Electronic Supplementary Information (ESI)

Efficient and thermally stable inverted perovskite solar cells by introduction of non-fullerene electron transporting material

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Experimental

Synthesis of ETM

The synthetic method of NDI-PM compound in the absence of catalyst have been previously reported in Ref. **[9]**. NDI-PM powder used in this work was purified by recrystallization in DMF solution without additional purification process.

Analysis of Crystal Characteristics

To analysis of crystal characteristics including intermolecular interactions and void characteristics of NDI-PM and PCBM crystals, the solvent-free crystal structures of NDI-PM and PCBM are obtained from Ref. **[9]** and **[13a]**, respectively. The intermolecular secondary-bonds were analyzed by Hirshfeld surface with its fingerprints **[15]** using *CrystalExplorer* (Version 3.1: S. K. Wolff, D. J. Grimwood, J. J. McKinnon, M. J. Turner, D. Jayatilaka, and M. A. Spackman, *CrystalExplorer(Version3.1)*, University of Western Australia, 2012). The void characteristics including content and shape in crystals were analyzed by MERCURY program **[16]** in Cambridge Structural Database (CSD).**[16]**

Device fabrication

To fabricate the perovskite solar cell, In-doped SnO_2 (ITO, 10 Ω, AMG) glass substrates were sequentially washed by ultrasonicator with 5% Hellmanex soap, ethanol, acetone, and then ITO glass substrates were treated by Ar plasma to remove the organic residues. A filtered poly(3,4-ethylenedioxythiophene):poly(styrenesulfonic acid) (PEDOT:PSS, AI4083, Clevios)/ methanol (1:1 vol:vol) was coated on a cleaned ITO glass substrate by spin-coating at 2000 rpm for 30 s and dried at150 ^{o}C for 20 min. For $MAPbI_3$ perovskite film, 40 wt% $MAPbI_3$ perovskite solution was prepared by mixing the methylammonium iodide powder (MAI, DS LOGICS CO., LTD.) and lead (II) iodide (PbI_2, Aldrich) (1:1 mol:mol) in *N,N*-dimethylformamide (DMF, Aldrich) at 60 ^{o}C for 30 min, and 100 μL hydriodic acid (HI, Aldrich) was added in 1mL $MAPbI_3$ perovskite solution at room temperature. 40wt% $MAPbI_3$ perovskite solution was spin-coated on the PEDOT:PSS/ITO substrate at 3000 rpm for 120 s , and then was dried on the hot plate at 100 ^{o}C for 2 min. For $FAPbI_{3-x}Br_x$ perovskite film, $PbI_2(DMSO)_2$ complex was prepared by dissolving 50 g PbI_2 in 150 mL dimetylsulfoxide (DMSO, Aldrich) at 60 ^{o}C for 30 min, and then 350 mL toluene slowly dropped into the PbI_2 solution. The white precipitate was filtered and was annealed in vacuum oven at 60 ^{o}C for 5h. 1 M PbI_2(DMSO) complex was dissolved in DMF at 60 ^{o}C for 5 min. The PbI_2(DMSO) complex solution was coated by spin coating at 3000 rpm for 30 s followed by spin-coating of 0.5 M FAI and MABr (0.85:0.15 mol:mol) mixture solution in *iso*-propanol (IPA, Aldrich) at 5000 rpm for 30 sec. The film tuned from clear to dark brown during spin-coating was dried on the hot plate at 150 ^{o}C 20 min. After preparing the perovskite film, a phenyl-C61-butyric acid methyl ester (PCBM, nano-C)/1,2-dichlorobenzen (1,2-DCB) solution (20 mg/1 mL) or NDI-PM/1,2-DCB solution (15 mg/ 1 mL) was coated on the perovskite film/PEDOT:PSS/ITO substrate by spin-coating at 3000 rpm for 60 s. Finally, Al counter electrode was deposited by thermal evaporation. The active area was fixed 0.16 cm^2.

Device characterization

The current density-voltage curves were measured by a solar simulator (Peccell, PEC-L01) with a potentiostat (IVIUM, IviumStat) at under illumination of 1 sun (100 mW/cm^2 AM 1.5G) and a calibrated Si-reference cell certificated by JIS (Japanese Industrial Standards). The J-V curves of all devices were measured by masking the active area with metal mask of 0.096 cm^2. To measure the hysteresis of J-V curves, the forward and reverse scan rate was set to 10 $mV \cdot 200\ ms^{-1}$ as a standard condition. The external quantum efficiency (EQE) was measured by a power source (ABET, 150W Xenon lamp, 13014) with a monochromator (DONGWOO OPTRON Co., Ltd., MonoRa-500i) and potentiostat (IVIUM, IviumStat). The morphorlogy of NDI-PN and PCBM film were obtained by measuring atomic force microscope (AFM, XE-100, park system). The PL life time of NDI-PN and PCBM were measured by a ChronosBH-ISS technology measuring equipment

Table S1. Fitting parameter for the TRPL decay curves of $MAPbI_3$, $MAPbI_3$/PCBM or NDI-PM, and $FAPbI_{3-x}Br_x$, $FAPbI_{3-x}Br_x$/PCBM or NDI-PM films.

