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Supporting Information

Effects of Self-Assembled Monolayer Modification of Nickel Oxide Nanoparticles Layer on the Performance and Application of Inverted Perovskite Solar Cells

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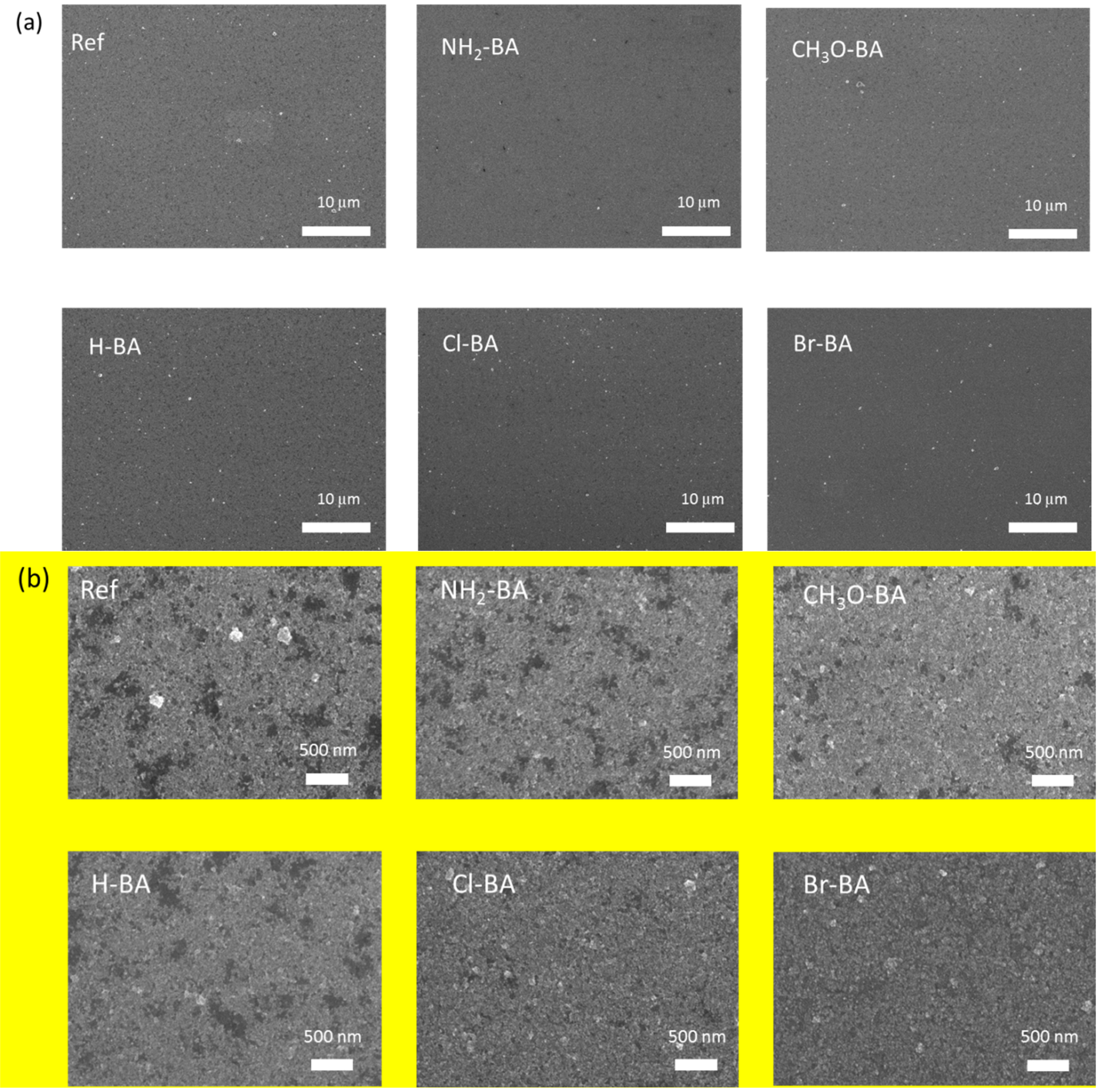

Figure S1. SEM images of NiO_x films with different SAMs at magnification of (a) 2500 times and (b) 20000 times.

