Supporting Information

A new unsymmetrical near-IR small molecule with squaraine chromophore for solution processed bulk heterojunction solar cells


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Device fabrication and characterization

The solution processed BHJ organic solar cells were fabricated as follow: The indium tin oxide (ITO) coated glass substrates were first cleaned with detergent, ultrasonicated in acetone and isopropyl alcohol, subsequently dried in an oven for overnight. PEDOT:PSS (Heraeus, Clevios PVP.Al 4083) in an aqueous solution was spin coated to form a film with thickness of approximately 40 nm and subsequently dried for 10 min at 140 °C under air. Small molecule JK216D were mixed with PC71BM in several weight ratios (1:1, 1:1.5 1:2, and 1:2.5) in CB solvent at a concentration of 20 mg/mL to form the blends. The blend solution was spin cast on the top of PEDOT:PSS layer to form the active layer and then dried for 2 hr to remove the residue of solvent. For the JK216D:PC71BM blend processed with solvent additives, different concentrations (1 v%, 2 v%, 3 v% and 4 v%) of DIO was added to the host CB solution and only the 1:2 w/w of JK216D and PC71BM was used. A thin film of aluminum (Al) (80 nm thick) was thermally deposited at a vacuum of 10⁻⁵ Torr on the top of active layer through a mask area of 0.20 cm². All the devices were fabricated and tested in ambient atmosphere without encapsulation. The hole only and electron only devices were with ITO/PEDOT:PSS/JK216D:PC71BM/Au and ITO/Al/JK216D:PC71BM/Al structures, respectively were fabricated in same method, to measure the hole and electron mobilities in the BHJ active layers. We have fabricated 10 devices processed with CB and 3v% DIO/CB solvents. The current-voltage characteristics of the fabricated devices were measured using a computer controlled in dark as well as under stimulated AM1.5 illumination of 100 mW/cm². A solar simulator consists of xenon lamp coupled with optical filter was used to give the stimulated irradiance at surface of the devices. The incident photon to current conversion efficiency (IPCE) of the devices was measured illuminating the devices through a light source and monochromator and resulting current was measured using a electrometer under short circuit conditions.
Figure S1. NMR spectra

Compound 3:
Compound 4: