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

Supporting Information

Versatile methods for improving the mechanical properties of bulk heterojunction layers to enable stretchable organic solar cells

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1,12-diazidododecane ($C_{12}N_3$) was obtained by a reaction of 1,12-dibromododecane (DBDD) with sodium azide NaN_3. This synthesis (Figure 3-2) was realized by the method described by Thomas.[1]

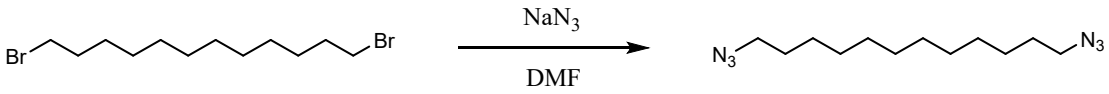

Figure S 1: Synthesis of 1,12-diazidododecane from 1,12-dibromododecane.

In a solution of 1,12-dibromododecane (2 g, 9 mmol) in DMF (15.0 mL) was added NaN_3 (1.18 g, 27.3 mmol). The mixture was stirred for 16 h at 60°C. Then, 100 mL of water and 25 mL of diethyl ether (Et_2O) were added. After phase separation, the aqueous solution was extracted with Et_2O (2x25 mL). The organic phase was washed with water (3x10 mL) and dried with magnesium sulfate. The solvent was evaporated, and the product was purified by column chromatography on silica (petroleum ether as eluent). ^{1}H NMR (250 MHz, $CDCl_3$) δ ppm: 3.26 (t, 4H), 1.60 (m, 4H), 1.32 (m, 16H).

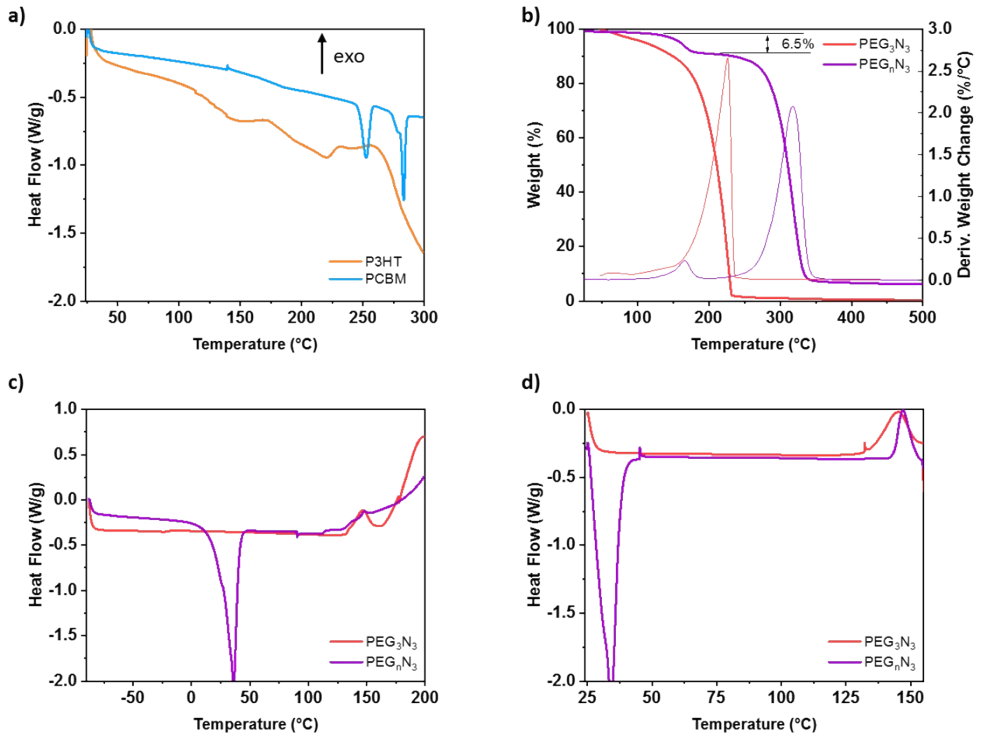

Figure S 2: Thermal gravimetric analysis and DSC plots of a) P3HT and $PC_{61}BM$, and b-d) cross-linkers PEG_3N_3 and PEG_nN_3 at different temperatures.