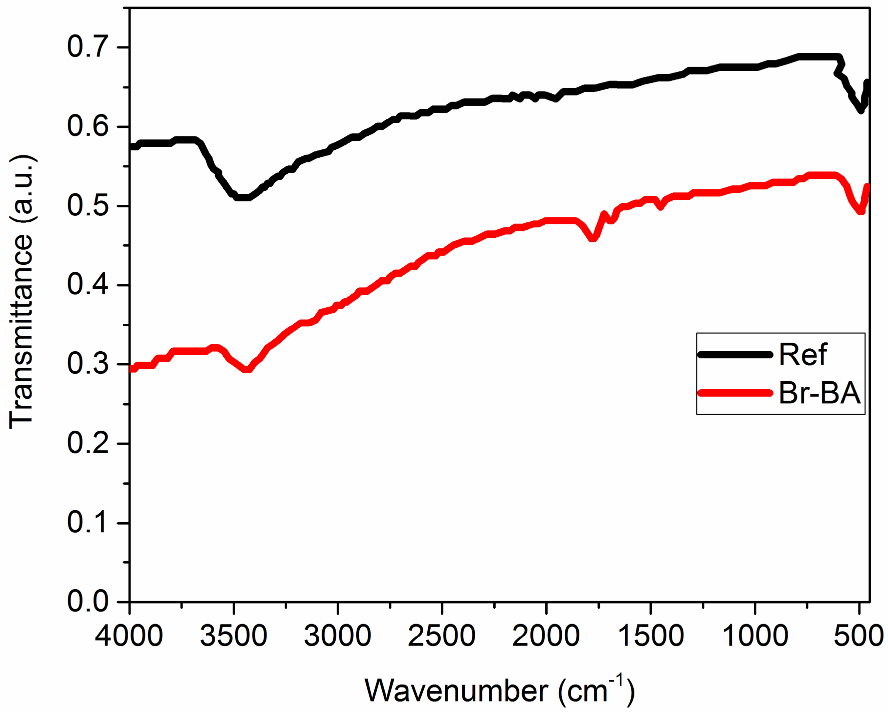

Figure S2. FTIR spectra of NiO_x without and with Br-BA modification. From the FTIR spectrum, the Ref group has a strong peak at 3450 cm^{-1} which is attributed to the O-H streching vibration. After Br-BA modification, the peak at 3450 cm^{-1} becomes weaker demonstrating the reaction of carboxyl functional group of Br-BA and hydroxyl functional group of NiO_x. Also, the new appearing peak ranging from 1700-1500 cm^{-1} corresponds to the aromatic C=C bending peaks, which comes from the Br-BA.

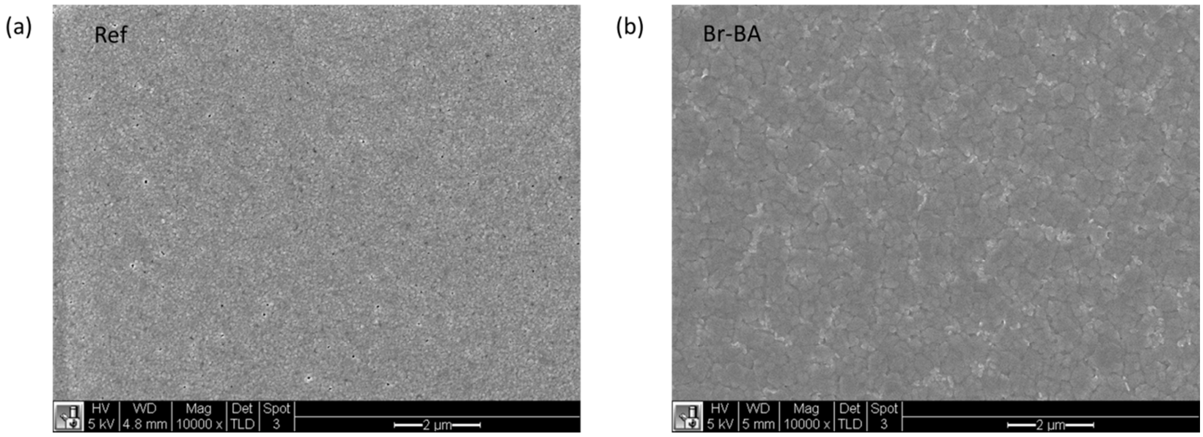

Figure S3. Large view of surface morphology of (a) Ref and (b) Br-BA modified NiO_x films. Scale bar is 2 µm.

