Electronic Supplementary Material (ESI) for RSC Advances


# Supporting Information

# A dual-functional additive improves the performance of molecular bulk heterojunction photovoltaic cells

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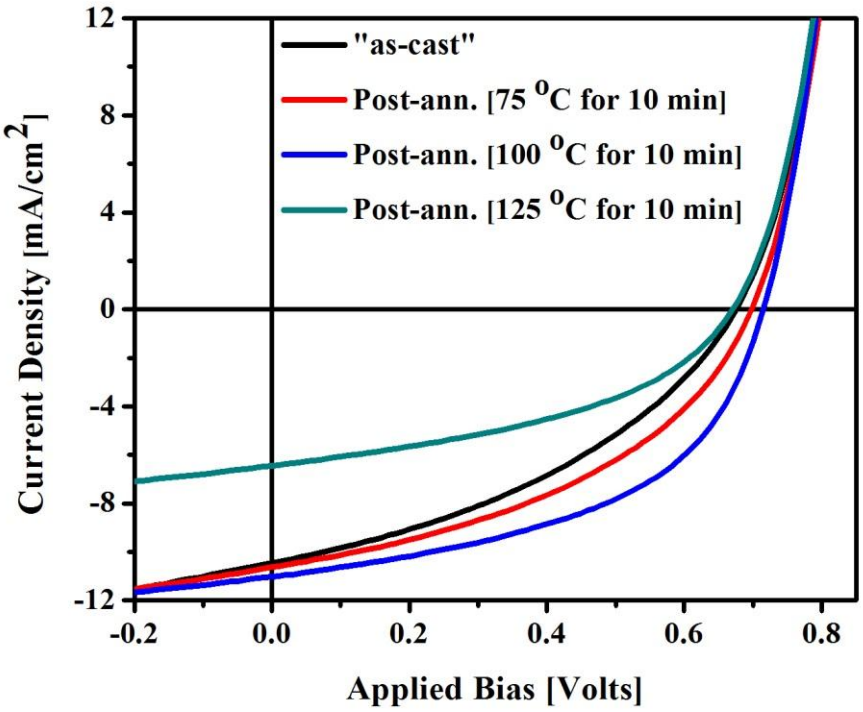



**Figure S1.** *J–V* characteristics of devices prepared without the additive and subjected to different post-annealing temperatures.

**Table S1.** Photovoltaic characteristics of devices prepared without the additive and subjected to different post-annealing temperatures.

| Annealing Temp. [$^{o}$C] | $J_{sc}$ [mA/cm$^2$] | $V_{oc}$ [V] | FF [%] | PCE [%] |
|---|---|---|---|---|
| "as-cast" | 10.46 | 0.68 | 38.66 | 2.75 |
| 75°C | 10.60 | 0.70 | 42.45 | 3.15 |
| 100 °C | 10.20 | 0.71 | 48.33 | 3.50 |
| 125°C | 6.45 | 0.67 | 43.04 | 1.86 |

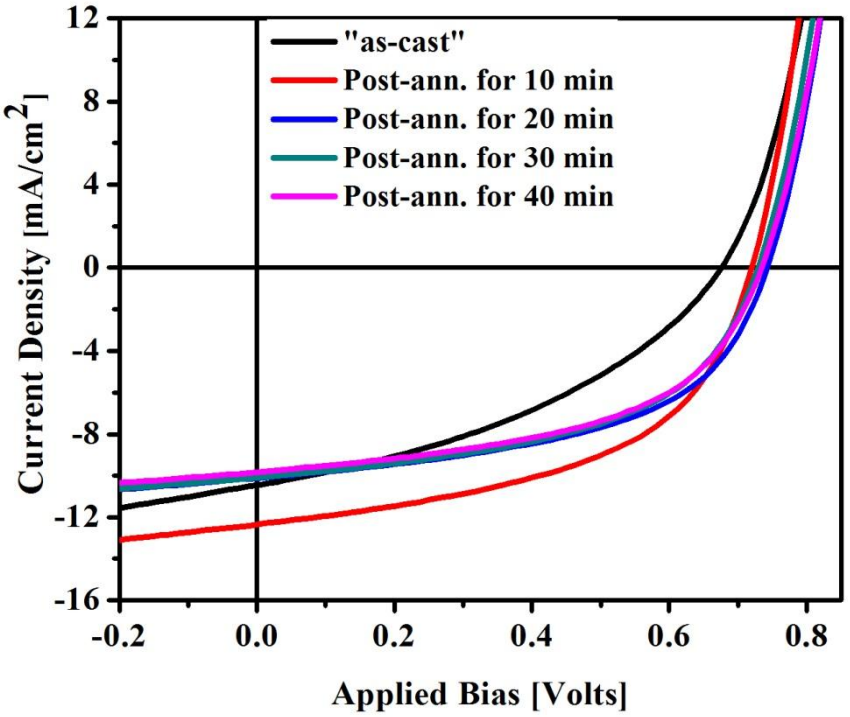



**Figure S2.** *J–V* characteristics of devices prepared with 0.1% of the additive CP3MS and post-annealing at 100 °C for different lengths of time.

