

Supplementary Information

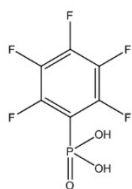
Efficient Hole Transport Layers with Widely Tunable Work Function for Deep HOMO Level Organic Solar Cells

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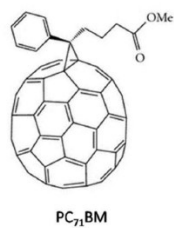
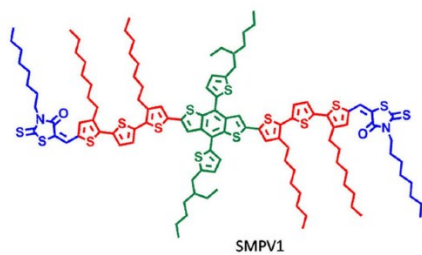


Fig. S1. Molecular structure of a) F5BnPA, b) SMPV1 and PC₇₁BM.

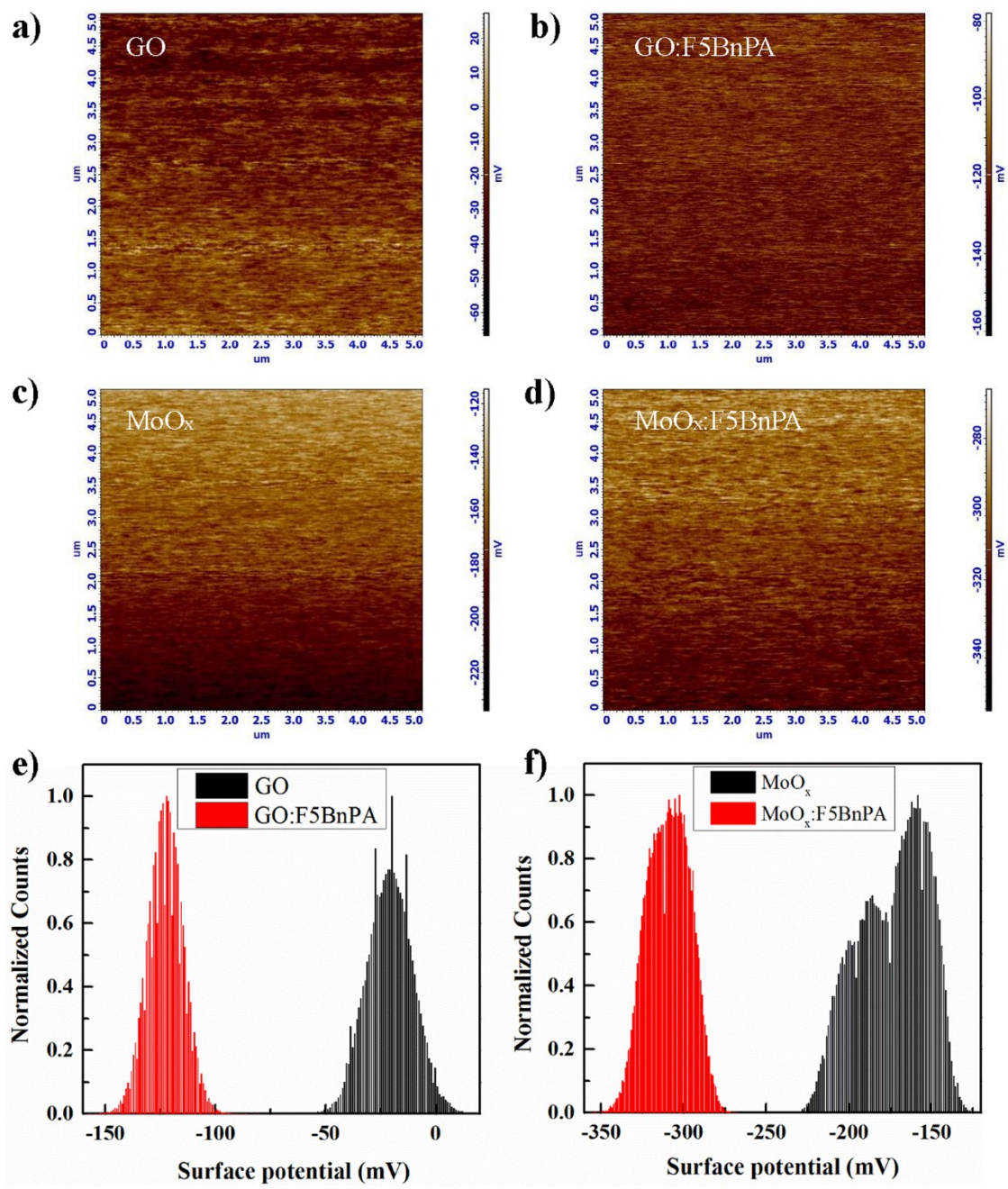


Fig. S2 Surface potential images of a) GO, b) GO:F5BnPA, c) MoO_x, d) MoO_x:F5BnPA. e-f) corresponding pixel analysis.

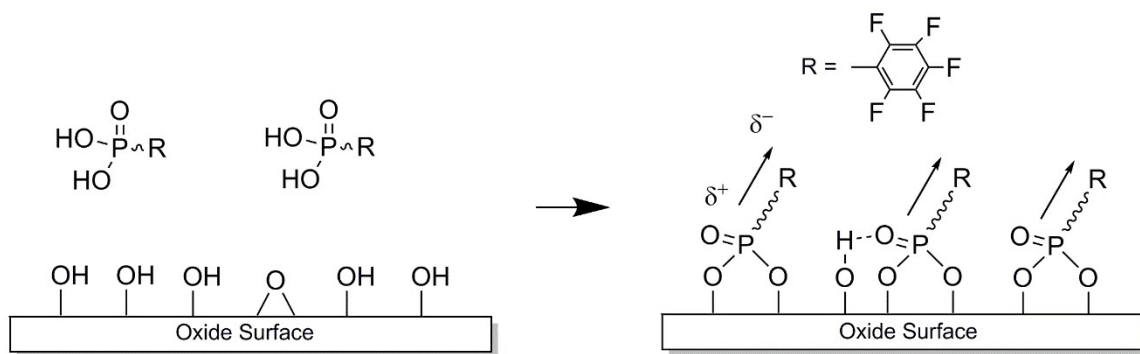


Fig. S3 Schematic of chemisorption of F5BnPA on oxide surface and dipole moment.

The thickness of GO and MoO_x are optimized through P3HT:PCBM based OSCs. The device structure is ITO/GO or MoO_x/P3HT:PCBM/Ca/Al. The devices are fabricated according to the details in the experimental section. The GO solution is diluted into a series of concentration (0.8, 0.6, 0.4, 0.2, 0.1 mg mL⁻¹). The synthesized molybdenum bronze solution is diluted by ethanol in a series of v/v ratio (1:2.5, 1:5, 1:7.5, 1:10, 1:12.5). The optimized concentration of GO solution in ethanol was 0.2 mg mL⁻¹, and the optimized ratio of molybdenum bronze solution was 1:7.5. The respective thickness are 2 nm and 8 nm, as measured by ellipsometer.

