

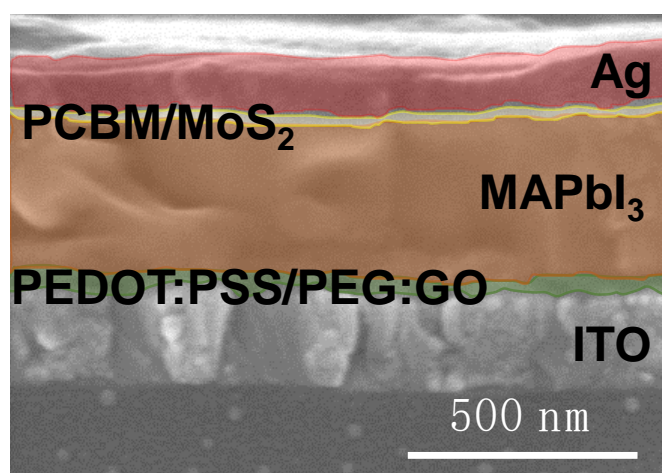
**Supplementary Information**  
**For Journal of Materials Chemistry A**

**Largely Enhanced  $V_{OC}$  and Stability in Perovskite Solar  
Cells with Modified Energy Match by Couple 2D Interlayers**

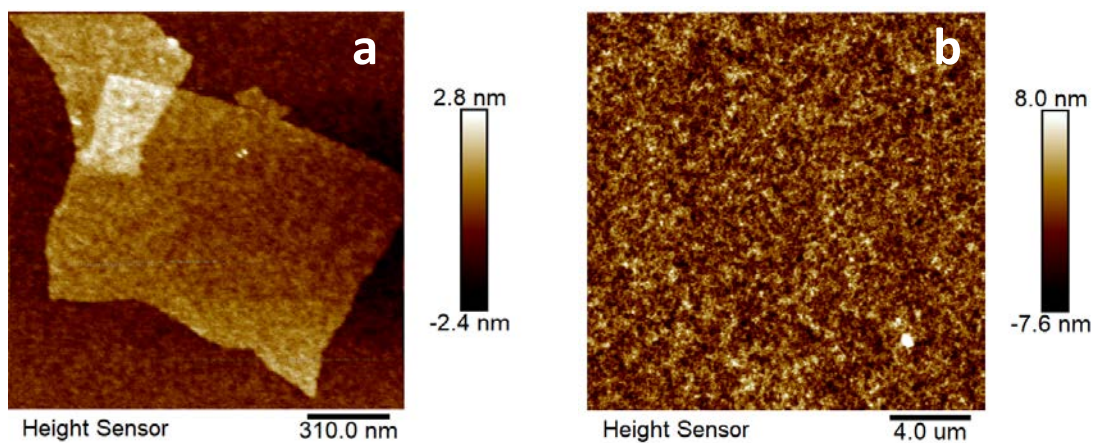
Yangyang Wang<sup>a</sup>, Sen Wang<sup>a</sup>, Xi Chen<sup>a</sup>, Zengrong Li<sup>a</sup>, Jie Wang<sup>a</sup>, Tianhao Li<sup>a</sup>,  
Xianyu Deng<sup>a\*</sup>

<sup>a</sup> Research Center for Advanced Functional Materials and Devices, Shenzhen Key  
Laboratory of Advanced Materials, School of Materials Science and Engineering,  
Harbin Institute of Technology, Shenzhen, 518055, China.

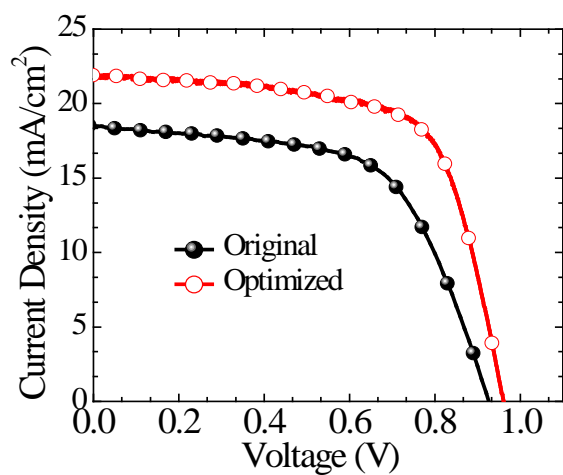
Email: xydeng@hit.edu.cn



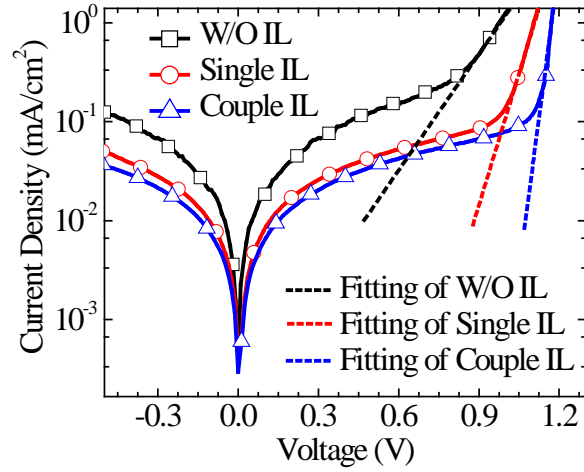
**Fig. S1.** Cross section SEM image of devices with both of MoS<sub>2</sub> and PEG:GO interfaces.



