Supplementary Material (ESI) for Journal of Materials Chemistry

SUPPLEMENTARY INFORMATION

Isomeric iminofullerenes as acceptors in bulk heterojunction organic solar cells

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1. Optical microscope images of P3HT:open APCBM and P3HT:closed APCBM films

Figure S1 shows optical microscope images of P3HT:open APCBM and P3HT:closed APCBM films (chloroform solvent) with and without annealing temperature. While no large features are observed in the film of P3HT:open APCBM under room and 120°C anneal condition, well ordered structures are observed in the P3HT:closed APCBM film after annealing at 120°C. This morphology difference between P3HT:open APCBM and P3HT:closed APCBM films is consistent with that of the TEM images in Figure 6 in the text.

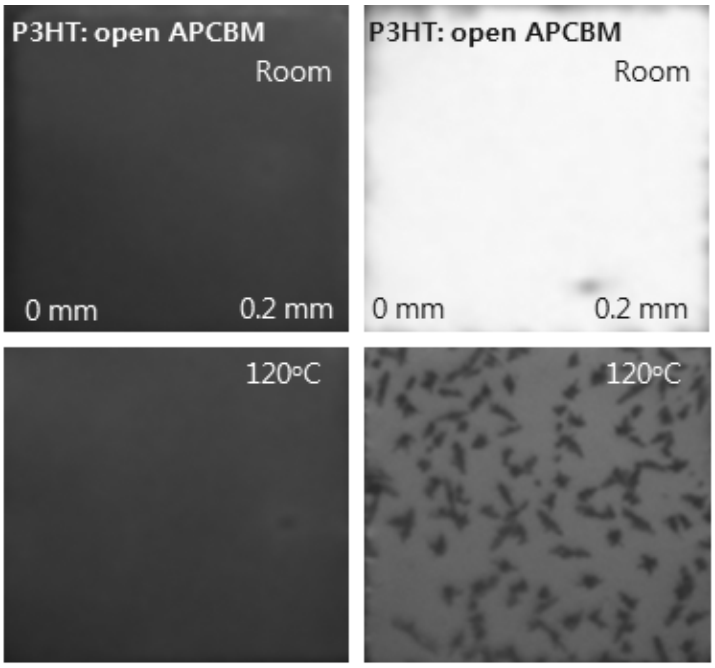

Figure S1. Optical microscope images of P3HT:open APCBM and P3HT:closed

APCBM films with and without annealing temperature.

2. Effect of organic solvent in morphology difference between P3HT:open APCBM and P3HT:closed APCBM films.

Figure S2 (a) shows optical microscope images of P3HT:open APCBM and P3HT:closed APCBM films cast from two different solvents -- chloroform (CF) and dichlorobenzene (DCB). The morphology difference between P3HT:open APCBM and P3HT:closed APCBM film become more pronounced when we change the solvent from CF to DCB. Figures S2 (b) and (c) show the morphology images of optical microscope and atomic force microscope (AFM) for the films cast from DCB.

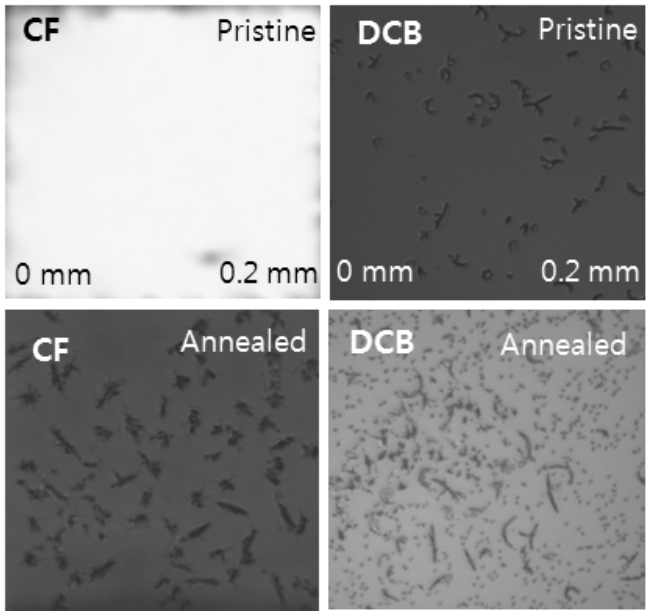

Figure S2 (a). Optical microscope images of P3HT:open APCBM and P3HT:closed APCBM films cast from CF and DCB solvent.