**Table S2.** Photovoltaic characteristics of devices incorporating 0.1% of the additive that had been subjected to post-annealing at 100 °C for different lengths of time.

| Annealing Time [min] | $J_{sc}$ [mA/cm$^2$] | $V_{oc}$ [V] | FF [%] | PCE [%] |
|---|---|---|---|---|
| "as-cast" | 10.46 | 0.68 | 38.66 | 2.75 |
| 10 | 12.36 | 0.72 | 51.14 | 4.55 |
| 20 | 10.13 | 0.74 | 52.43 | 3.93 |
| 30 | 10.09 | 0.73 | 51.45 | 3.79 |
| 40 | 9.85 | 0.73 | 51.87 | 3.73 |

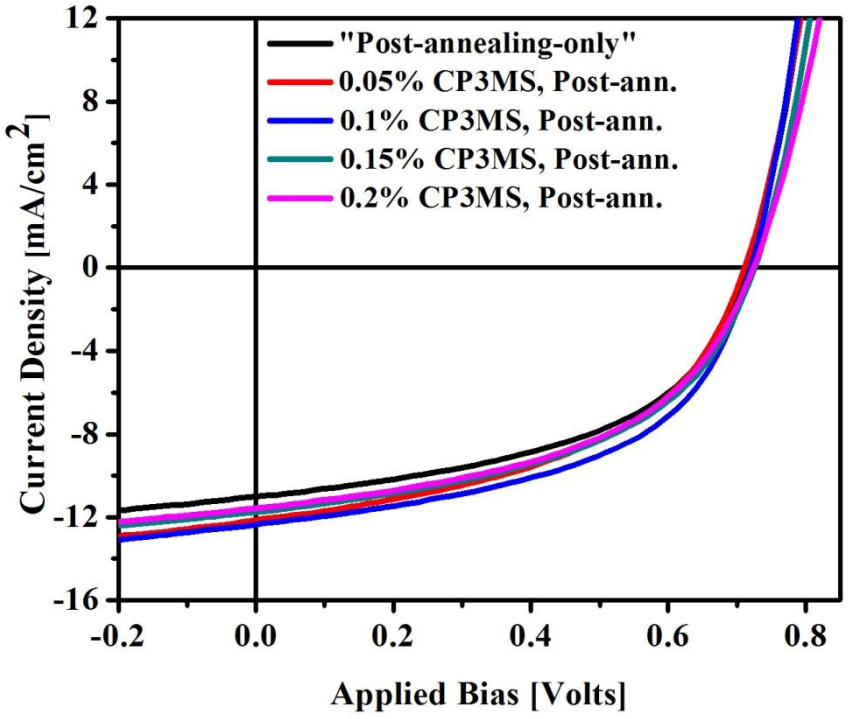



**Figure S3.** *J–V* characteristics of devices prepared with different CP3MS concentrations and post-annealing at 100 °C for 10 min.

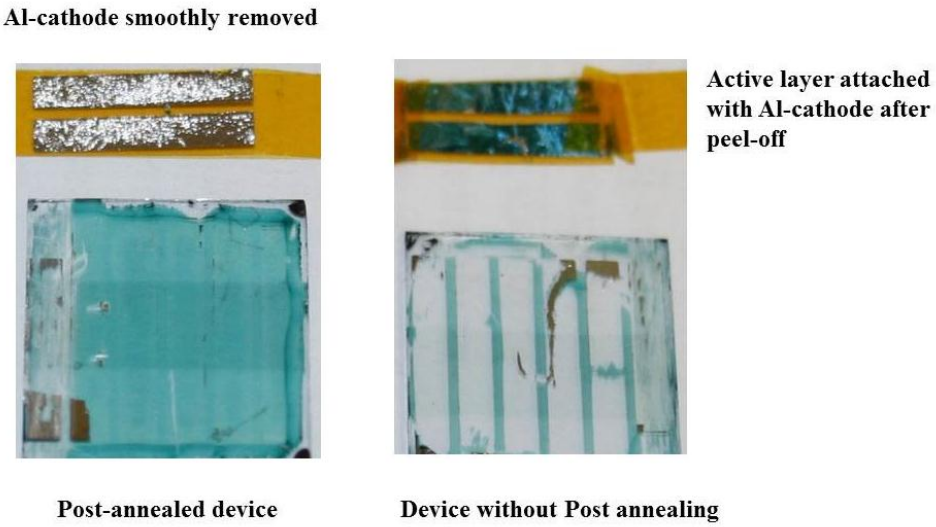



**Figure S4.** Digital camera images showing the effect of post-annealing treatment on the interface between the active layer and the metal cathode.