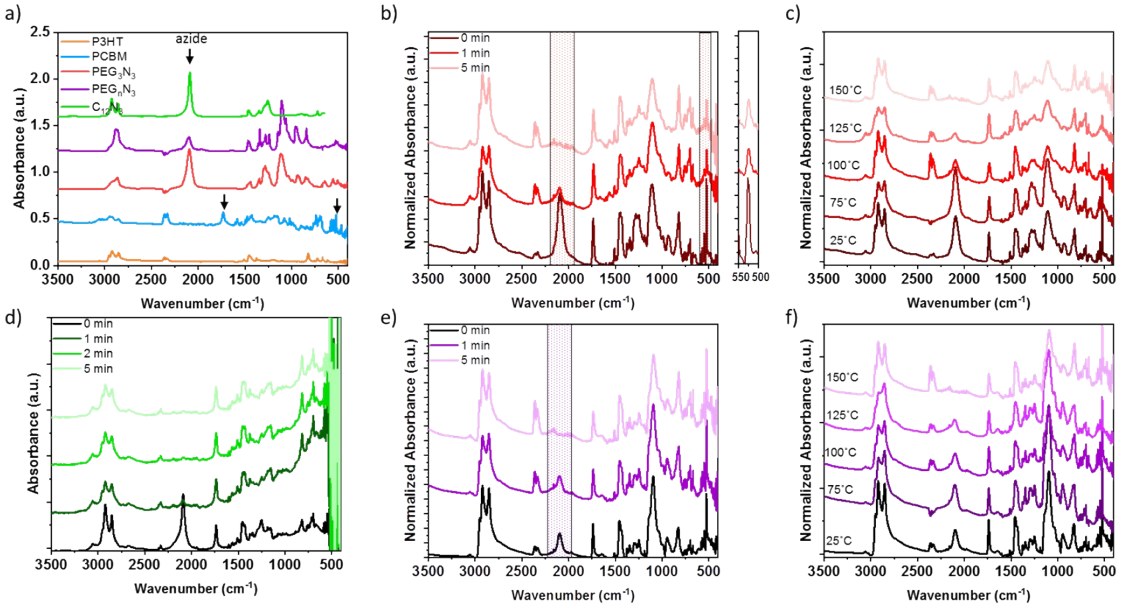

Figure S 3: FTIR spectra of a) the precursors before cross-linking. b) Kinetic of cross-linking via monitoring P3HT:$PC_{61}BM$:PEG_3N_3 after thermal annealing at 150°C. c) Temperature effect on P3HT:$PC_{61}BM$:PEG_3N_3, for 5min. d) Kinetic of P3HT:$PC_{61}BM$:$C_{12}N_3$ and e)P3HT:$PC_{61}BM$:PEG_nN_3 after thermal annealing at 150°C. f) Dependence of the temperature on the cross-linking of P3HT:$PC_{61}BM$:PEG_nN_3 during 5 min of curing.

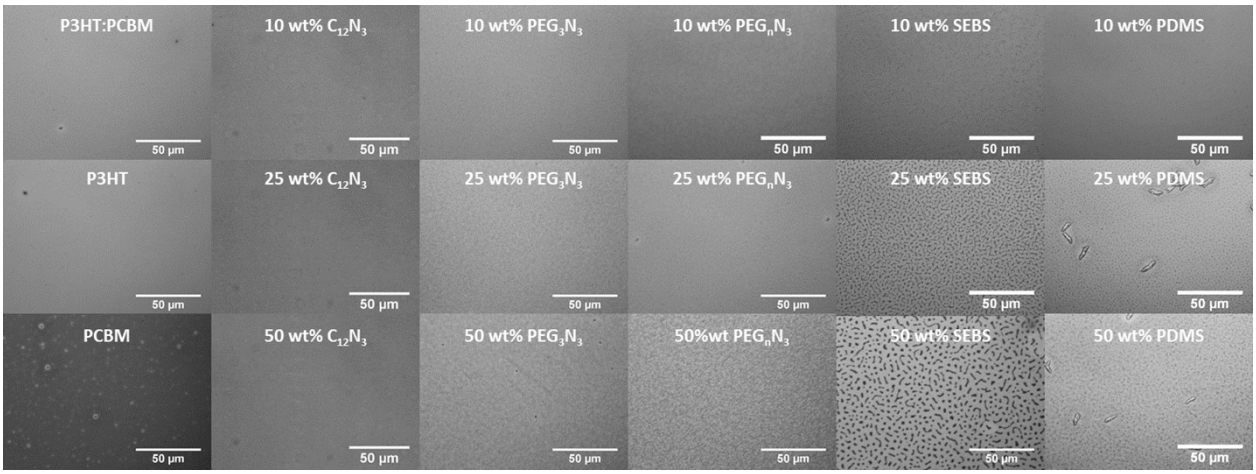

Figure S 4: Optical micrographs of P3HT, $PC_{61}BM$, and P3HT:$PC_{61}BM$ in the presence of additives as indicated in the picture after annealing.

