Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Spontaneous interlayer formation in OPVs by additive migration due to additive-metal interactions

Igal Deckman,[a] Moshe Moshonov,[a] Stas Obuchovsky,[a] Reuven Brener,[b] and Gitti L. Frey [a]

Supporting Information

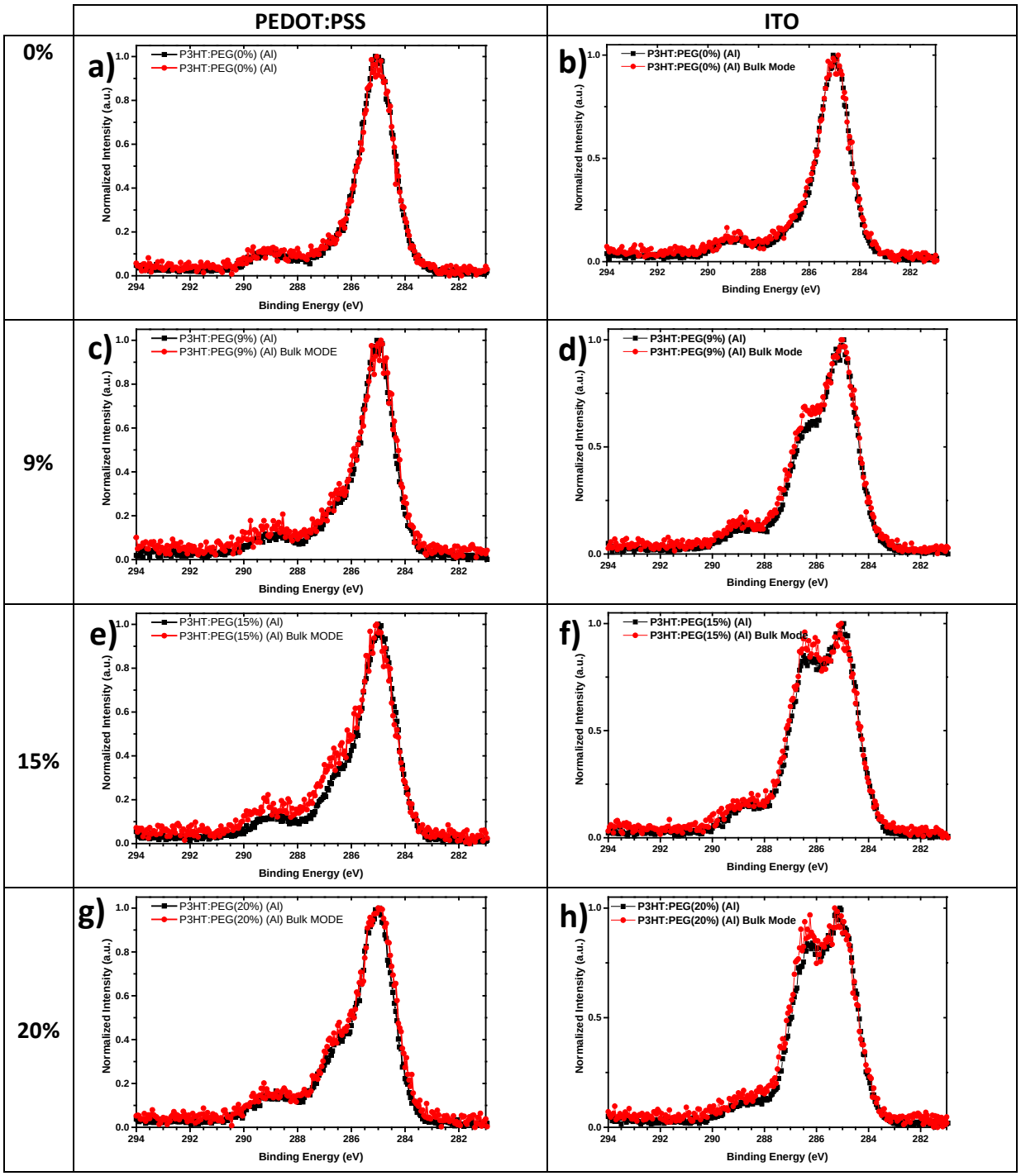


Figure S1- High energy resolution C1s XPS spectra in the standard analysis mode (black lines) and bulk analysis mode (red lines) of P3HT:PEG blends with different PEG content (wt% indicated on the left) on ITO/PEDOT:PSS (left column) or ITO (right column). All spectra are normalized to the intensity of the C-C/C-H peak (285 eV) obtained from the corresponding Al-covered areas.

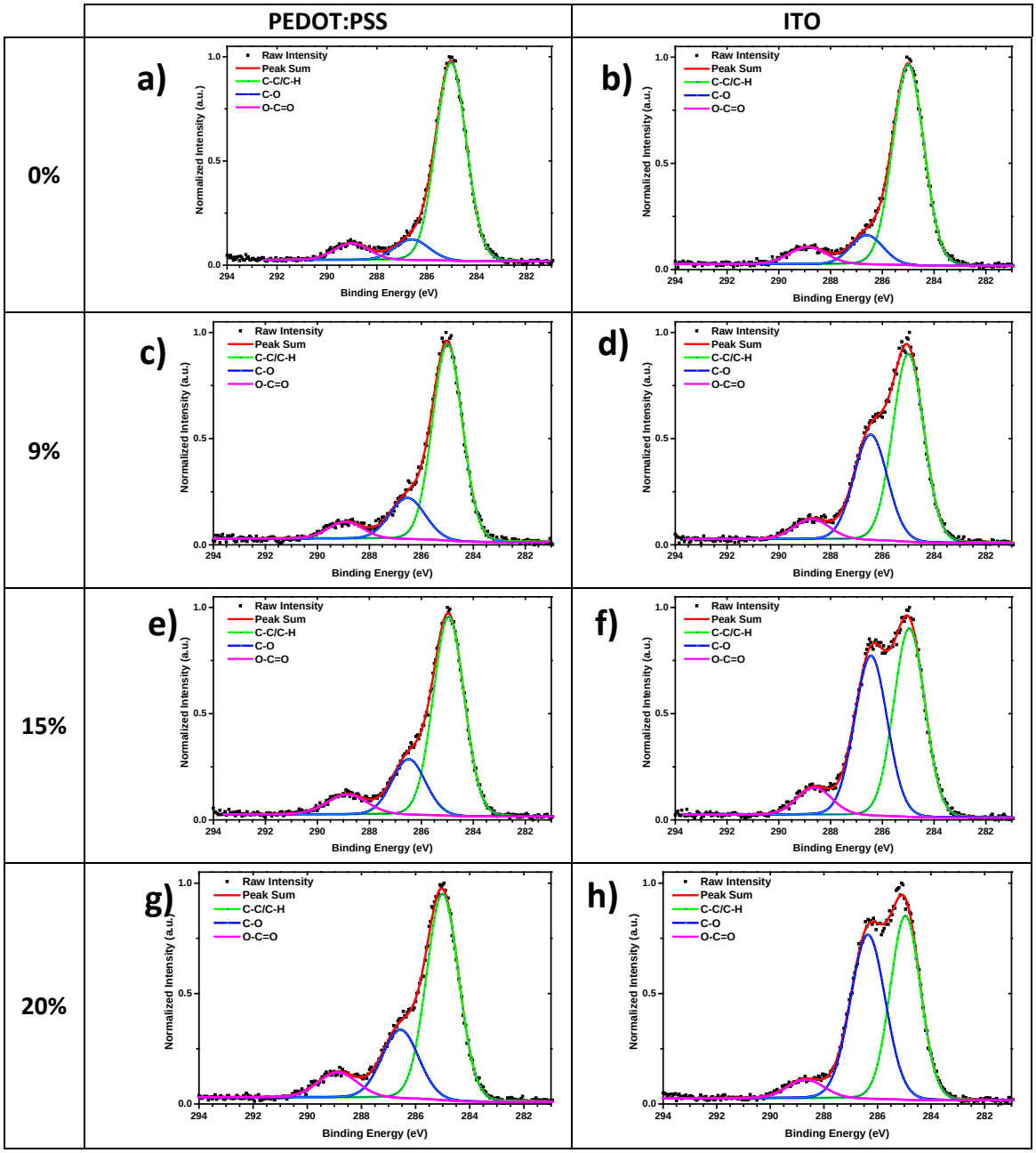


Figure S2- Line fitting of the high resolution C1s XPS spectra obtained in standard analysis mode from Al-covered P3HT:PEG blends with different PEG content (wt% indicated on the left) deposited on ITO/PEDOT:PSS (left column) or ITO (right column). Three peaks are fitted to each spectra: the green line associated with the C-C/C-H bonding in both PEG and P3HT (285.0 eV); the blue line associated with the C-O bonding in PEG (286.6 eV); and the magenta line associated with O-C=O contamination moieties (288.6 eV). The red lines in each graph show the cumulative fitted spectra.

The peak at 286.6eV binding energy can also be attributed to organic contaminants adsorbed on the sample's surface due to air exposure. The contribution of this general contamination is represented in the C-O peak in the XPS spectra of Al-covered pristine P3HT films (see blue lines in Figure S2a and S2b of the Supporting information). The small peak at 288.6 eV (magenta line in Figure S2), associated with O–C=O bonds resulting from unintentional oxidation or contamination of the surfaces, did not show significant changes for all spectra in Figure 4c and 4d indicating similar low contamination levels in all films. Since the contamination levels are similar in all films covered by the same metal, than an increase of the C-O peak over the values attained for the pristine-P3HT films on both substrates provides conclusive evidence of an increase in PEG concentration at the blend/Al interface.