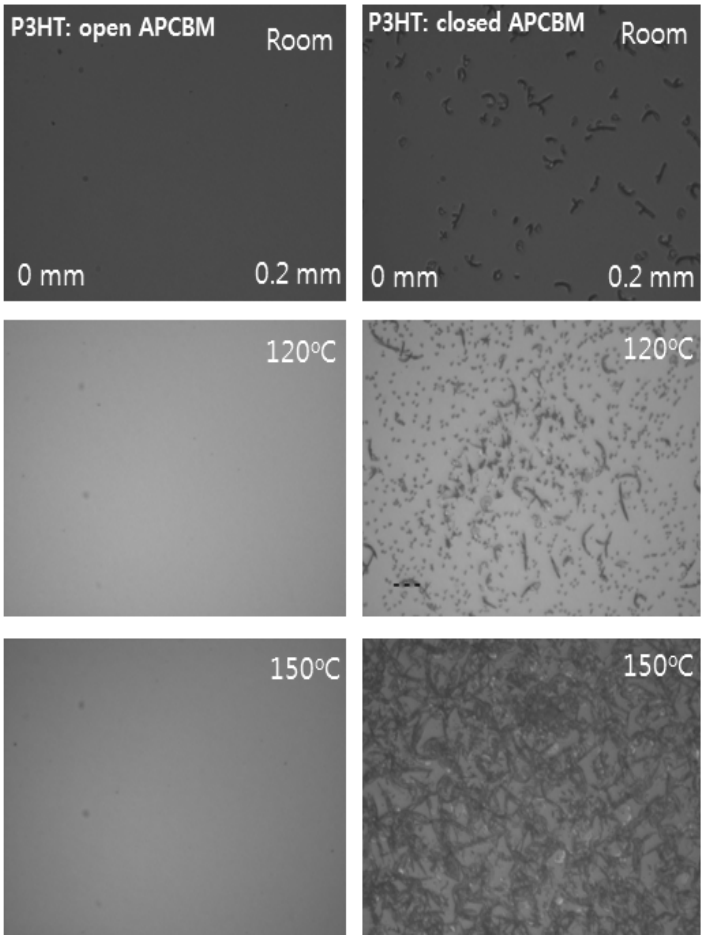

Figure S2 (b). Optical microscope images of P3HT:open APCBM and P3HT:closed APCBM films cast from DCB solvent with and without annealing temperature.