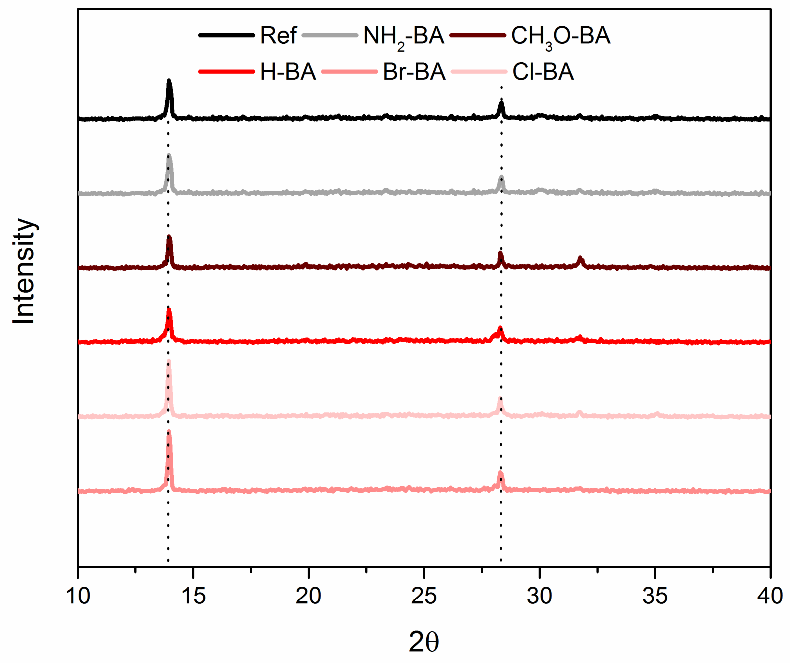

Figure S4. XRD patterns of the $MAPbI_3$ perovskite films deposited on various R-BA modified NiO_x films spun on glass substrates.

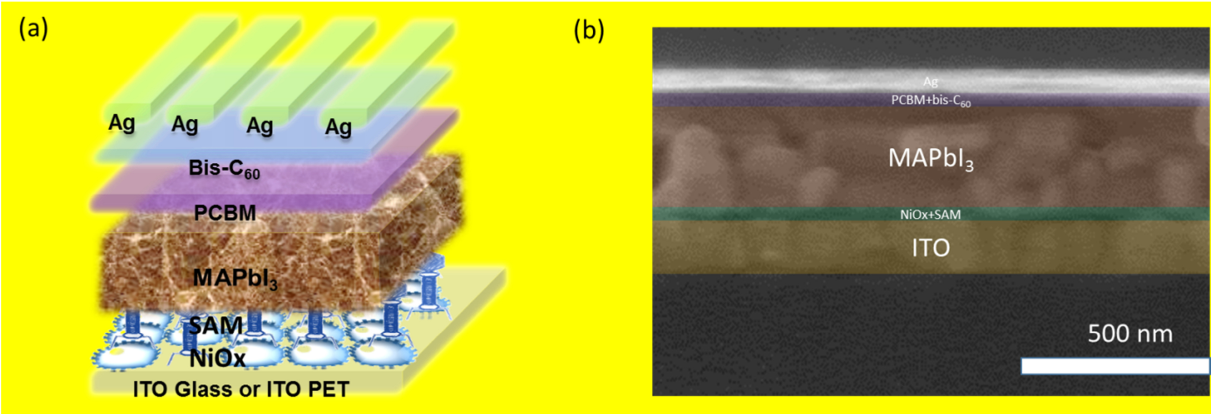

Figure S5. (a) Device structure of the PVSCs made in this study; (b) Cross section image of ITO/NiO_x/SAM/$MAPbI_3$/PCBM/bisC_{60}/Ag