Sample	A_1 (%)	τ_1 (ns)	A_2 (%)	τ_2 (ns)	τ_{avg} (ns)
$MAPbI_3$	65.79	4.45	34.21	13.60	9.03
$MAPbI_3$ /NDI-PM	60.49	2.51	39.51	5.84	4.18
$MAPbI_3$ /PCBM	58.92	1.08	41.08	3.76	2.42
$FAPbI_3$	50.72	4.41	49.28	14.88	9.65
$FAPbI_3$ /NDI-PM	60.87	2.06	39.13	5.22	3.64
$FAPbI_3$ /PCBM	55.87	1.60	44.13	4.33	2.96

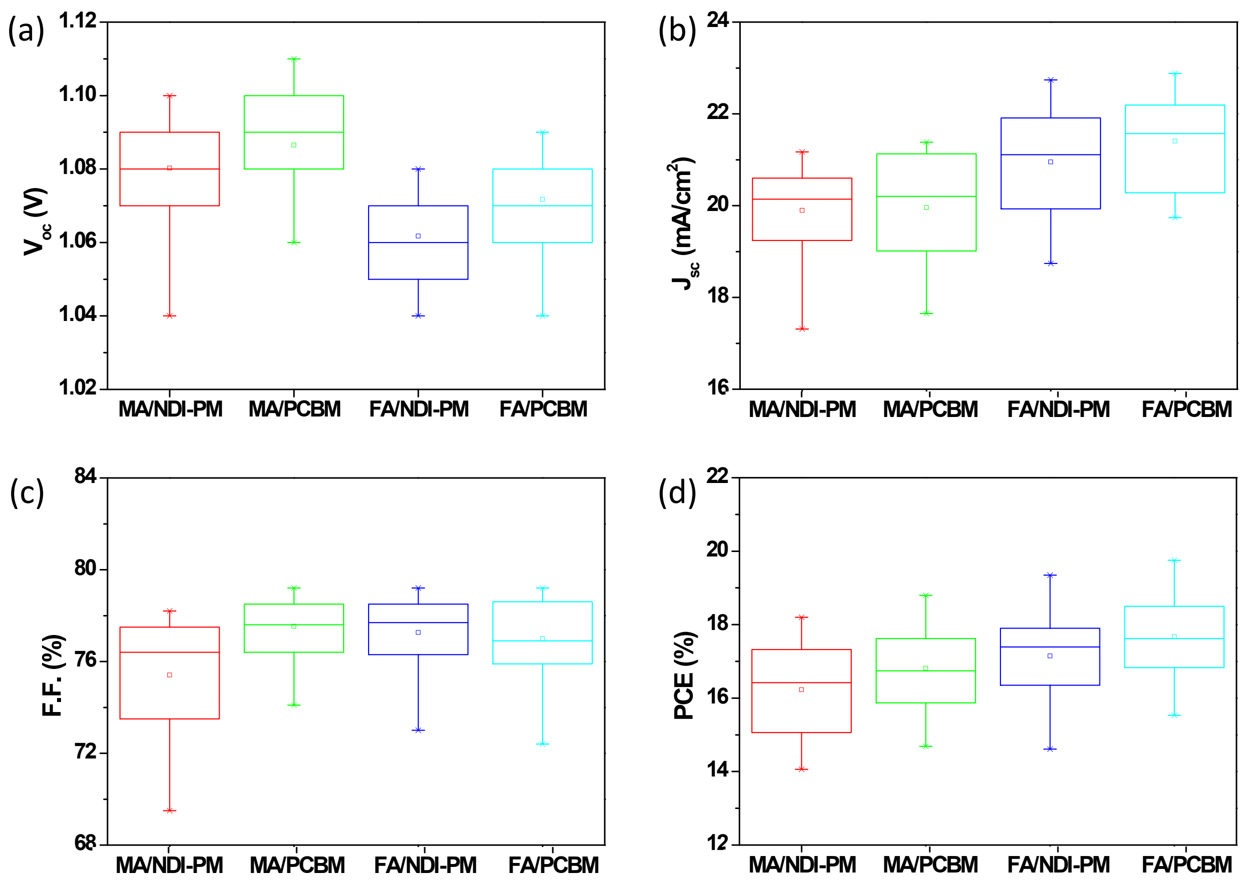

Fig. S1. Device statics (a) V_{oc} , (b) J_{sc} , (C) FF, and (d) PCE of the inverted $MAPbI_3$ and $FAPbI_{3-x}Br_x$ perovskite planar solar cells with NDI-PM and PCBM ETM.