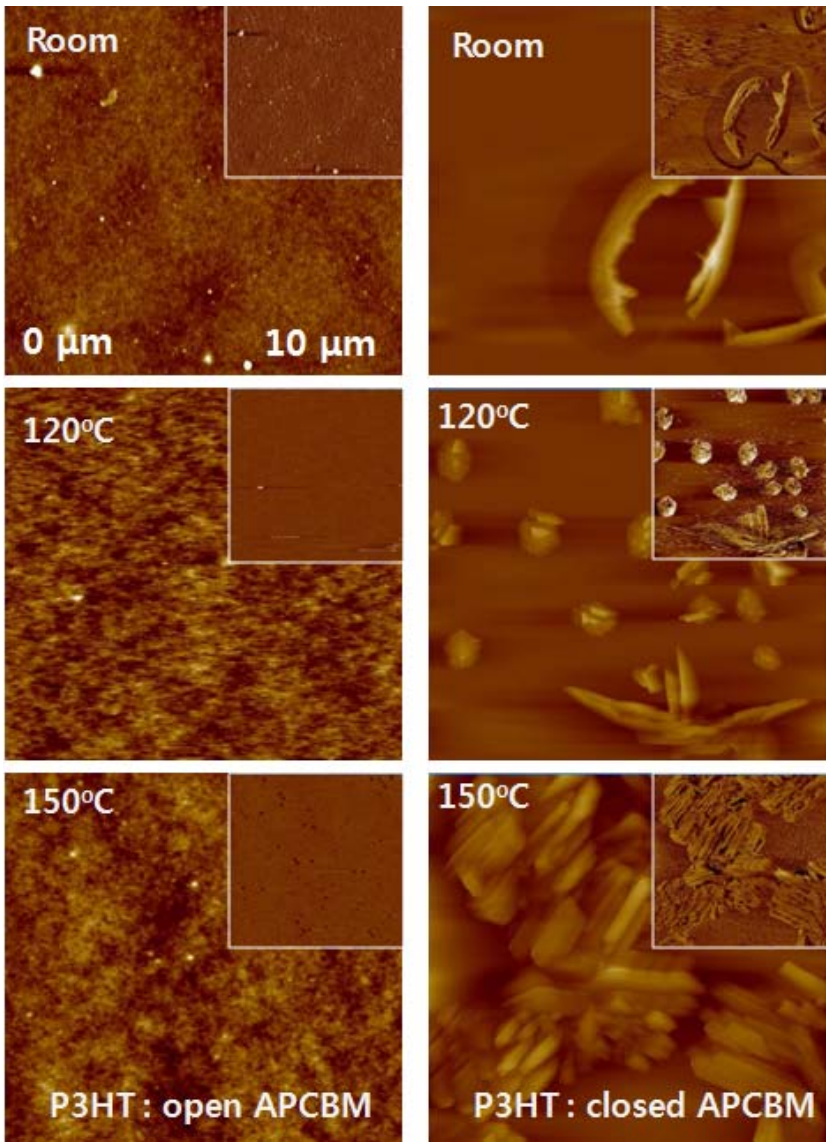

Figure S2 (c). Atomic force microscope images of P3HT:open APCBM and P3HT:closed APCBM films with and without annealing temperature. The insets exhibit phase images.

3. The detailed experimental procedures

Device Fabrication: Solar cells were fabricated on an indium tin oxide (ITO)-coated glass substrate in the following structure; ITO-coated glass substrate/ poly(3,4-ethylenedioxy -thiophene)(PEDOT:PSS)/P3HT: each APCBM mixture/Al. The ITO-coated glass substrate was first cleaned with detergent, ultrasonicated in acetone and isopropyl alcohol, and subsequently dried overnight in an oven. PEDOT:PSS (Baytron PH) was spin-cast from aqueous solution to form a film of thickness of 40nm. The substrate was dried for 10 min at 140°C in air and then transferred into a glove box to spin-cast the charge separation layer. A solution containing a mixture of P3HT : each APCBM (1:1) in chloroform solvent with concentration of 1 wt.% was then spin-cast on top of the PEDOT/PSS layer. Then, an aluminum (Al, 100nm) electrode was deposited by thermal evaporation in a vacuum of about 5 x 10^{-7} Torr. Current density-voltage (J-V) characteristics of the devices were measured using a Keithley 236 Source Measure Unit. The processing was carried out in a glove-box under nitrogen and at room temperature. Solar cell performance utilized an Air Mass 1.5 Global (AM 1.5 G) solar simulator with an irradiation intensity of 1000 W m^{-2}. An aperture (12.7mm^2) was used on top of the cell to eliminate extrinsic effects such as cross-talk, waveguiding, shadow effects etc. The spectral mismatch factor was calculated by comparison of solar simulator spectrum with AM 1.5 spectrum at room temperature.

TEM measurement: Specimens were prepared by first casting a P3HT:APCBM blend thin film on glass. Films were annealed in a nitrogen environment simulating the post-annealing conditions in functional solar cells. The films were then removed from the nitrogen environment and were scored with a diamond scribe to define sample size. The substrate and film were immersed in deionized water for 20 minutes and sonicated to promote delamination. Resulting pieces of the film were transferred to a PELCO copper TEM grid with a carbon/Formvar support grid. TEM specimens were allowed to dry under low heat to remove excess water from the transfer process. Light field imaging was performed in an FEI T20 TEM, using a small objective aperture for contrast from crystalline parts of the sample (i.e the closed APCBM agglomerates) and defocus for additional phase contrast from the relatively amorphous polymer material.