Electronic Supplementary Information

Photo-cross-linked perylene diimide derivative materials as efficient electron transporting layers in inverted polymer solar cells

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Experimental

Device fabrication and characterization: The indium tin oxide (ITO)-coated (10 Ω/sq) glass substrate was cleaned by ultrasonication in deionized water, acetone, and isopropyl alcohol and then kept in 80 ˚C for 30 min. The PDIM powder was dissolved in water for the preparation of 1, 3, 5, 7, and 10 mg/ml solutions. The PDIM solution was spin-coated onto UV/Ozone-treated ITO substrates and thermal-annealed at 150 ˚C for 10 min in air. Then, the PDIM film was photoirradiated under ultraviolet (UV) light (365 nm) for 5 min to induce the cross-linking.[1,2] The average thicknesses of 1, 3, 5, 7, and 10 mg/ml PDIM films were 1.5, 2.5, 3.5, 5.0, and 6.5 nm, respectively. The photoactive layer was spin-coated onto the PDIM films with a speed of 1500rpm for 40s using a solution mixed with PTB7-Th (10 mg), $PC_{71}BM$ (15 mg), and 1,8-diiodictance (5 vol.%) in 1 ml chlorobenzene (CB). Finally, 3-nm molybdenum trioxide (MoO_3) and 100-nm Ag with the active area of 4.64 mm^2 were deposited as the hole transporting layer and the electrode, resepectively, via a thermal evaporation in a vacuum at 10^{-6} Torr. The current-voltage curve of the solar cells was measured under 100 mW/cm^2 using a Keithley2400 equipment and a 450 W Class AAA solar simulator. Cyclic voltammetry was conducted on an electrochemical workstation (Metrohm Autolab, AUT302M, FRA2) with an Ag/AgCl reference electrode, a platinum wire counter electrode, and a glassy carbon as the working electrode in 0.1 mol/L tetrabutylammonium hexafluorophosphate (n-Bu4NPF6) dissolved in acetonitrile solution at a potential scan rate of 100 mV/s. The ferrocene/ferrocenium (Fc/Fc+) redox couple was used as a calibration reference. The lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO) of PDIM film was calculated from the onset reduction potential and the onset oxidation potential. The surface image, work function, transmittance, and absorbance of PDIM films were measured by atomic force microscopy (Park system, XE7), ultraviolet

photoelectron spectroscopy (UPS) with a He-1 ($h\nu$ = 21.2 eV) UV source (Thermo Scientific), and UV-visible spectroscopy.

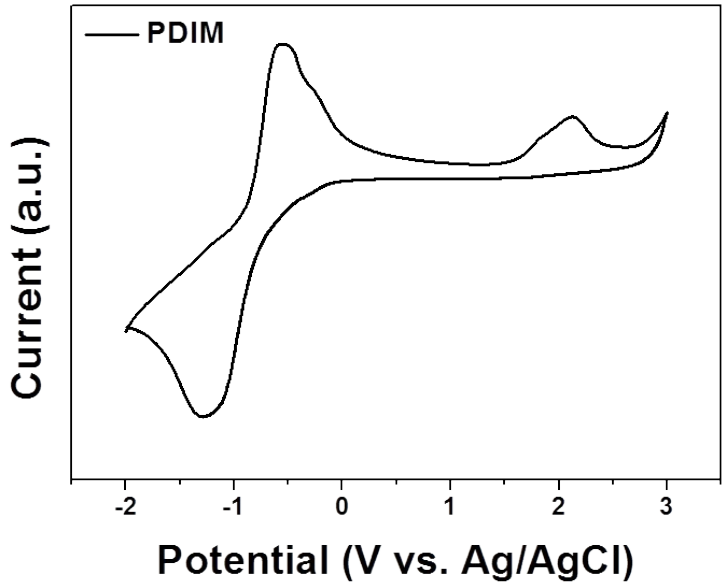

Figure S1. Cyclic voltammetry of PDIM.