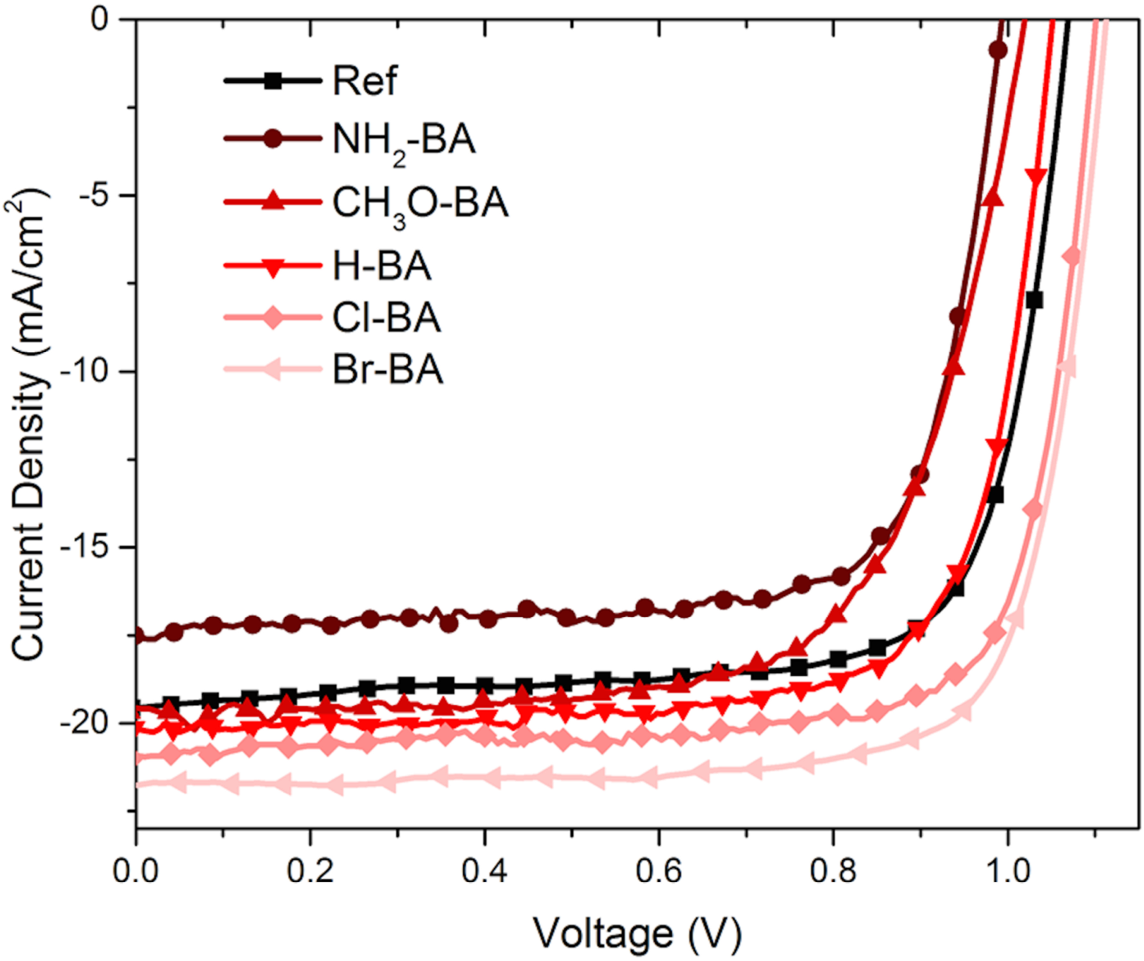

Figure S6: J-V curves of PVSC with and without SAM modification.