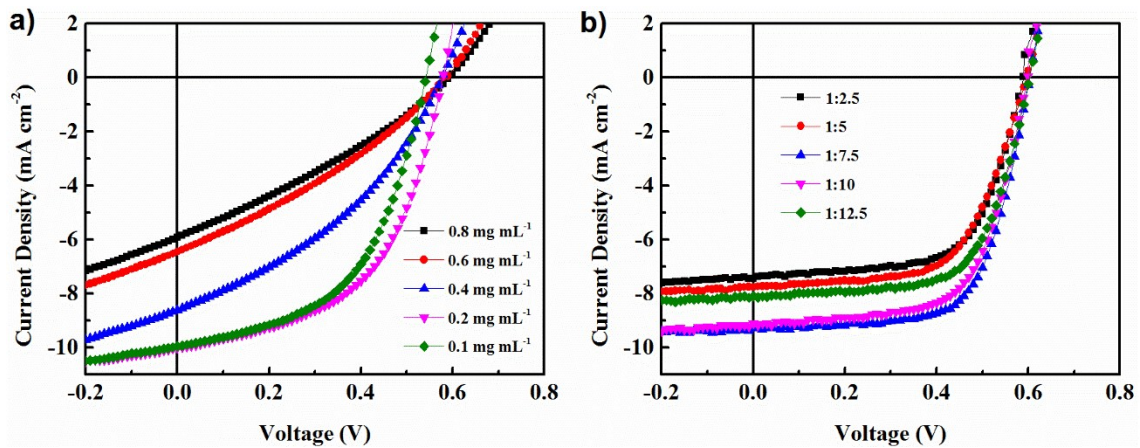


Fig. S4. *J-V* characteristics of P3HT:PCBM based OSCs using different thickness of a) GO and b) MoO_x.

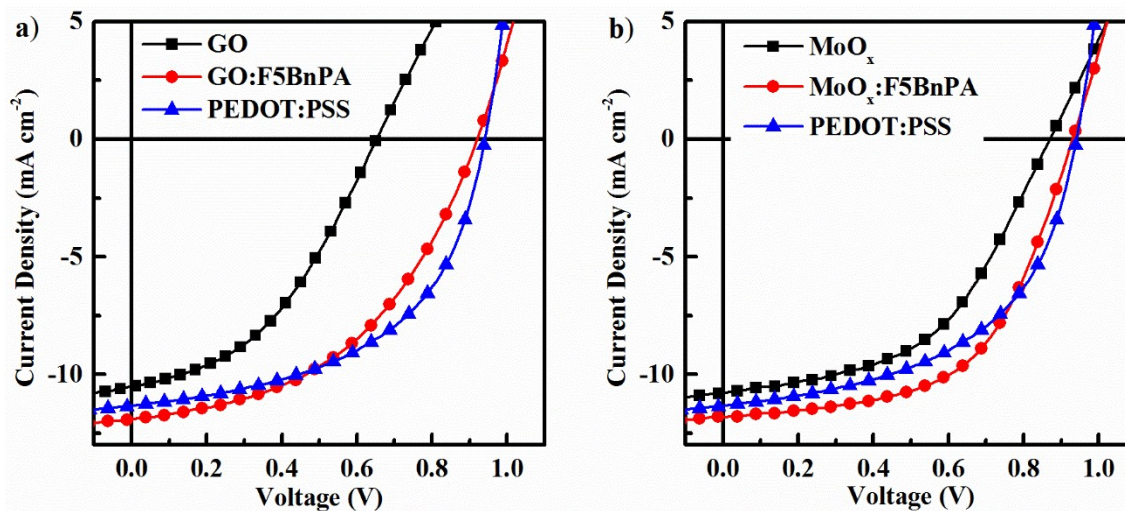


Fig. S5. J - V characteristics of P3HT:PCBM based OSCs using different HTLs (the concentrations of F5BnPA are both 0.5 mg mL^{-1}) under illumination of simulated 100 mW cm^{-2} AM 1.5G irradiation.

Table S1. Device performance of OSCs with the structure of ITO/HTL/SMPV1:PC₇₁BM/Ca/Al.

	J_{sc} (mA cm^{-2})	V_{oc} (V)	FF (%)	PCE (%)
GO	11.03 ± 0.27	0.65 ± 0.01	43.28 ± 0.76	3.10 ± 0.14
GO:F5BnPA	11.96 ± 0.11	0.92 ± 0.01	46.59 ± 1.00	5.13 ± 0.18
MoO _x	10.96 ± 0.20	0.88 ± 0.01	50.81 ± 0.30	4.92 ± 0.10
MoO _x :F5BnPA	11.69 ± 0.27	0.91 ± 0.01	55.92 ± 0.90	5.96 ± 0.19
PEDOT:PSS	11.27 ± 0.47	0.94 ± 0.01	52.42 ± 2.40	5.54 ± 0.30