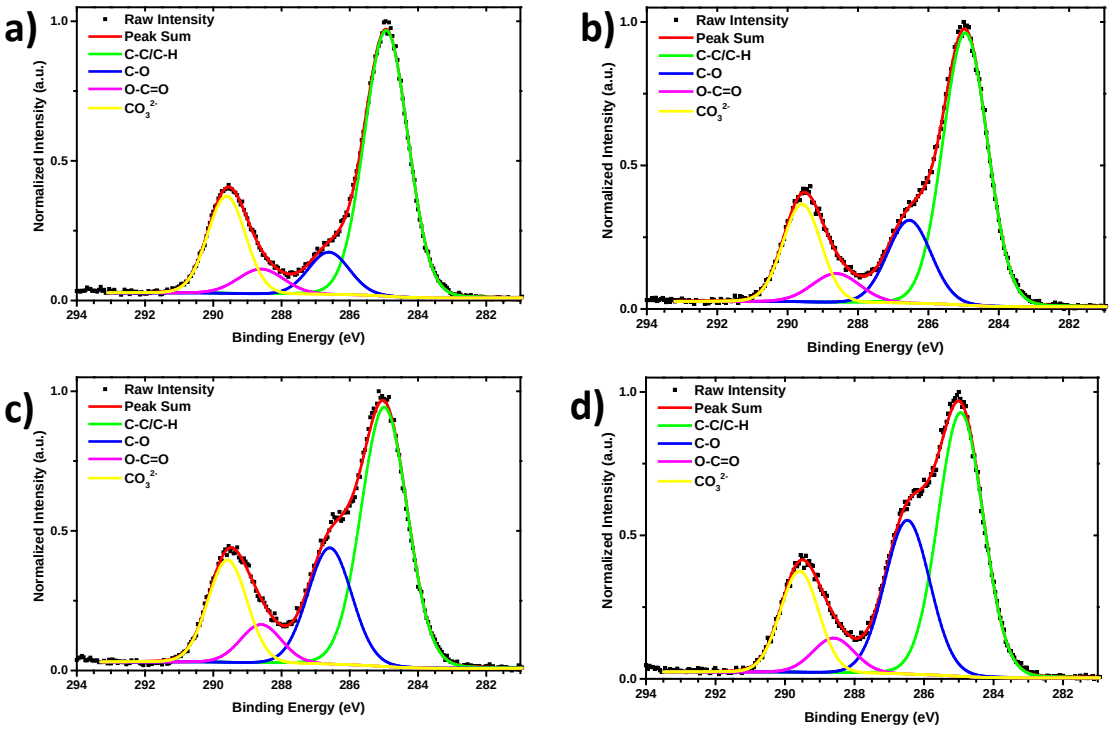


Figure S3- Line fitting of the high resolution C 1s XPS spectra obtained in standard analysis mode for Ca-covered P3HT:PEG blends with different PEG content a) 0 wt%, b) 9 wt% and c) 15 wt% d) 20% deposited on ITO. Four peaks are fitted to each spectra: the green line associated with the C-C and C-H bonding in both PEG and P3HT (285.0 eV); the blue line associated with the C-O bonding in PEG (286.6 eV); the magenta line associated with O-C=O contamination moieties (288.6 eV); and the yellow line associated with carbonate CO_3^{2-} contamination moieties (289.5 eV). The red lines in each graph show the cumulative fitted spectra.

