Electronic Supplementary Information for Journal of Materials Chemistry A

Electronic Supplementary Information

High efficiency aqueous-processed MEH-PPV/CdTe Hybrid solar cells with a PCE of 4.20%

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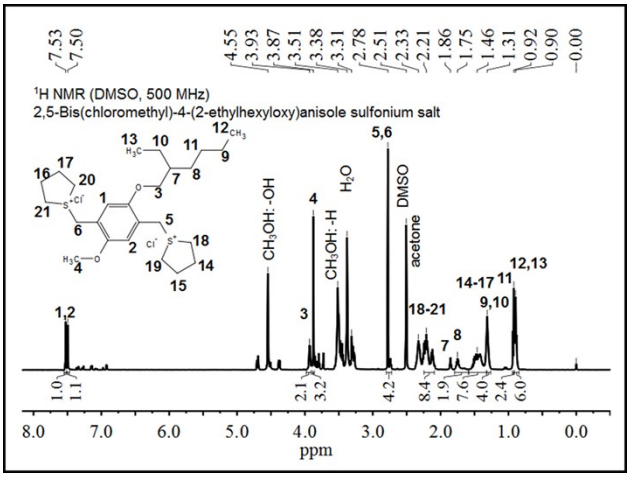

Fig. S1 The ^{1}H NMR spectrum and structure of 2,5-Bis(chloromethyl)-4-(2-ethylhexyloxy)anisole sulfonium salt (DMSO, 500 MHz).

The 2,5-Bis(chloromethyl)-4-(2-ethylhexyloxy)anisole sulfonium salt characterization: ^{1}H NMR (DMSO, 500 MHz, δ, ppm): 7.53 (s, 1H), 7.50 (s, 1H), 3.94 (s, 2H), 3.88 (s, 3H), 2.78 (s, 4H), 2.21 (s, 8H), 1.86 (s, 1H), 1.75 (s, 2H), 1.46 (s, 8H), 1.31 (s, 4H), 0.92 (s, 2H), 0.90 (s, 6H).

The ^{1}H NMR spectrum and structure of sulfonium salt were shown in Fig. S1. The signals around 7.50 and 7.53 ppm were attributed to the hydrogen atoms in phenyl. The characteristic peaks around 3.88-3.94 ppm were assigned to the protons in the alkoxy adjacent to oxygen atoms. The appearance of a singlet at 2.78 ppm was assigned to the hydrogen atoms in the methylene bonded to benzene ring. The signals around 1.86, 1.75, 1.31, 0.90 and 0.92 ppm were attributed to the protons assigned to the protons in hexyloxy. The multiplets around 2.21 and 1.46 ppm were assigned to the hydrogen atoms in tetrahydrothiophene rings. Other peaks are assigned to the solvents of reactions.

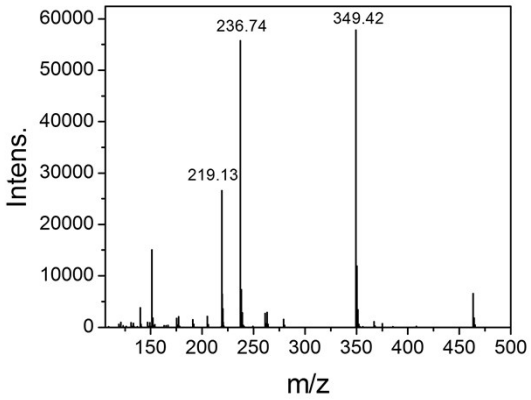

Fig. S2 The mass spectrometer of 2,5-Bis(chloromethyl)-4-(2-ethylhexyloxy)anisole sulfonium salt.

The mass spectra result shows a strong peak at m/z is 219.13. Because 2,5-Bis(chloromethyl)-4-(2-ethylhexyloxy)anisole sulfonium salt molecular has two positive charges. the molecular weight of sulfonium salt is 438 $g \cdot mol^{-1}$, which is matched with standard molecule.

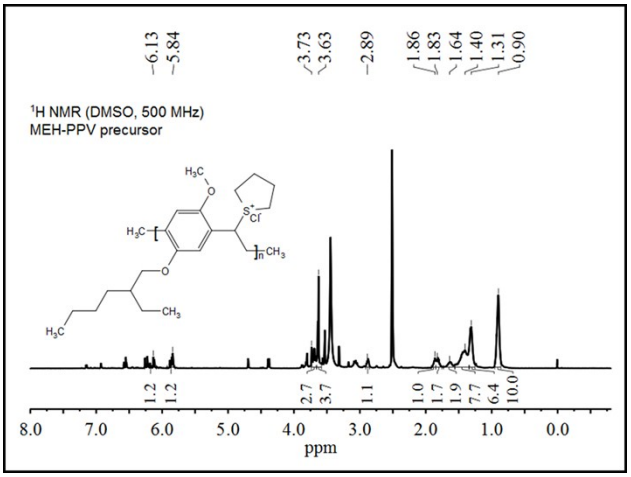

Fig. S3 The ^{1}H NMR spectrum and structure of MEH-PPV precursor (DMSO, 500 MHz).

The MEH-PPV precursor characterization: ^{1}H NMR (DMSO, 500 MHz, δ, ppm): 6.13 (s, 1H), 5.84 (s, 1H), 3.73 (s, 3H), 3.63 (s, 4H), 2.89 (s, 1H), 1.86 (s, 1H), 1.83 (s, 2H), 1.64 (s, 2H), 1.40 (s, 8H), 1.31 (s, 6H), 0.90 (s, 10H).

As for MEH-PPV precursor, the ^{1}H NMR spectrum and structure are shown in Fig. S3. The signals around 5.84 and 6.13 ppm were attributed to the hydrogen atoms in phenyl. The characteristic peaks around 3.63-3.73 ppm were assigned to the protons in the alkoxy adjacent to oxygen atoms. The appearance of peaks at 2.89 and 1.64 ppm were assigned to the hydrogen atoms in the methylene bonded to benzene ring. The signals around 1.86, 1.83, 0.90 ppm were attributed to the protons assigned to the protons in hexyloxy. The signals around 1.31 ppm were attributed to the hydrogen atoms in the methyl terminal groups. The multiplets around 1.40 ppm were assigned to the hydrogen atoms in THT rings. Other peaks are assigned to the solvents of reactions.

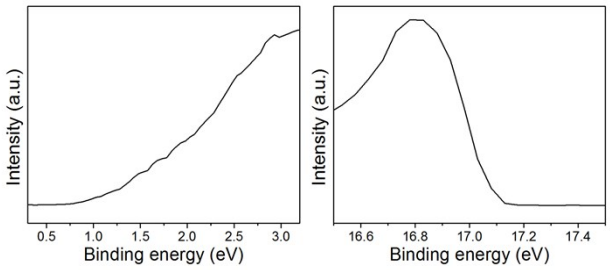

Fig. S4 Ultraviolet photoelectron spectra of MEH-PPV. Based on the intersection of baseline with the tangent line of the spectra, the HOMO energy levels of MEH-PPV is determined as -5.22 eV.