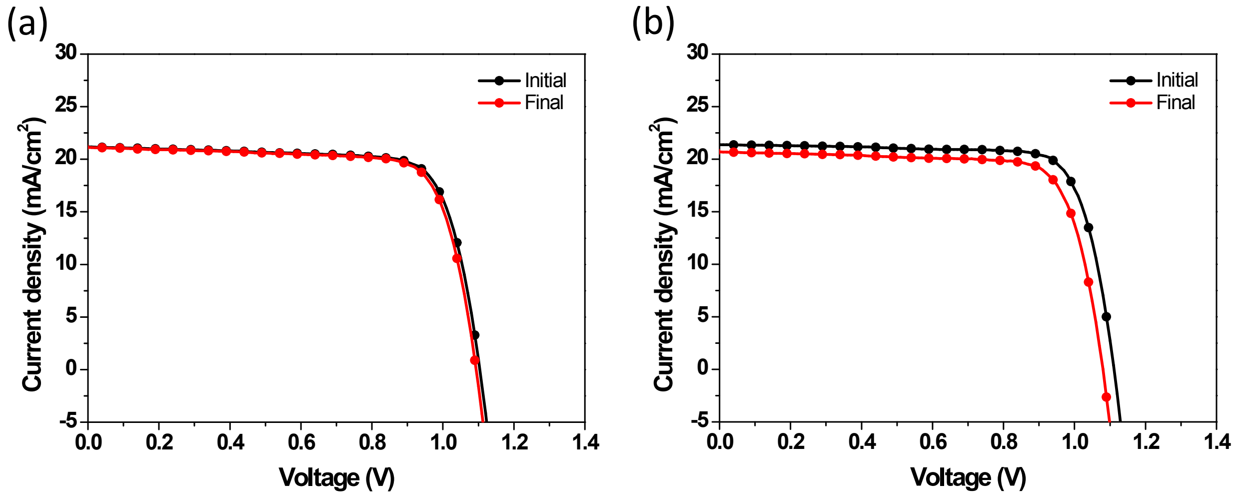

Fig. S2. I-V curves of NDI-PM and PCBM based devices before (0 min) and after heat-treatment (100 min) on the hot-plate at 90 °C

Table S2. Summary of photovoltaic properties of NDI-PM and PCBM based devices before and after heat-treatment.

ETM	Perovskite	Scan direction	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
NDI-PM/initial	$MAPbI_3$	Forward	1.10	21.2	77.2	18.0
NDI-PM/final	$MAPbI_3$	Forward	1.09	21.1	76.9	17.7
PCBM/initial	$MAPbI_3$	Forward	1.11	21.4	78.8	18.7
PCBM/final	$MAPbI_3$	Forward	1.08	20.7	77.5	17.3

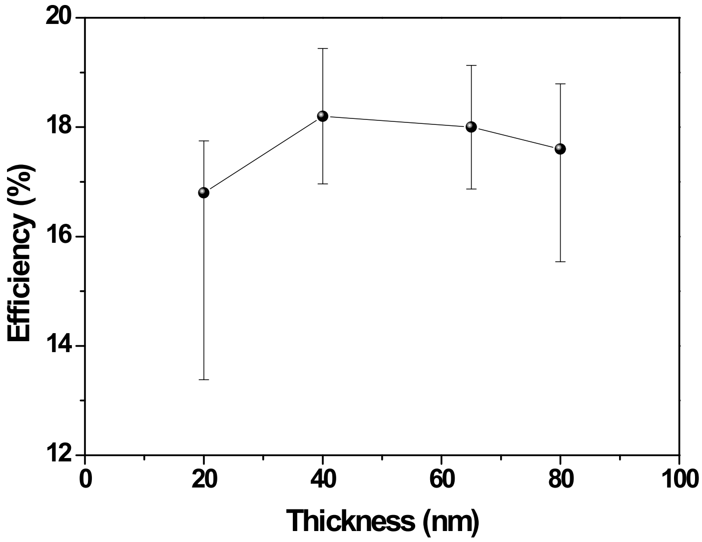

Fig. S3 Device efficiency of inverted $MAPbI_3$ perovskite planar solar cells with different thickness of NDI-PM.