Unintentional contaminations are represented by the carbonate peaks (289.5 eV) in the Ca covered films, and by an almost negligible O-C=O peak (288.6 eV) in the Au covered films, show similar levels in each set of films indicating similar contamination levels in each batch. Following the analysis of the XPS results presented in Figure 4, we consider the C-O peak of pristine homo-P3HT films covered by Au or Ca (green lines in Figure 6) representative of the contaminants on the sample surface.

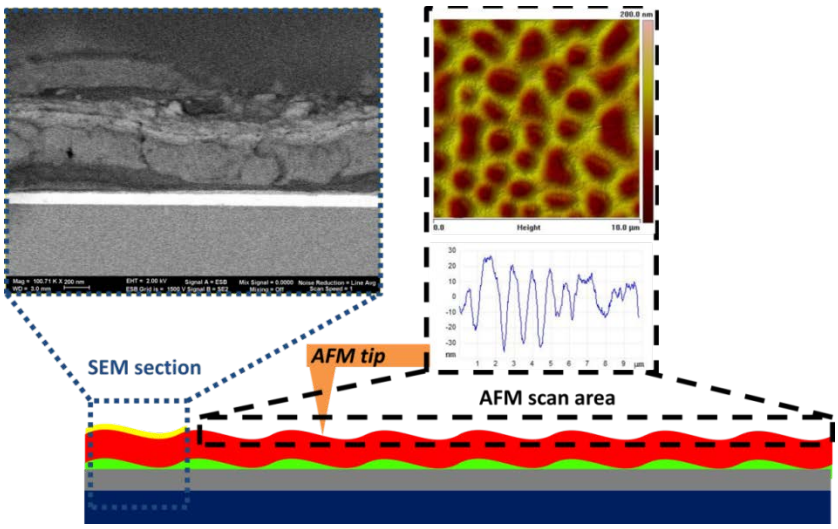


Figure S4-Shematic illustration of the P3HT:PEG bilayer and its characterization by HRSEM cross section and AFM surface topography.