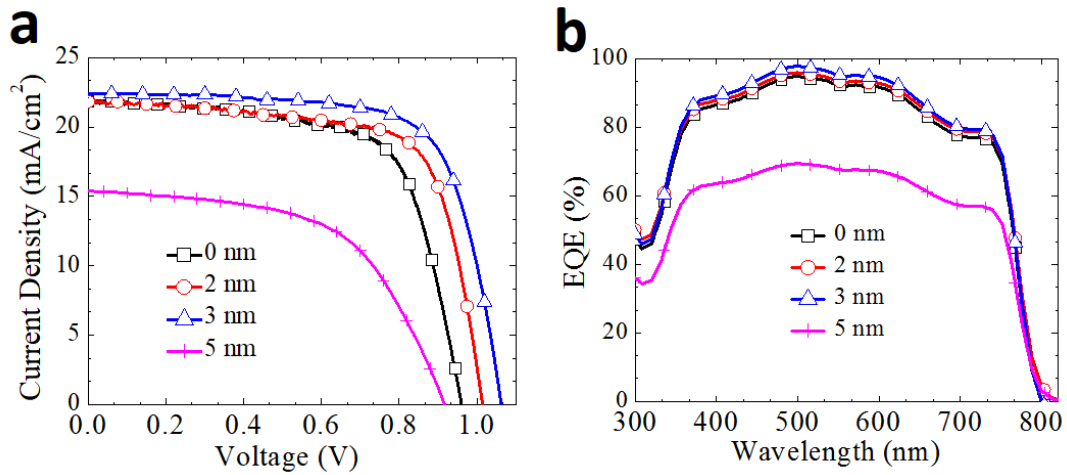
**Fig. S2.** The AFM images of PEG:GO/PEDOT:PSS (a) and 3 nm MoS<sub>2</sub> (b) films deposited on the underlayers.



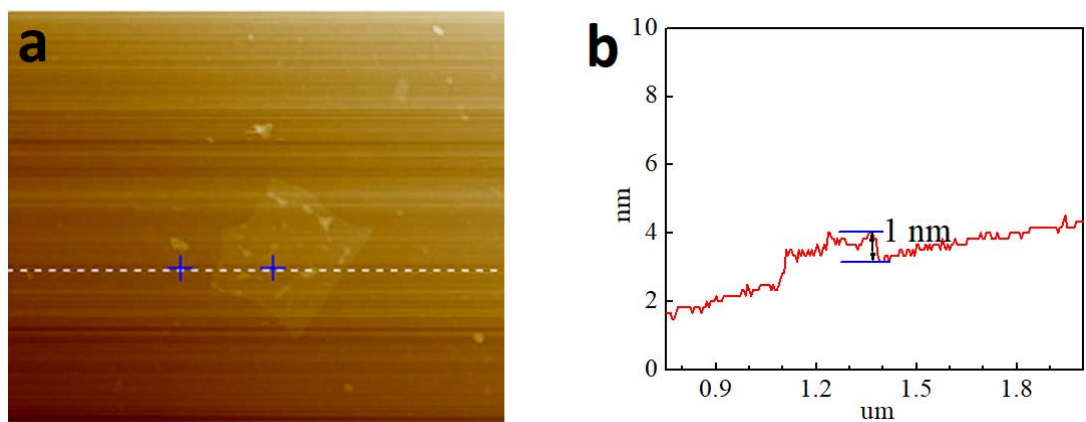
**Fig. S3.** J-V curves of devices based on films prepared via the original process in our earlier work and the optimized process in this work.



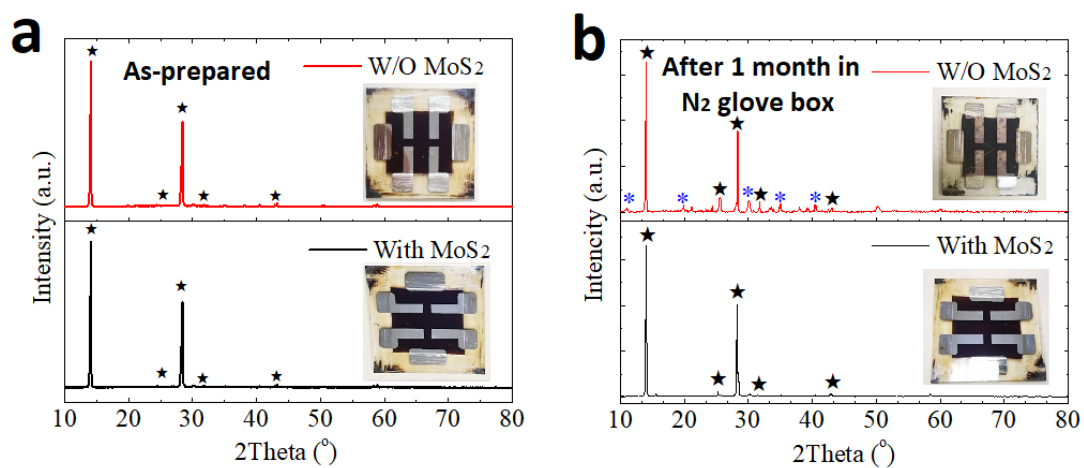
**Fig. S4.** J-V curves of devices with different ILs in the dark.