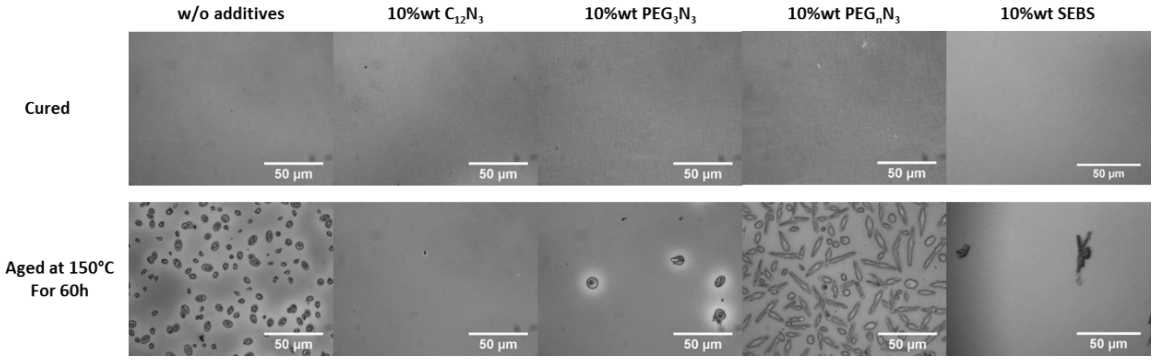

Figure S 5: Microscopic images of $PC_{61}BM$ aggregation in P3HT:$PC_{61}BM$ layer in the presence of additives at 10 wt% before and after aging for 60 h at 150°C.

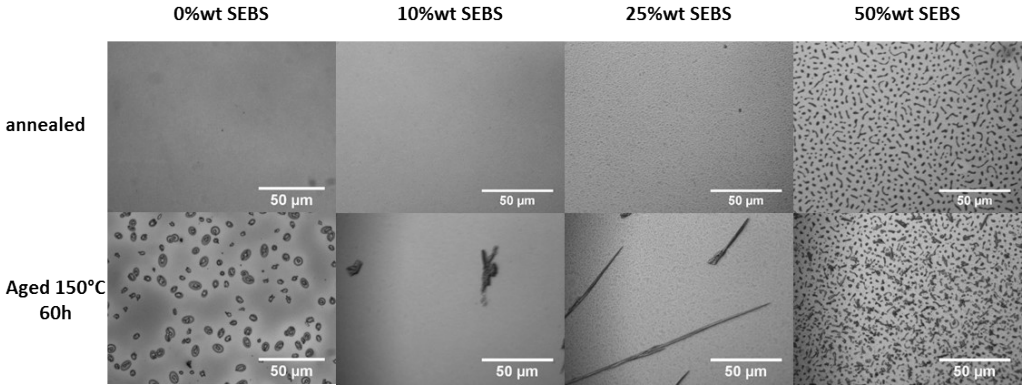

Figure S 6: Effect of the thermal aging on P3HT:$PC_{61}BM$ morphology taken by microscope regarding the SEBS content. The microscopic images show before and after aging of 60 h at 150°C.

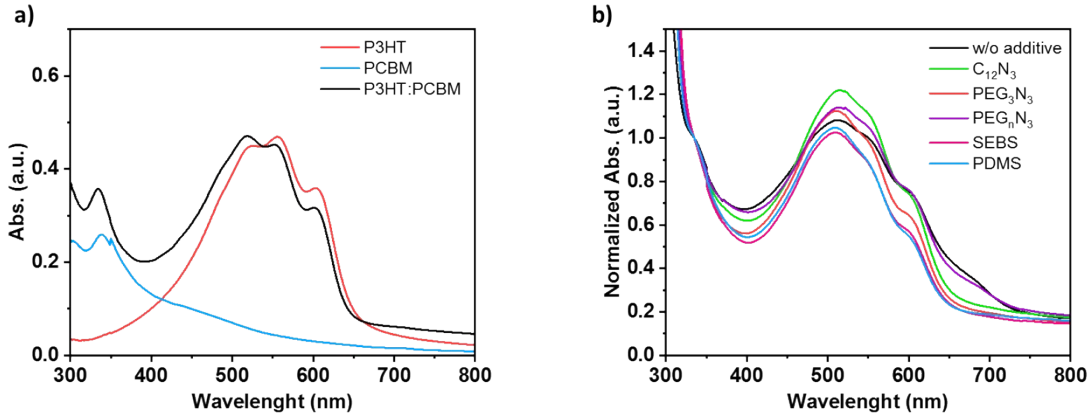

Figure S 7: UV-vis absorbance spectra obtained of a) casted $PC_{61}BM$, P3HT, and P3HT:$PC_{61}BM$ (1:0.8) blend and b) annealed P3HT:$PC_{61}BM$ film in the presence of additives at 50 wt%.