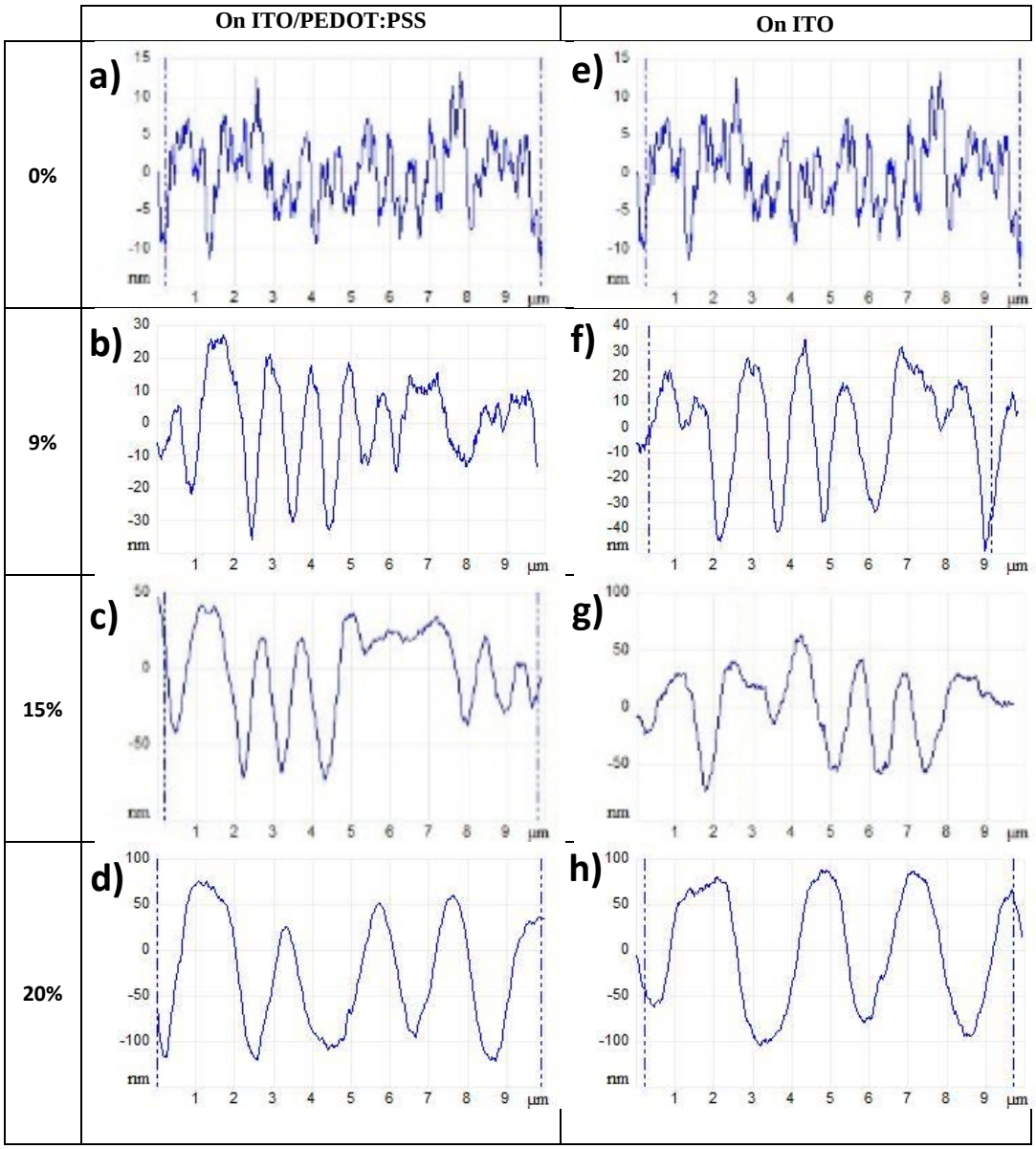
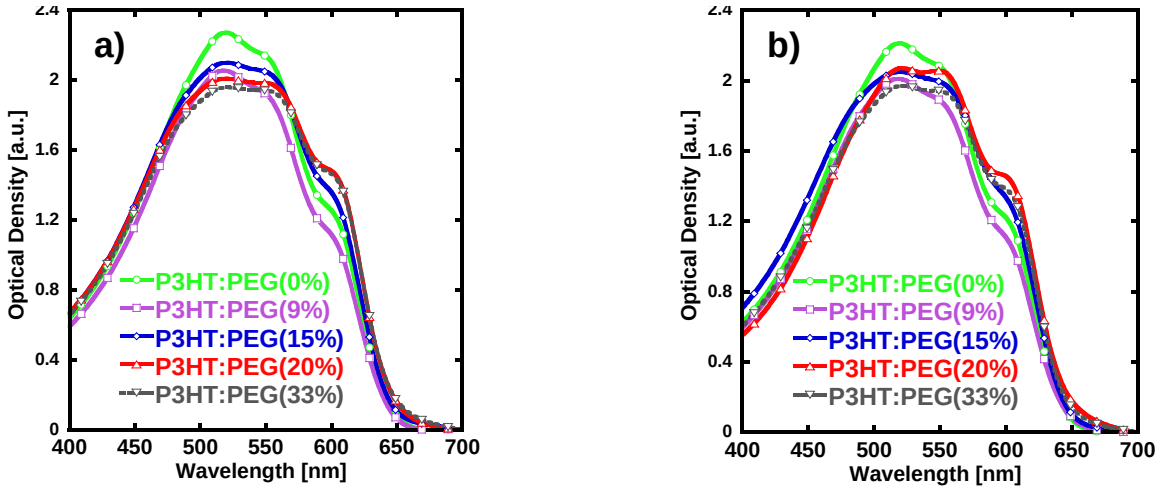