**Fig. S5.** MoS<sub>2</sub> thickness-dependent device performances. Current density–voltage (J–V) (a) and EQE (b) characteristics of devices modified by MoS<sub>2</sub> with different thickness of 0, 2, 3 and 5 nm.



**Fig. S6.** AFM image (a) and section profiles (b) of PEG:GO films deposited on PEDOT:PSS.



**Fig. S7.** The aging test for devices modified without or with MoS<sub>2</sub> films. (a) The XRD spectrum of perovskite films in as-prepared devices shown in inserted figures. (b) The XRD spectrum of perovskite films in devices that were stored for 1 month in glove box shown in inserted figures.

**Tab. S1.** Different performances of devices based on films prepared via the original process and optimized in later work.

<b>Device</b>	<b>V<sub>oc</sub> (V)</b>	<b>J<sub>sc</sub> (mA/cm<sup>2</sup>)</b>	<b>FF (%)</b>	<b>PCE (%)</b>
<b>Original</b>	0.923	18.501	60.8	10.38
<b>Optimized</b>	0.962	21.743	67.6	14.15

**Tab. S2.** The parameters of ITO/PEDOT:PSS/MAPbI<sub>3</sub>/PCBM/MoS<sub>2</sub>/Ag devices with different thickness of the MoS<sub>2</sub> layer.

<b>Thickness of MoS<sub>2</sub></b>	<b>V<sub>oc</sub> (V)</b>	<b>J<sub>sc</sub> (mA/cm<sup>2</sup>)</b>	<b>FF (%)</b>	<b>PCE (%)</b>
<b>0 nm</b>	0.962	21.743	67.6	14.15
<b>2 nm</b>	1.017	21.814	70.4	15.62
<b>3 nm</b>	1.062	22.423	71.0	16.89
<b>5 nm</b>	0.917	15.392	56.2	7.94

**Tab. S3.** EIS parameters for the electrode films shown in Figure 5 (a, b).

<b>Electrode Film</b>	<b>R<sub>s</sub> (Ω)</b>	<b>R<sub>1</sub> (Ω)</b>
<b>PEDOT:PSS film without GO:PEG</b>	30	1660
<b>PEDOT:PSS film with GO:PEG</b>	20	2970
<b>Ag film without MoS<sub>2</sub></b>	17	790
<b>Ag film with MoS<sub>2</sub></b>	9	1390

**Tab. S4.** PL life times fitted by a bi-exponential decay model for the data in Figure 5 (c, d).

Electrode Film	$\tau_1$ (ns)	$\tau_2$ (ns)
ITO/ PEDOT:PSS/MAPbI <sub>3</sub>	4.4	35.2
ITO/ PEDOT:PSS/GO:PEG/MAPbI <sub>3</sub>	1.8	15.2
MAPbI <sub>3</sub> /PCBM/MoS <sub>2</sub> /Ag	3.9	30.4
MAPbI <sub>3</sub> /PCBM/Ag	1.0	12.2

**Tab. S5.** A comparison of performances obtained using halide perovskites MAPbI<sub>3</sub> in inverted planar heterojunction perovskite solar cells with different cathode metals reported in our work and others.

Cathode Metal	Work	Voc (V)	Jsc (mA·cm <sup>-2</sup> )	FF	PCE (%)	ETL	Perovskite	HTL	Reference
	Function of Cathode Metal								
Ag	4.7	1.135	22.834	0.73	19.14	PCBM/MoS <sub>2</sub>	MAPbI <sub>3</sub>	PEDOT:PSS	Our
Al	4.3	1.132	22.850	0.73	18.88	PCBM/MoS <sub>2</sub>	MAPbI <sub>3</sub>	PEDOT:PSS	Work
Al	4.3	0.98	19.8	0.70	13.58	ICBA/C60/BCP	MAPbI <sub>3</sub>	PTAA	
Cu	4.6	1.03	19.8	0.73	14.88	ICBA/C60/BCP	MAPbI <sub>3</sub>	PTAA	[1]
Au	5.1	0.98	19.8	0.63	12.22	ICBA/C60/BCP	MAPbI <sub>3</sub>	PTAA	

## References

- (1) Y. Deng, Q. Dong, C. Bi, Y. Yuan, J. Huang, Adv. Energy Mater. 6 (2016) 1600372.