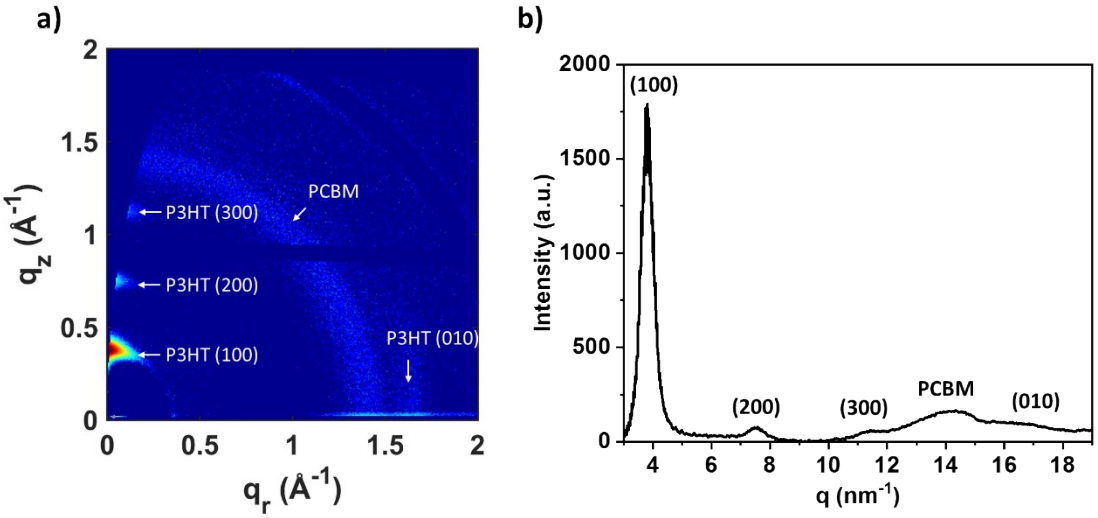

Figure S 8: a) Two-dimensional GIWAXS image of P3HT:$PC_{61}BM$ thin film and b) the resulting integration.

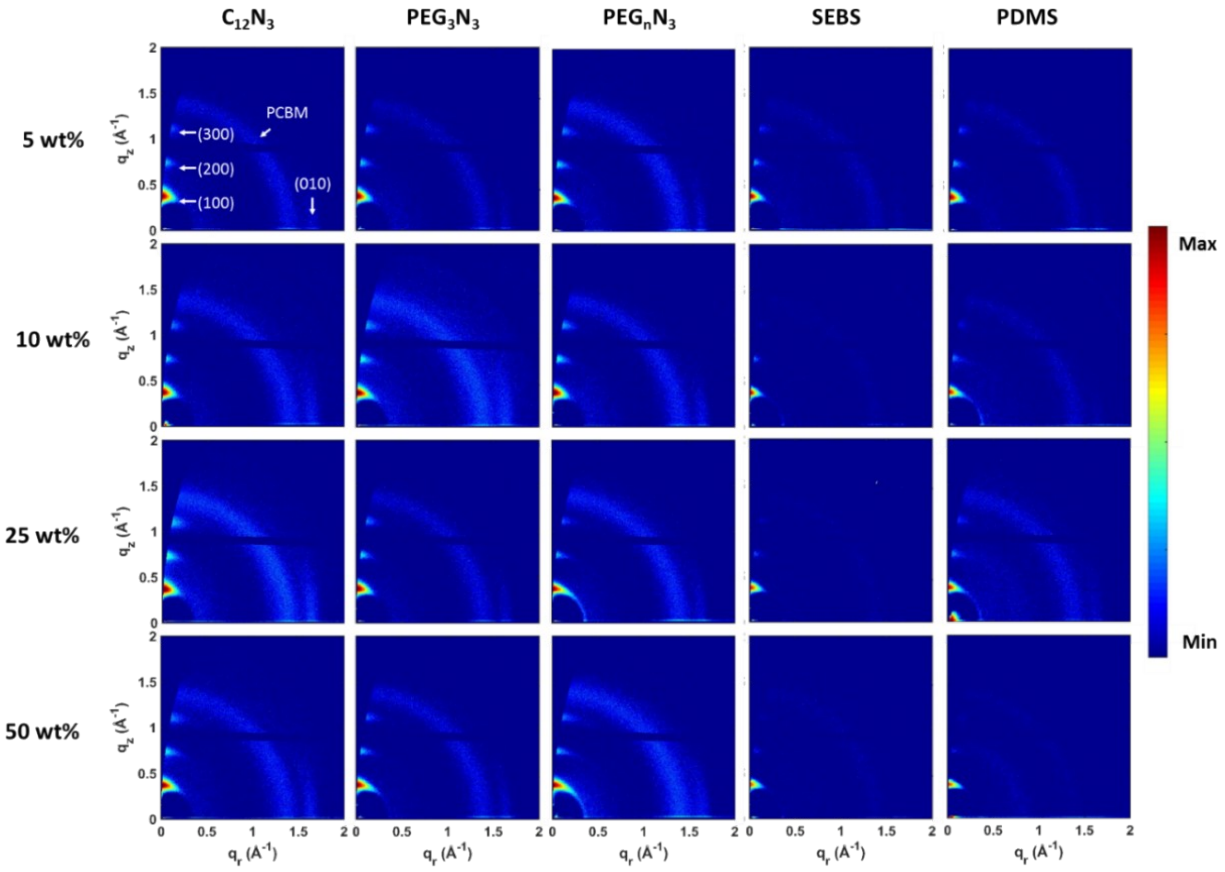

Figure S 9: 2D grazing incidence X-ray diffraction patterns of annealed P3HT:$PC_{61}BM$ blend with additives

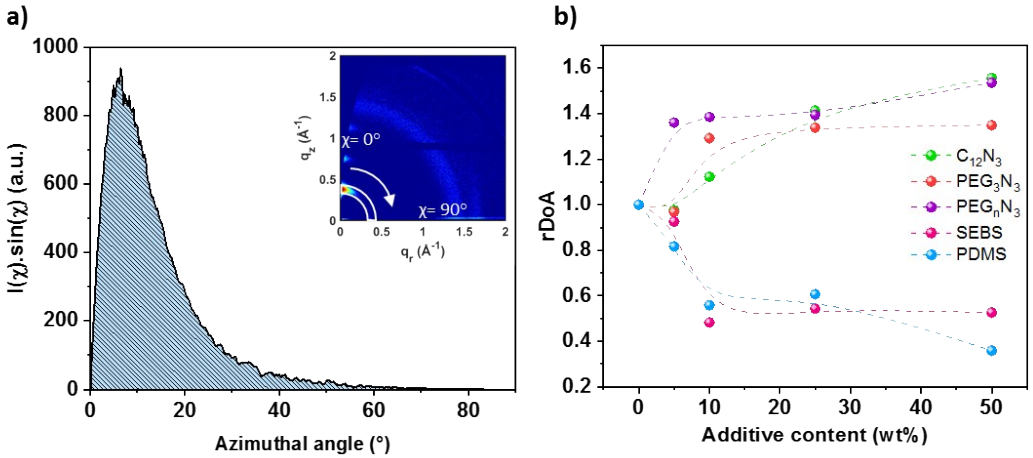

Figure S 10: a) Example of azimuthal integration of (100) P3HT lamella peak. b) The relative degree of aggregation to neat P3HT:$PC_{61}BM$ of (100) peak

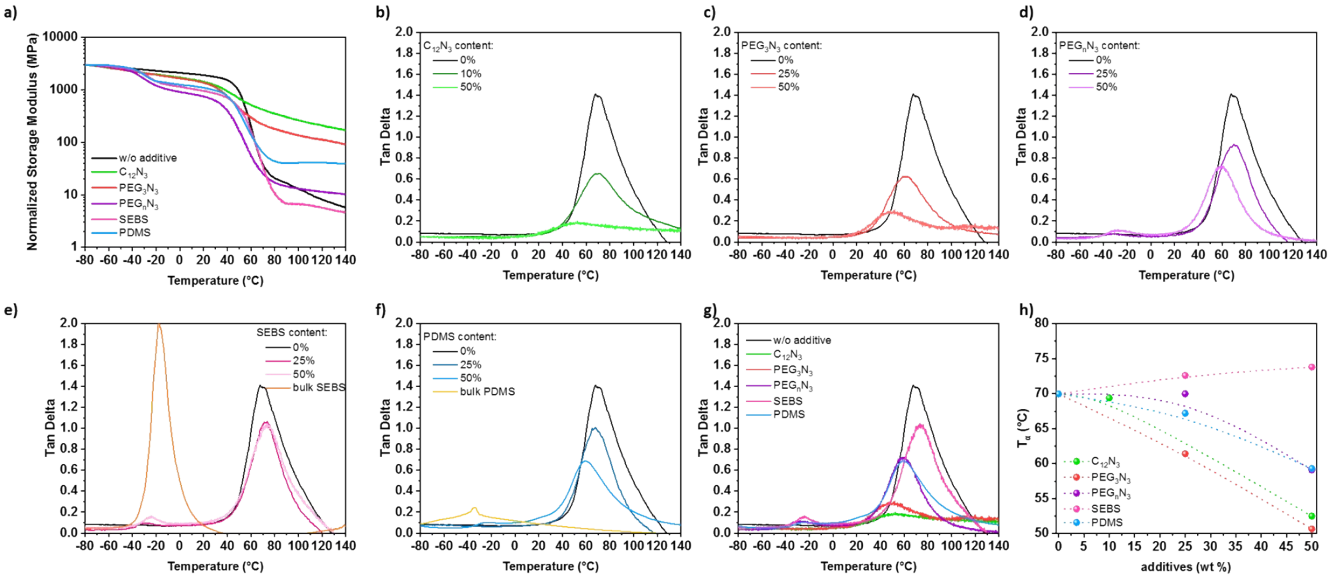

Figure S 11: Temperature dependence of a) storage modulus and Tan δ for the P3HT:$PC_{61}BM$:additive in presence of b) $C_{12}N_3$, c) PEG_3N_3, d) PEG_nN_n, e) SEBS, and f) PDMS. g) Comparison of Tan δ for P3HT:$PC_{61}BM$:additive composites (1:0.8:0.4), i.e., in the presence of 50 wt% additive and h) Summary of the glass temperature.

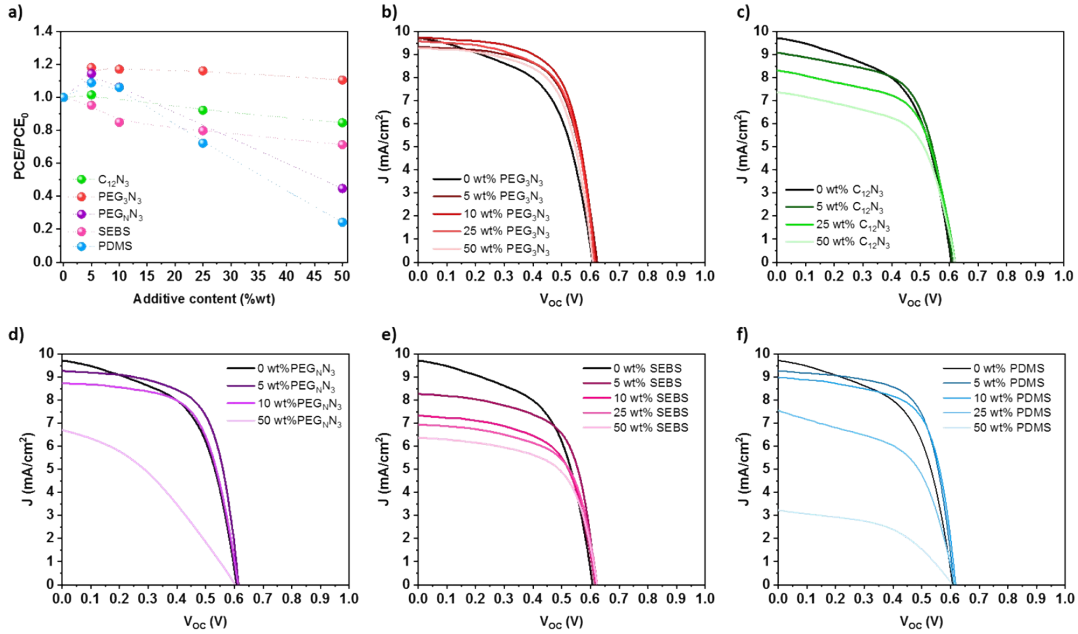

Figure S 12: Photovoltaic curves associated with P3HT:$PC_{61}BM$ solar cells in the presence of additives.

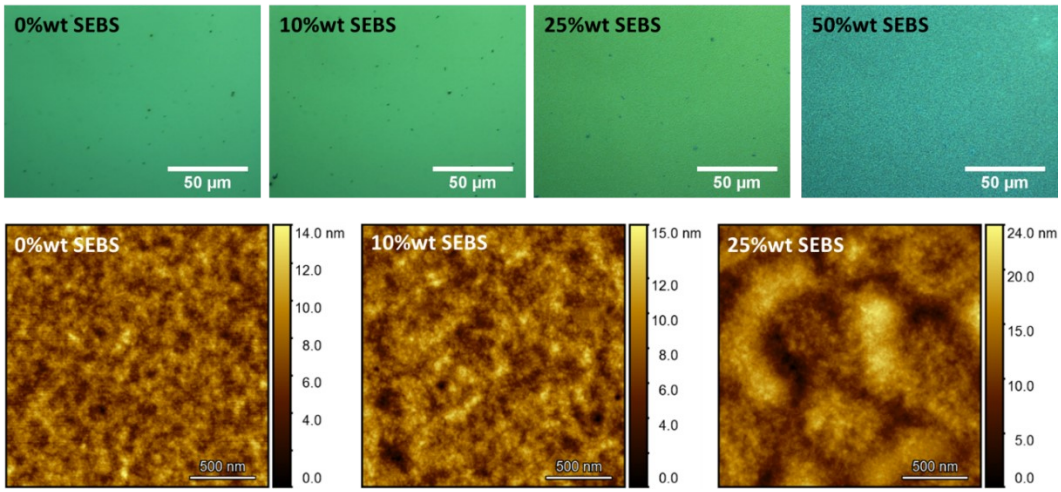

Figure S 13: PCE10:$PC_{71}BM$:SEBS morphology characterized by optical microscopy (top row) and atomic force microscopy (bottom row).

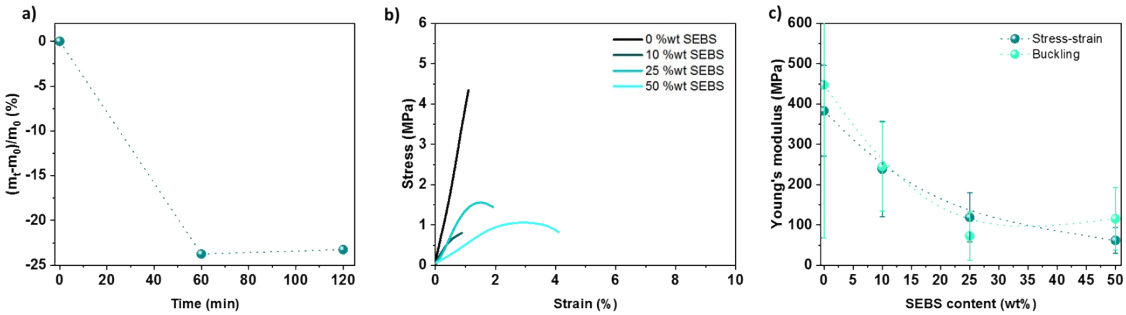

Figure S 14: a) Mass loss of PCE10:$PC_{71}BM$ under vacuum at 50°C after MeOH treatment. b) Characterization stress-strain after vacuum drying at 50°C for 90 min. c) Young's moduli by stress-strain or buckling methods with different amount of SEBS (wt%/wt $PC_{71}BM$).

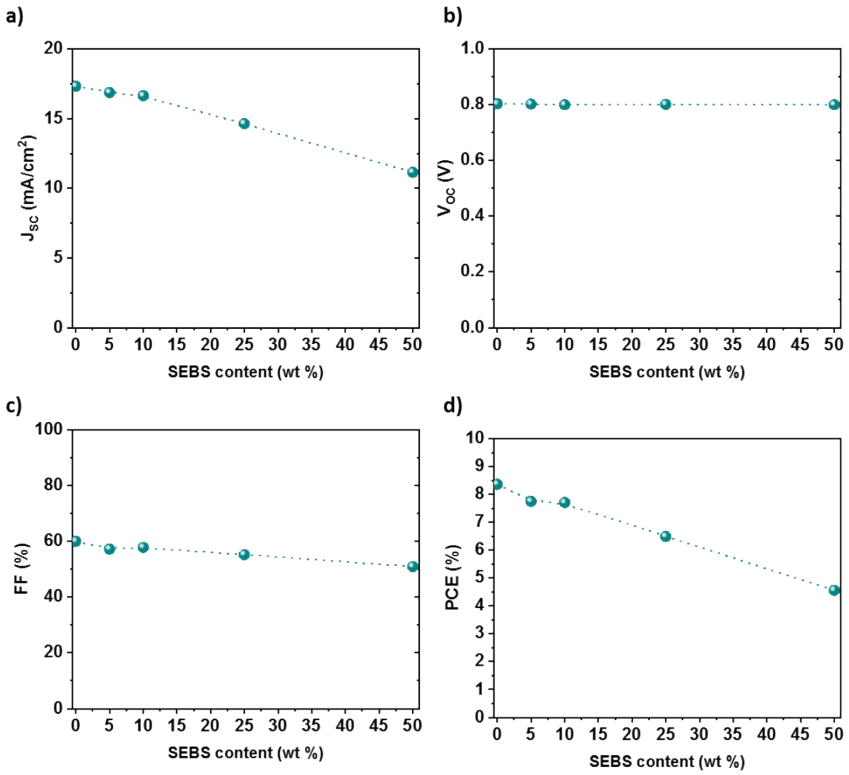

Figure S 15: Evolution of the photovoltaic characteristics of PCE10:$PC_{71}BM$ blend in the function of SEBS additive content.