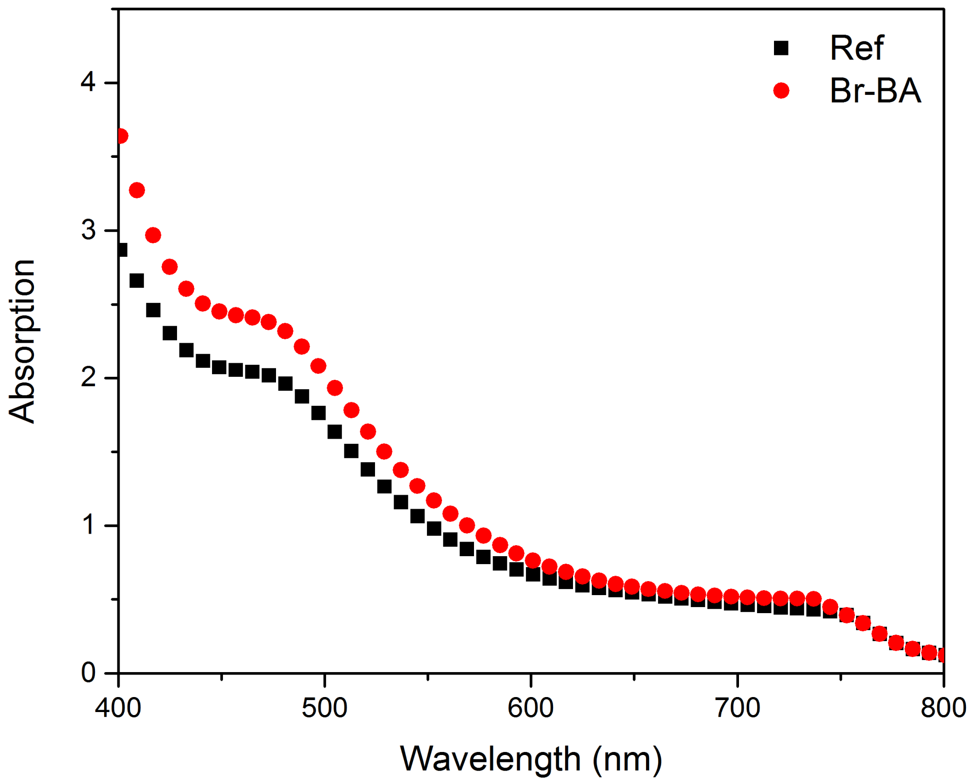

Figure S7. Absorption spectrum of the PVSCs with and without Br-BA modification.

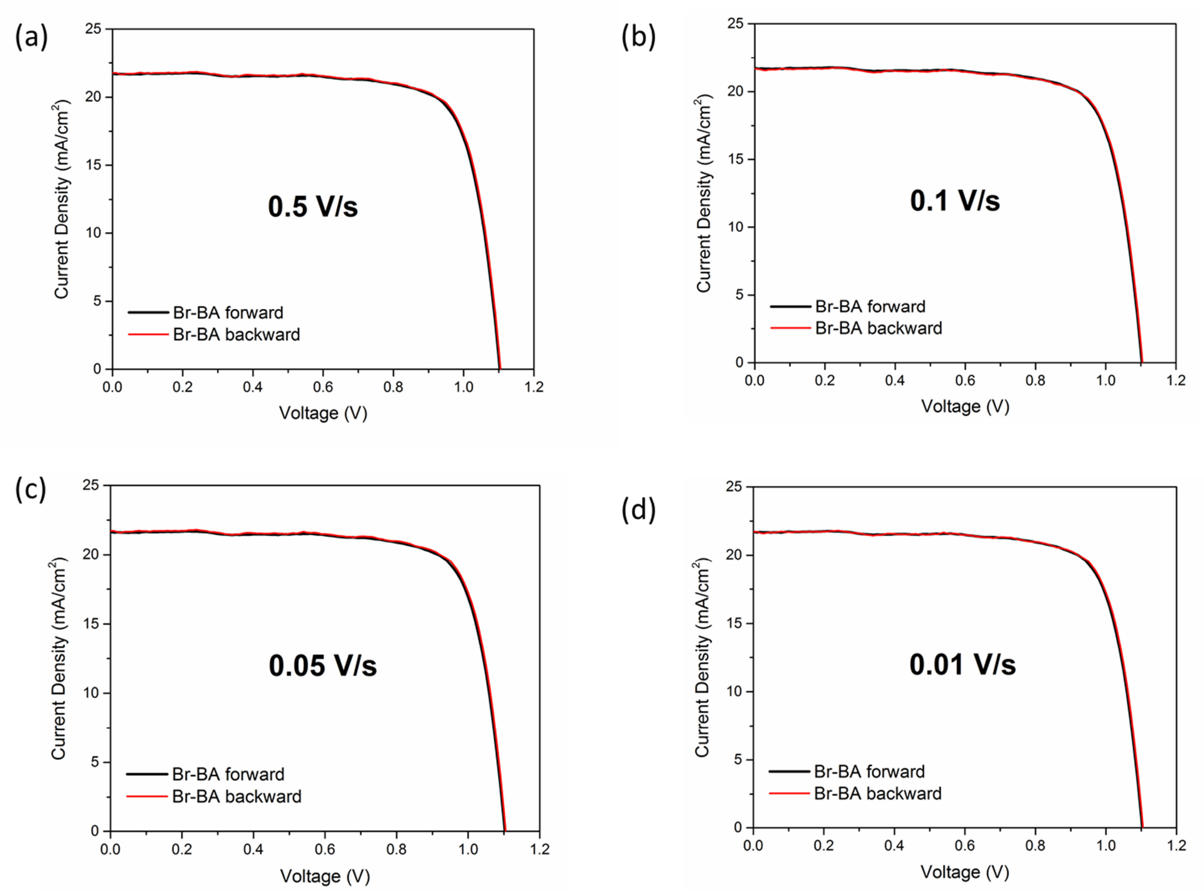

Figure S8. J-V curves of the Br-BA modified PVSCs at various scan rates: (a) 0.5, (b) 0.1, (c) 0.05, and (d) 0.01 V s^{-1}.

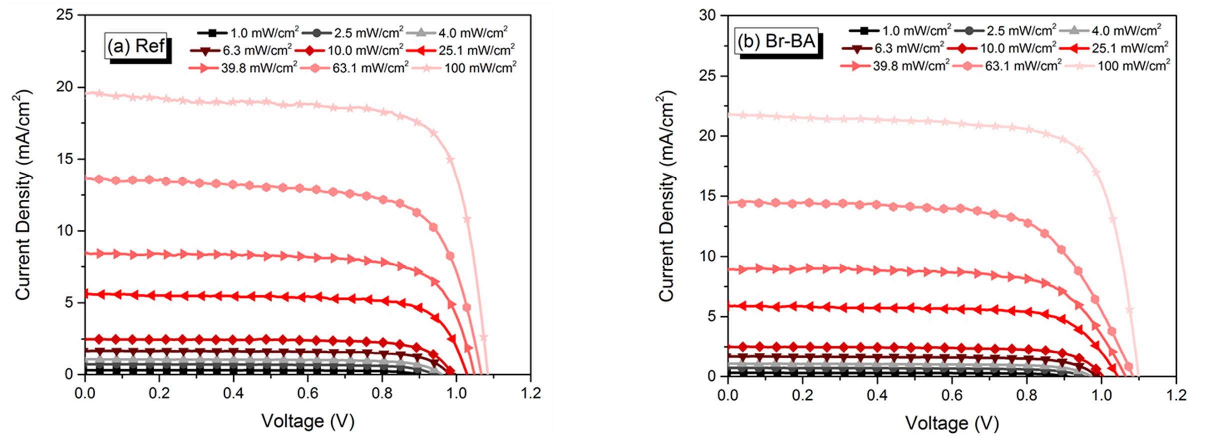

Figure S9. J-V curves of (a) the Ref and (b) Br-BA modified PVSCs at various light intensities.

Table S1. Photovoltaic parameters of various SAM-modified PVSCs.

SAMs	V_{oc}	J_{sc}	FF (%)	PCE (%)
None	1.07	19.6	74.2	15.5
$-NH_2$	0.99	17.5	74.1	12.8
$-OCH_3$	1.02	19.1	70.6	13.8
-H	1.05	20.3	76.2	16.2
-Cl	1.10	21.0	76.0	17.6
-Br	1.11	21.7	76.3	18.4
-Br on ITO/PET	1.10	20.7	71.3	16.2

Table S2. Summary of the recent works focusing on the application of NiO_x HTL in PVSCs