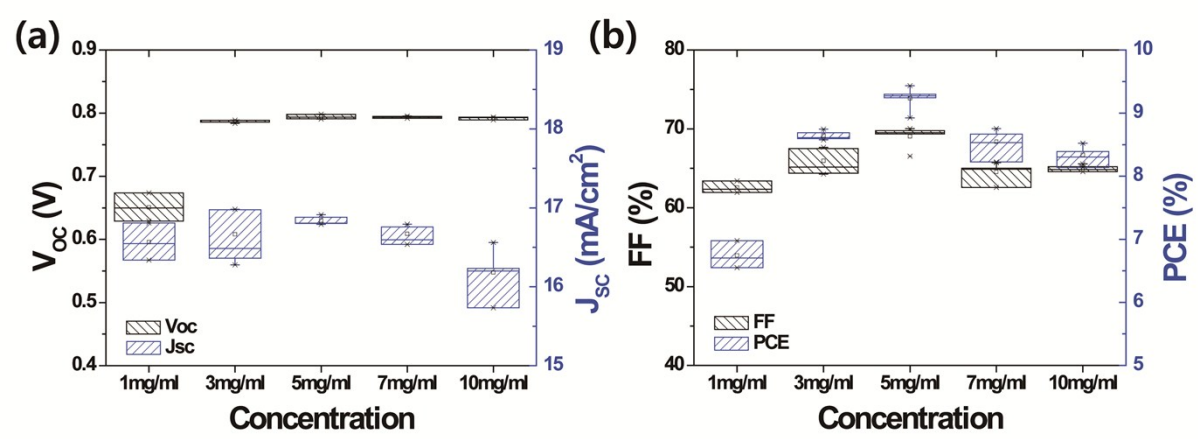

Figure S2. Influence of different PDIM-concentration on (a) open-circuit voltage (Voc) and short-circuit current density (Jsc) and (b) fill factor (FF) and power conversion efficiency (PCE).

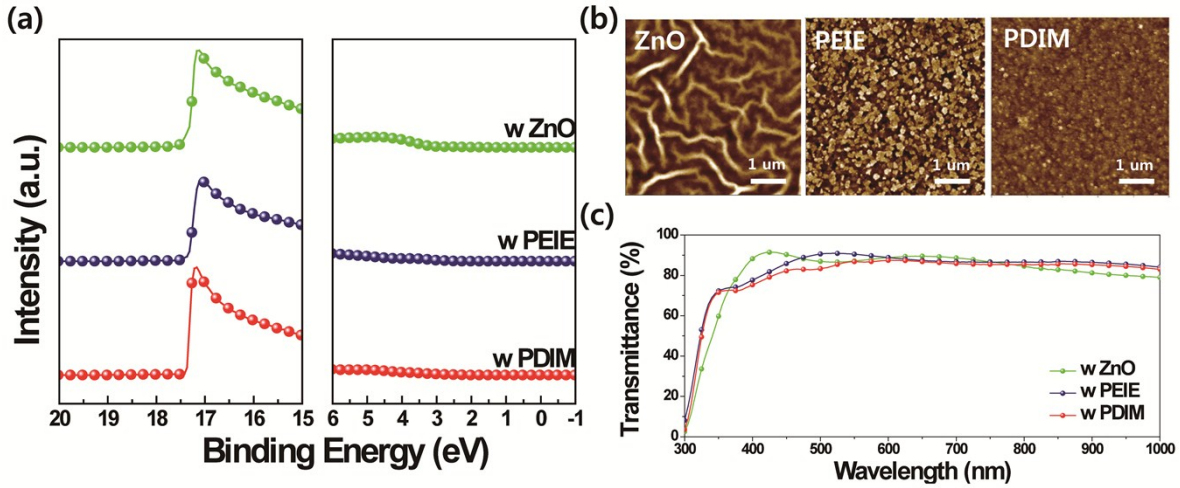

Figure S3. (a) UPS spectra, (b) AFM topographic images, and (c) transmittance of ZnO, PEIE, and PDIM films.

References

1. F. Bella, N. Vlachopoulos, K. Nonomura, S. M. Zakeeruddin, M. Grätzel, C. Gerbaldi, A. Hagfeldt, *Chem. Commun.*, 2015, **51**, 16277-16424.
2. S. Kim, J. H. Koh, X. Yang, W. S. Chi, C. Park, J. W. Leem, B. Kim, S. Seo, Y. Kim, J. S. Yu, J. H. Kim, E. Kim, *Adv. Energy Mater.*, 2014, **4**, 1301338-1-1301338-8.