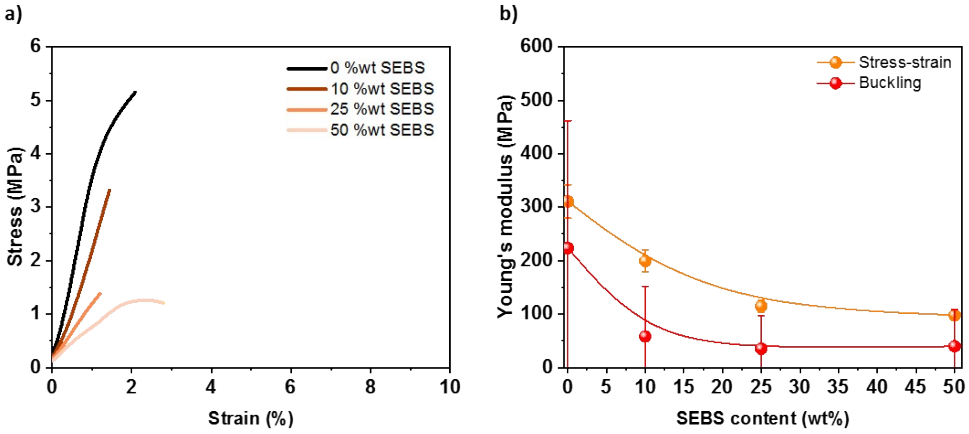

Figure S 16: Determination of Young's moduli: a) stress-strain curves of PCE13:IT-4F with 0, 10, 25, and 50 wt% SEBS and b) comparison of Young's moduli by buckling method or direct measurements by stress-strain.

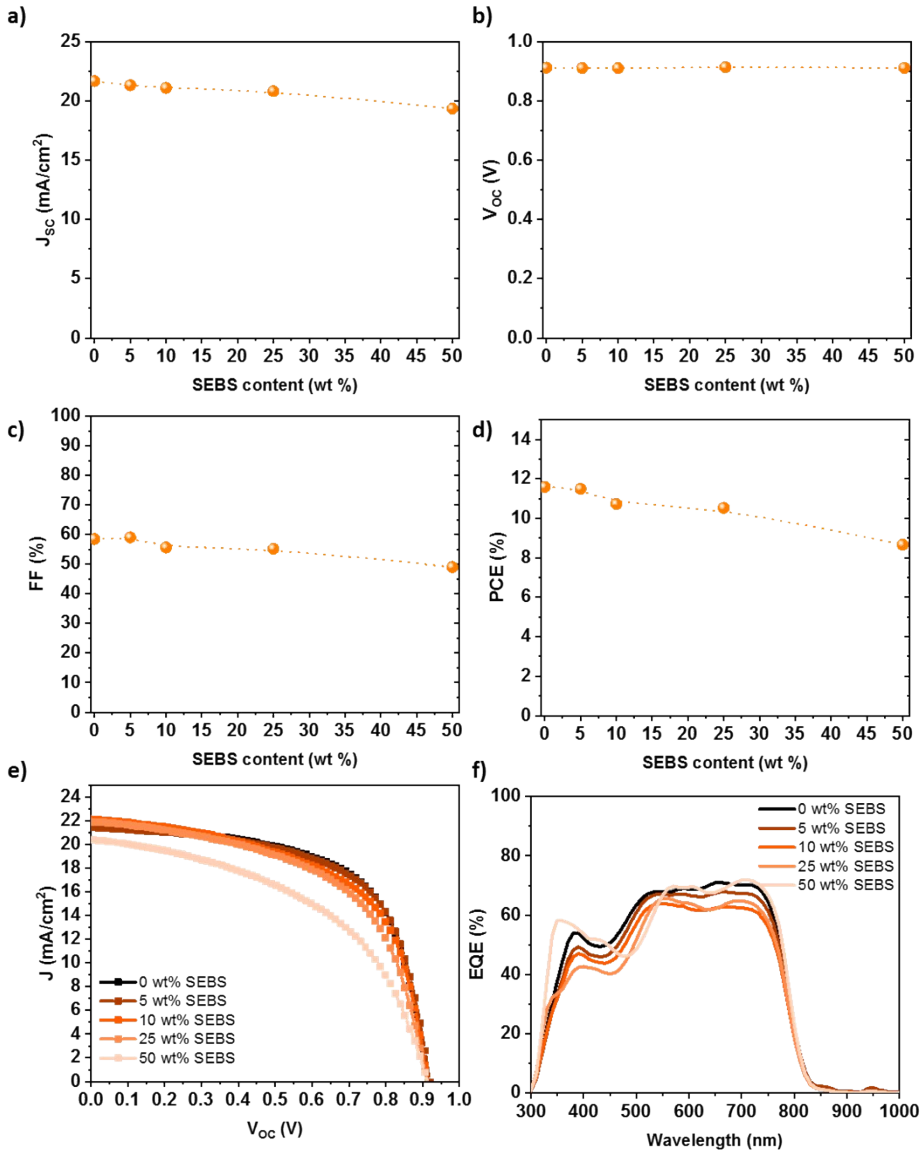

Figure S 17: Photovoltaic performances of PCE13:IT-4F with different amounts of SEBS elastomer.

References

[1] J. R. Thomas, X. Liu, P. J. Hergenrother, *J. Am. Chem. Soc.* **2005**, *127*, 12434.