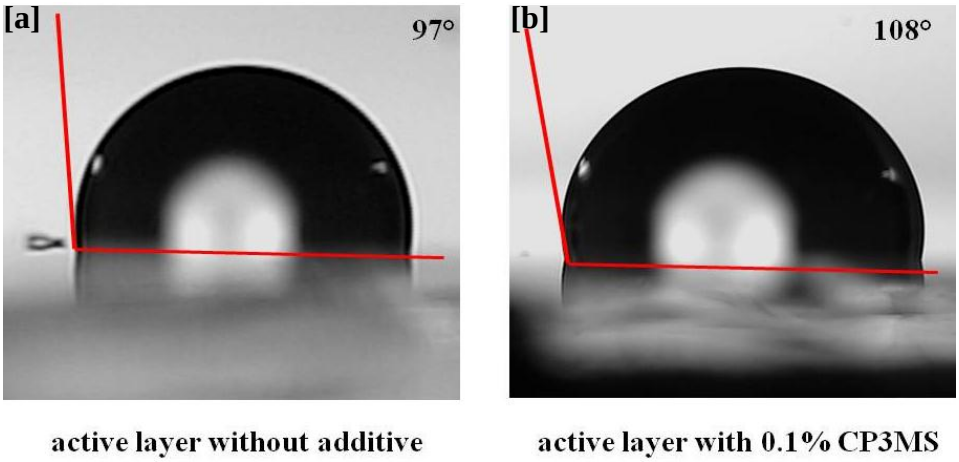
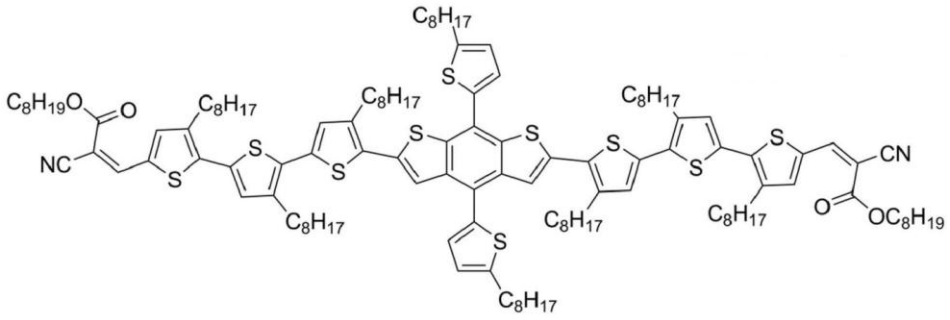



**Figure S5.** Images of contact angles of active layers without additive (a) and with 0.1% CP3MS additive (b)




**Scheme S1.** Chemical structure of benzodithiophene (BDT)-based molecule (TBDTCNR)

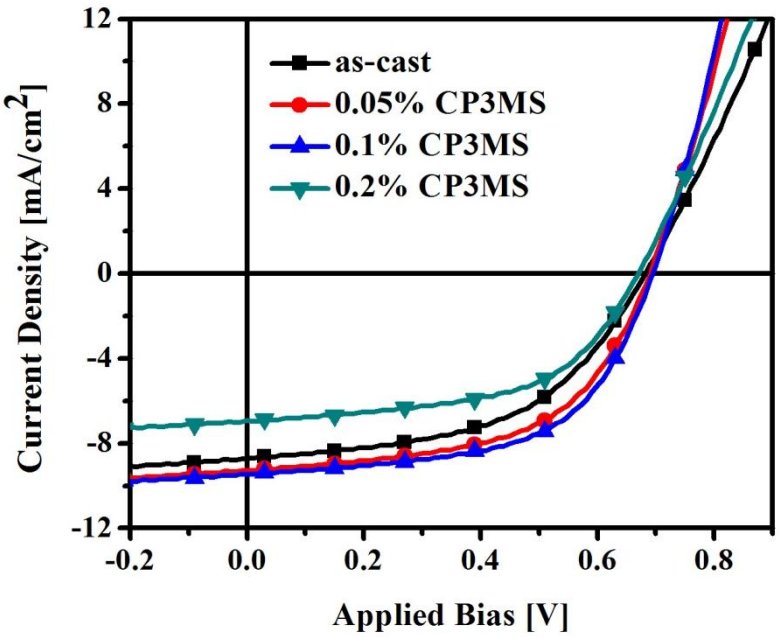



**Figure S6:** *J–V* characteristics of devices prepared with different CP3MS concentrations for benzodithiophene (BDT)-based molecule (TBDTCNR)

**Table S3.** Photovoltaic characteristics of devices prepared with different CP3MS concentrations for benzodithiophene (BDT)-based molecule (TBDTCNR).

| Additive Conc. [%] | $J_{sc}$ [mA/cm$^2$] | $V_{oc}$ [V] | FF [%] | PCE [%] |
|---|---|---|---|---|
| "as-cast" | 8.70 | 0.68 | 51.56 | 3.05 |
| 0.05% CP3MS | 9.26 | 0.69 | 55.25 | 3.53 |
| 0.10% CP3MS | 9.46 | 0.70 | 57.38 | 3.80 |
| 0.20% CP3MS | 6.92 | 0.67 | 55.22 | 2.56 |