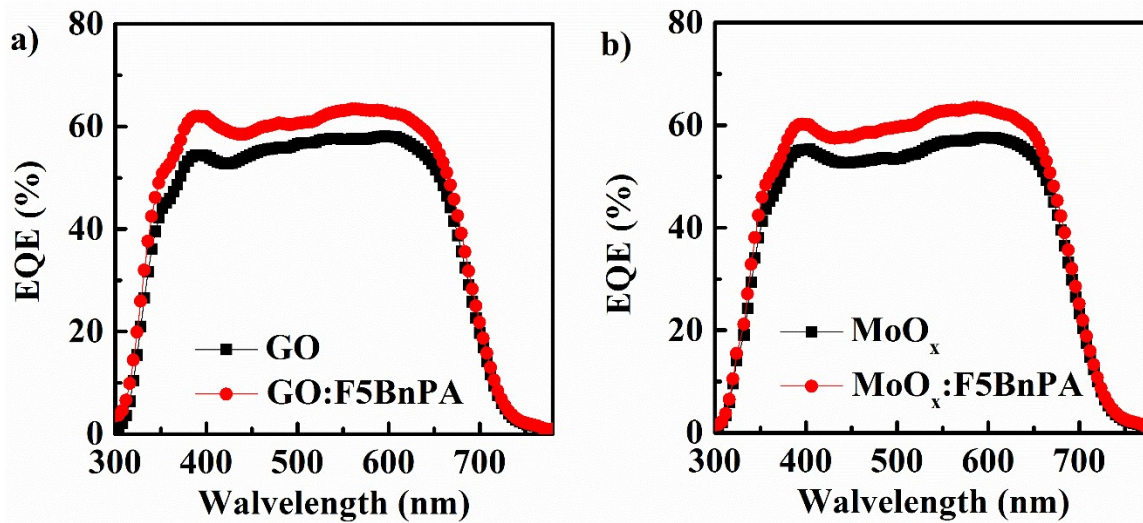


Fig. S6. EQE of the OSC structure of ITO/HTLs/Active layers/Ca/Al.

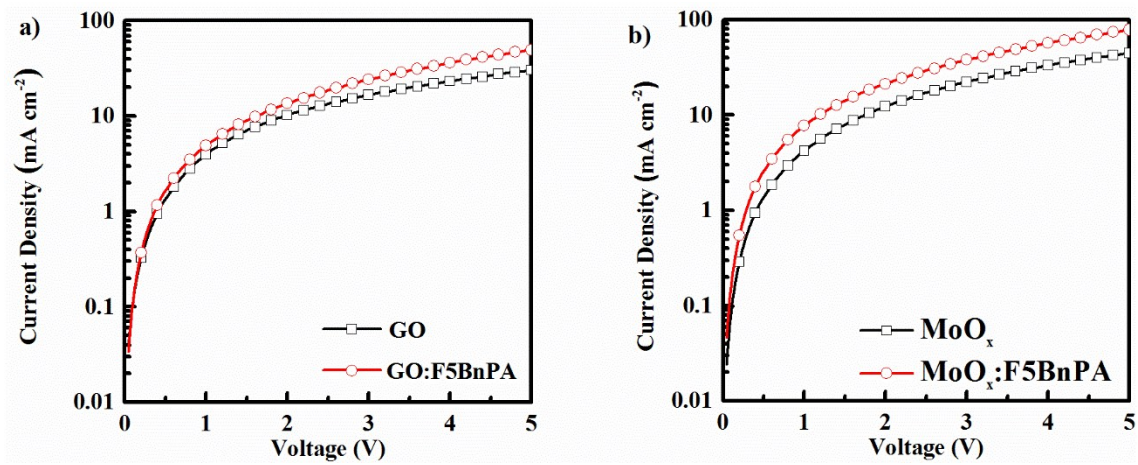


Fig. S7. J-V characteristics of hole only devices with the structure of ITO/HTL/SMPV1:PC₇₁BM/MoO_x/Ag.