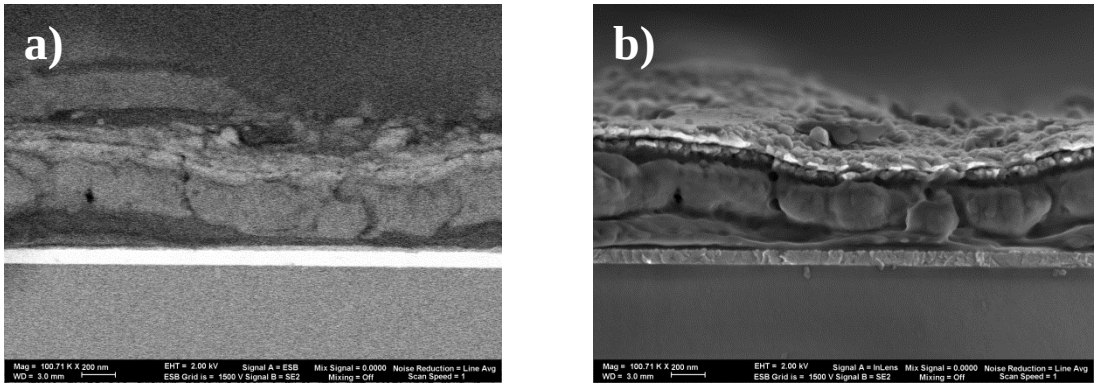


