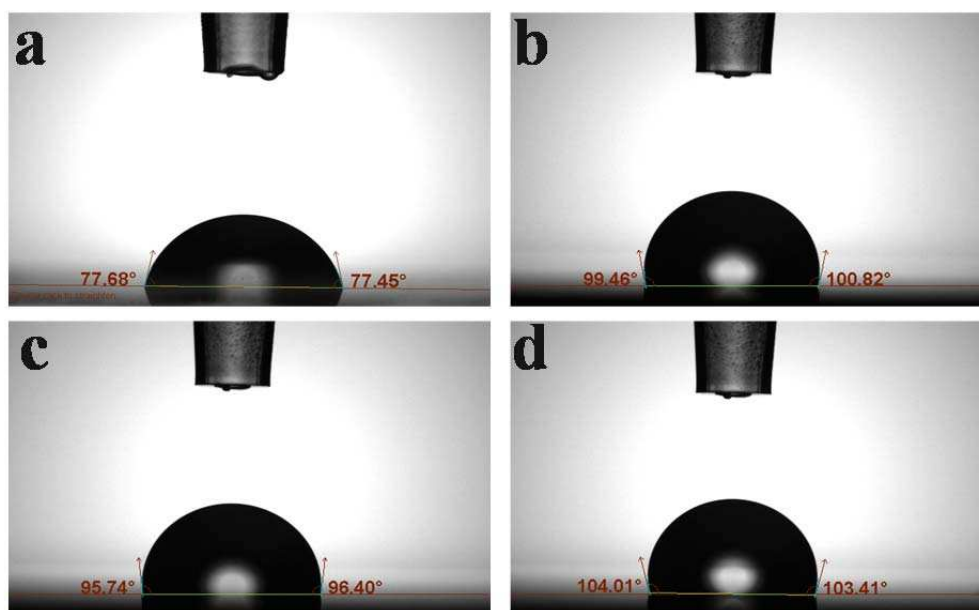


Figure S8. Surface hydrophobicity analysis. The water contact angle images of (a) spiro-OMeTAD, (b) PCDTBT, (c) PCDTBT1 and (d) PCDTBT8.

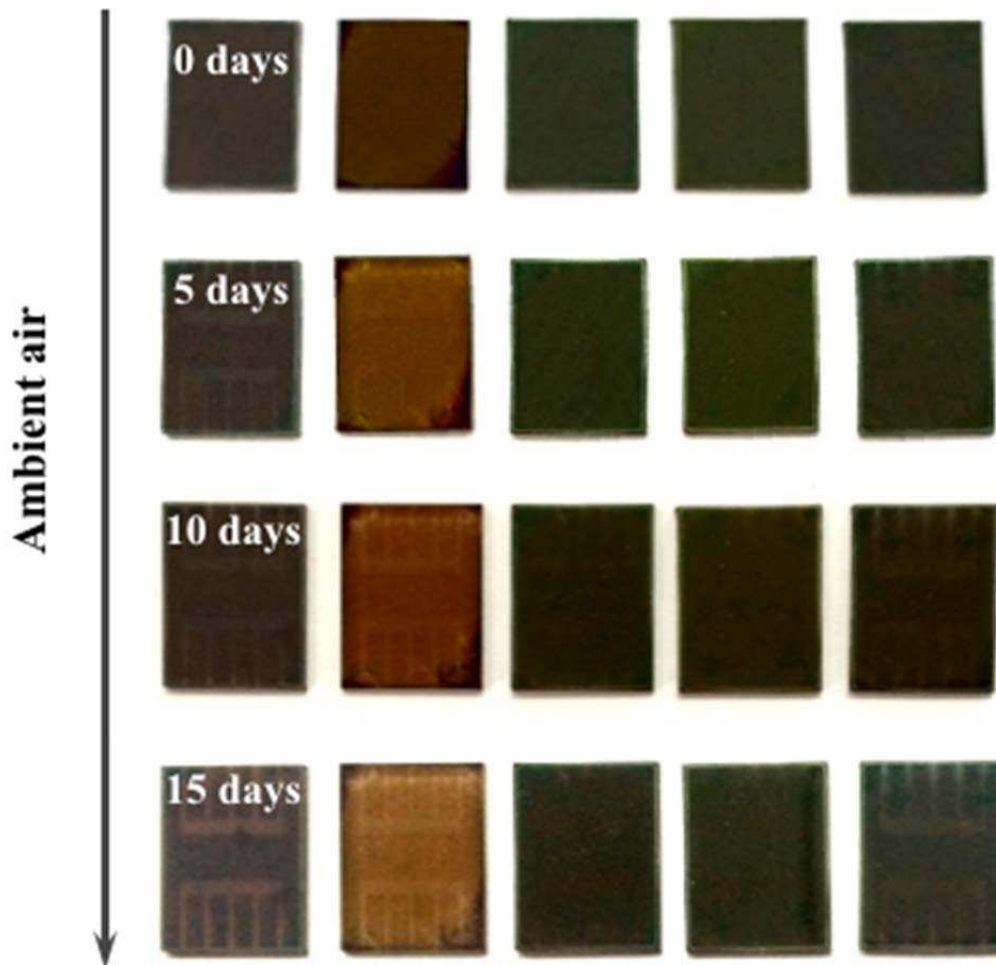


Figure S9. Stability test of perovskite devices. Images of perovskite, perovskite/ spiro-OMeTAD, perovskite/PCDTBT1, perovskite/PCDTBT and perovskite/PCDTBT8 (from left to right, respectively) films under different durations of exposure in ambient (40~70 RH%).