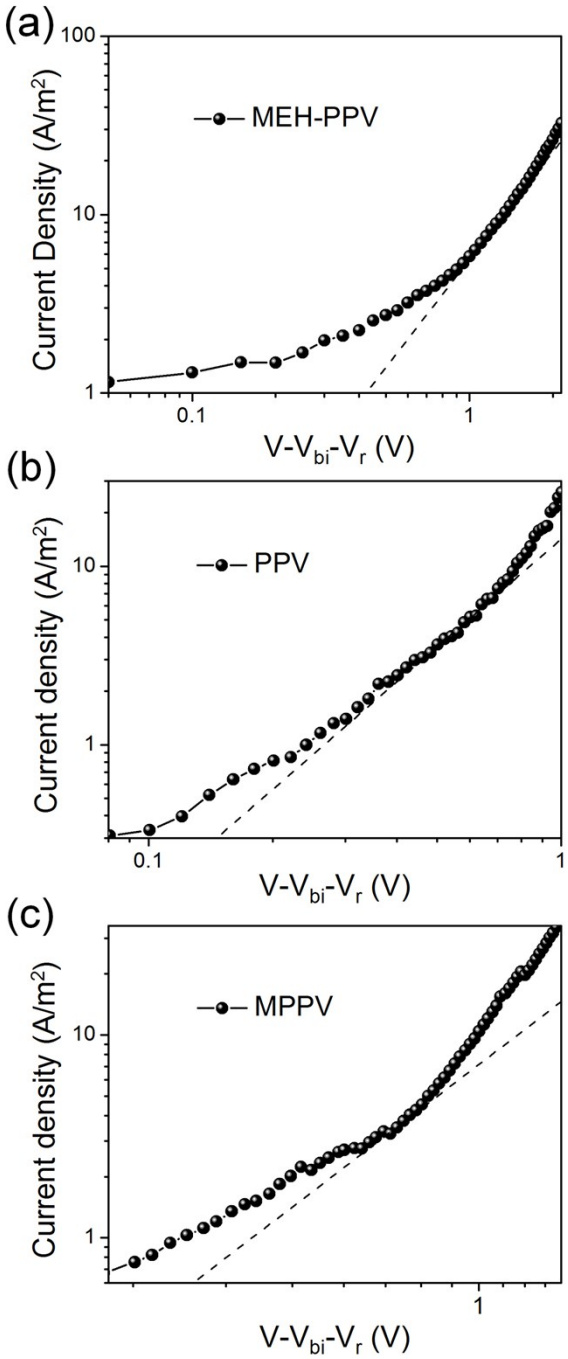

Fig. S5 *J-V* characteristics of the hole-only devices. (a) MEH-PPV film. (b) PPV film. (c) MPPV film. The slope of the tangent line equals 2.

The carrier mobility is calculated according to equation (1)

$$J=9\varepsilon_0\varepsilon_r\mu(V-V_{bi}-V_r)^2/8L^3 \quad (1)$$

where ε_0 is the permittivity of free space, ε_r is the dielectric constant of MEH-PPV (assumed as 3), μ is the hole mobility, V is the applied voltage, V_r is the voltage drop due to contact resistance and series resistance across the electrodes, V_{bi} is the built-in voltage, and L is the film thickness. By SCLC method, the hole mobility of MEH-PPV, PPV and MPPV are measured as 3.29×10^{-6} $cm^2V^{-1}s^{-1}$, 4.70×10^{-5} $cm^2V^{-1}s^{-1}$ and 1.07×10^{-5} $cm^2V^{-1}s^{-1}$ respectively.

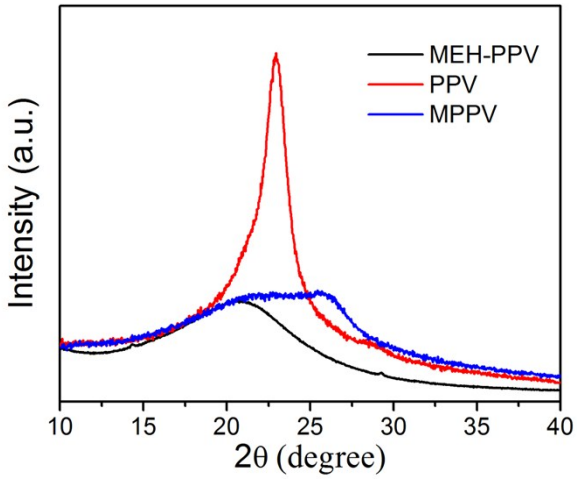

Fig. S6 X-ray diffraction spectrum of MEH-PPV, PPV and MPPV films.