Figure S5- AFM line profiles of P3HT:PEG blend films with various PEG content (wt% indicated on the left) on ITO/PEDOT:PSS (left panels) and ITO (right panels).



Figurer S6- Absorption spectra of P3HT: PEG blend films on PEDOT:PSS (a) or ITO (b), with varying PEG content (wt %).



Figurer S7-HRSEM cross section images of P3HT: PEG (20 wt %) on ITO/PEDOT: PSS covered ~100 nm of Al (a) backscattered and (b) secondary electron images.

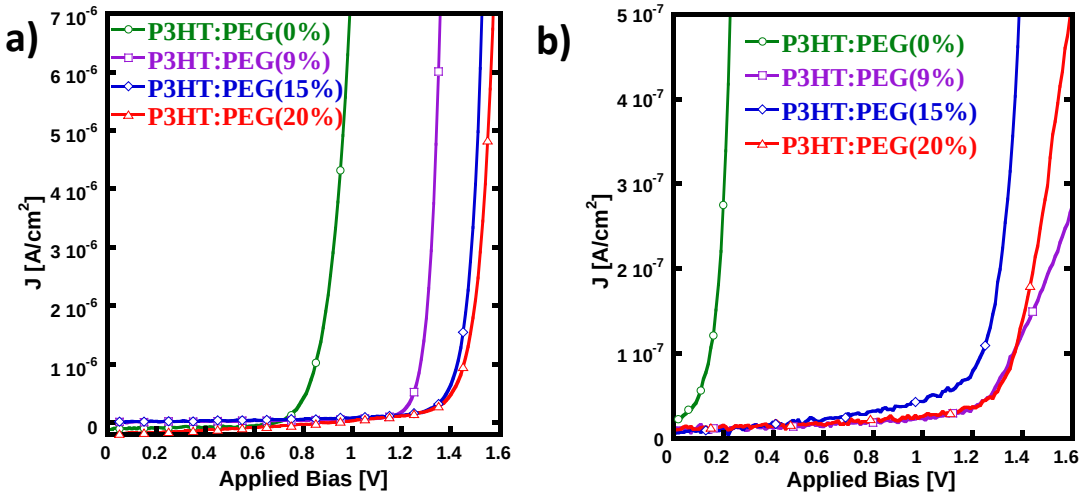


Figure S8- J-V curves measured in the dark of: a) ITO/PEDOT:PSS/P3HT:PEG/Al, and b) ITO/P3HT:PEG/Al devices with various PEG content.

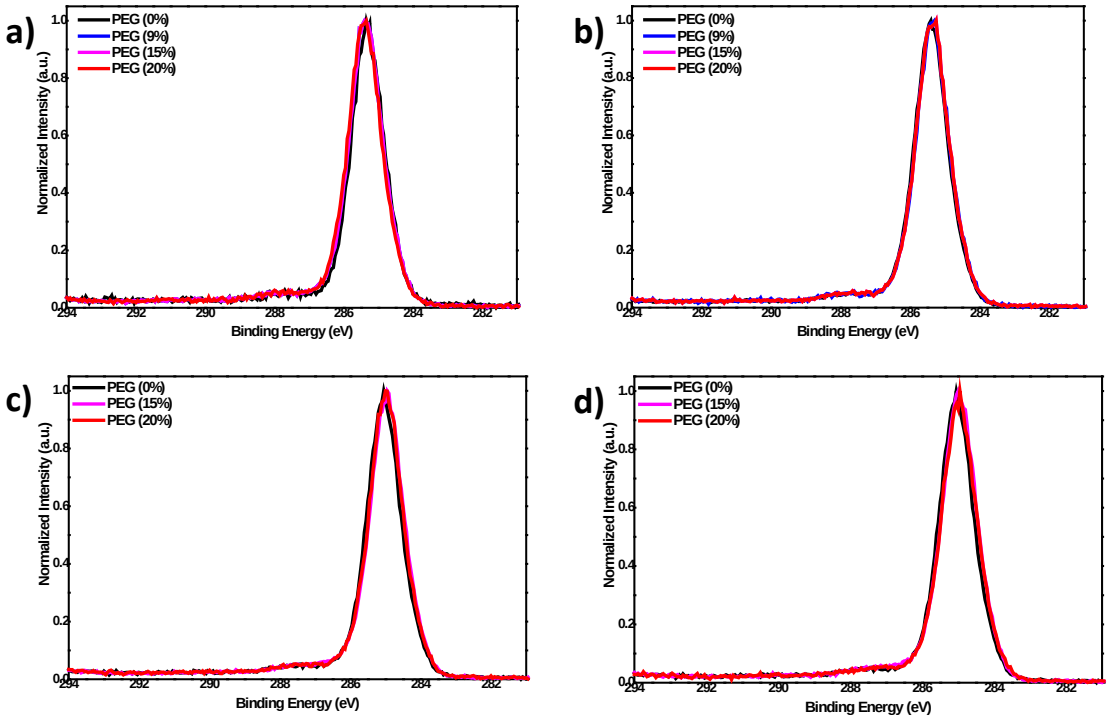


Figure S9- Normalized high energy resolution C1s XPS spectra of the bare areas of adjacent to Ca-covered (a and b) or Au-covered (c and d) surfaces of P3HT:PEG blends with different PEG content deposited on ITO/PEDOT:PSS (a and c) or ITO (b and d).