Device structure	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)	High T [a)]	Reference
ITO/ NiO_x(solution)/ $CH_3NH_3PbI_3$/ PCBM/ Al	1.05	15.4	47	7.6	Y (300 °C)	[1]
ITO/ NiO_x(solution)/ NiO_{nc}/ $CH_3NH_3PbI_3$/ PCBM/ BCP/ Al	1.04	13.2	69	9.5	Y (300 °C)	[2]
FTO/ NiO_x(sol-gel)/ $CH_3NH_3PbI_3$/ PCBM/ Au	0.88	16.3	64	9.1	Y (500 °C)	[3]
ITO/ NiO_x(sputtered)/ NiO_{nc}/ $CH_3NH_3PbI_3$/ PCBM/ BCP/ Al	0.96	19.8	61	11.6	Y (400 °C)	[4]
FTO/ NiO_x(spray pyrolysis)/ meso-Al_2O_3/ $CH_3NH_3PbI_3$/ PCBM/ BCP/ Ag	1.04	18.0	72	13.5	Y (500 °C)	[5]
ITO/ Cu: NiO_x(sol-gel)/ $CH_3NH_3PbI_3$/ PCBM/ bis-C_{60}/ Ag	1.11	19.0	73	15.4	Y (400 °C)	[6]
FTO/ NiO_x(sputtered)/ NiO_{nc}/ $CH_3NH_3PbI_3$/ PCBM/ BCP/ Au	1.10	15.2	59	9.83	Y (450 °C)	[7]
ITO/ NiO_x(PLD)/ $CH_3NH_3PbI_3$/ PCBM/ LiF/ Al	1.06	20.2	81	17.3	N (150 °C)	[8]
ITO/ Cu: NiO_x(combustion)/ $CH_3NH_3PbI_3$/ C_{60}/ bis-C_{60}/ Ag	1.05	22.2	76	17.8	N (150 °C)	[9]
FTO/ NiO_x(Li:Mg) (spray pyrolysis)/ $CH_3NH_3PbI_3$/ PCBM/ Ti(Nb)O_x/ Ag	1.09	20.4	83	18.4	Y (500 °C)	[10]
ITO/ NiO_x(sol-gel)/ DEA/ $CH_3NH_3PbI_{3-x}Cl_x$/ PCBM/ Ag	0.95	20.9	80	15.9	Y (500 °C)	[11]
ITO/ NiO_x(solution)/ $CH_3NH_3PbI_3$/ PCBM/ PDINO/ Ag	1.11	20.57	76.5	17.5	N (140 °C)	[12]
ITO/ NiO_x(NPs)/ $CH_3NH_3PbI_3$/ PCBM/ Ag	1.07	20.58	74.8	16.5	N (130 °C)	[13]
ITO/ NiO_x(sol-gel)/ $CH_3NH_3PbI_3$/ PCBM/ Ag	1.09	19.9	76.9	16.7	Y (300 °C)	[14]
ITO/ NiO_x(NPs)/ $CH_3NH_3PbI_3$/ PCBM/ bis-C_{60}/ Ag	1.03	21.8	78.4	17.6	N (25 °C)	[15]
ITO/ NiO_x(NPs)/ $CH_3NH_3PbI_3$/ C_{60}/ bis-C_{60}/ Ag	1.05	22.6	72.1	17.1	N (25 °C)	[16]
ITO/ NiO_x(NPs)/ $CH_3NH_3PbI_3$/ PCBM/ BCP / Ag	1.03	20.66	74.2	15.9	N (25 °C)	[17]
FTO/ Cs: NiO_x(sol-gel)/ $CH_3NH_3PbI_3$/ PCBM/ Zr(Acac)/ Ag	1.12	21.77	79.3	19.35	Y (275 °C)	[18]
ITO/ NiO_x (NPs)/ SAM/ $CH_3NH_3PbI_3$/ PCBM/ bis-C_{60}/ Ag	1.11	21.7	76.3	18.4	N (25 °C)	This work

[a)] High T denotes high temperature processed NiO_x films, which are not compatible with the roll-to-roll fabrication.

Table S3. Summary of the recent works of low-temperature processed NiOx film based flexible perovskite solar cells (F-PVSCs) with PCE ≥ 10% made on PET substrate.

Device structure	V_{oc} (V)	J_{sc} (mA/cm2)	FF (%)	PCE (%)	Power per weight (W/g)	Reference
ITO/ NiO_x (NPs)/ $CH_3NH_3PbI_3$/ C_{60}/ bis-C_{60}/ Ag	0.997	20.7	70.5	14.5	/	[15]
ITO/ NiO_x (NPs)/ $CH_3NH_3PbI_3$/ PCBM/ BCP / Ag	1.04	17.44	64.2	11.84	/	[17]
ITO/ NiO_x (PLD)/ $CH_3NH_3PbI_3$/ PCBM/ LiF/ Al	1.04	18.7	68.9	13.4	/	[13]
ITO/ NiO_x (NPs)/ $CH_3NH_3PbI_3$/ PCBM/ PDINO/ Ag	0.975	20.9	69.63	14.19	23.26	[16]
ITO/ NiO_x (NPs)/ SAM/ $CH_3NH_3PbI_3$/ PCBM/ bis-C_{60}/ Ag	1.1	20.7	71.3	16.2	26.92	This work

Table S4. Calculation of power per weight (w/g)

Materials	Thickness	Weight (g/m^2)	Power
PET/ITO	1.4 µm	5.6	
NiO_x	20 nm	1.5×10^{-4}	
$MAPbI_3$	250 nm	0.4167	(one-sun)$1000 W/m^2\times$PCE $= 1000\times16.2\% W/m^2$ $= 162 W/m^2$
PCBM/bis-C_{60}	40 nm	8.34×10^{-5}	
Ag	120 nm	1.26×10^{-3}	
Total		6.0182	

Therefore, the power per weight of F-PVSC= 162÷ 6.0182= 26.92 W/g

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