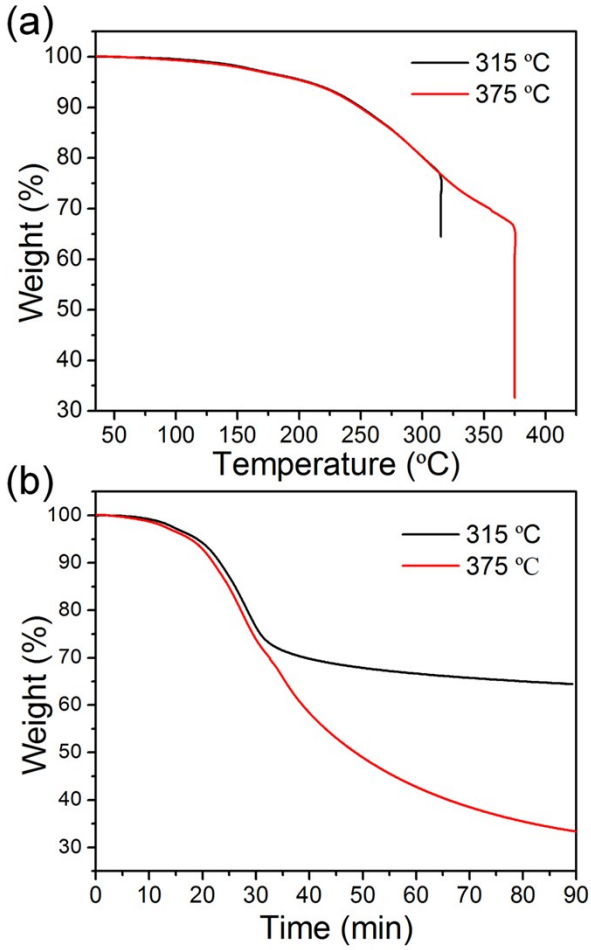

Fig. S7 TGA curves of MEH-PPV precursor at 315 ºC and 375 ºC. (a) Temperature-weight curves. (b) Time-weight curves.

Firstly, MEH-PPV precursor is annealed from room temperature (25 ºC) to 315 ºC or 375 ºC for 10 ºC/min. Secondly, the precursor is annealed at 315 ºC or 375 ºC for 1h. From TGA curves in Fig. S6, after 90 min, the weight of MEH-PPV precursor is about 65 % at 315 ºC, which represents HCl and tetrahydrothiophene (THT) is eliminated. At 375 ºC, the weight of MEH-PPV precursor is about 30 %, which represents the polymer is decomposed.

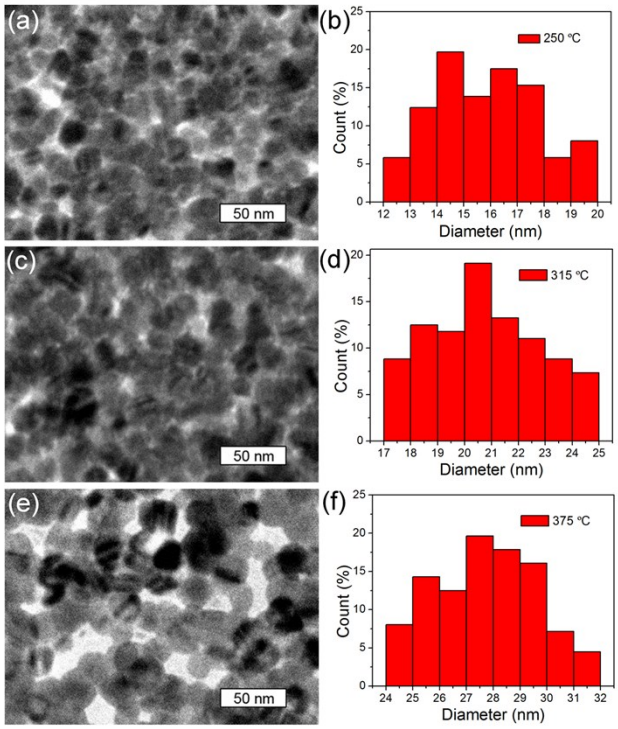

Fig. S8 TEM images of MEH-PPV:CdTe films after annealing at (a) 250 °C, (c) 315 °C and (e) 375 °C for 1 h. And corresponding size distribution of CdTe in MEH-PPV:CdTe films after annealing at (b) 250 °C, (d) 315 °C and (f) 375 °C for 1 h.