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


# Supporting Information

## Dehydration of Molybdenum Oxide Hole Extraction Layers via Microwave Annealing for Efficiency and Lifetime Improvement in Organic Solar Cells

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**Table S1.** Possible Mo oxides in $MoO_x$ films and indexing of the various peaks observed in the XRD spectra in Figure 2 b of the main manuscript.

| **2θ (degrees)** | **Possible Compound** | **Crystallographic Plane** |
|---|---|---|
| 23.32 | $MoO_3$ | [1 0 0], [0 2 0], [1 1 0] |
| | $Mo_9O_{26}$ | [-1 3 1], [ -1 1 1] |
| 25.07 | $Mo_9O_{26}$ | [-2 1 1] |
| 25.71 | $MoO_3$ | [0 0 2], [0 2 0], [0 4 0], [2 1 0] |
| | $Mo_9O_{26}$ | [-1 1 2] |
| 27.32 | $MoO_3$ | [0 1 1], [0 2 1] |
| | $Mo_9O_{26}$ | [2 -3 1], [-3 1 0] |
| | $Mo_4O_{11}$ | [6 1 0] |
| | $Mo_9O_{23}$ | [1 1 2] |
| | $Mo_{17}O_{47}$ | [3 2 1] |
| 38.99 | $MoO_3$ | [1 0 2], [0 6 0], [0 2 0] |
| 45.87 | $MoO_3$ | [0 0 8], [2 0 0] |
| | $Mo_9O_{23}$ | [1 2 1] |
| 49.24 | $MoO_3$ | [0 2 0], [2 2 0], [0 0 2] |
| | $Mo_9O_{26}$ | [5 1 5] |
| 51.48 | $Mo_4O_{11}$ | [-8 1 3] |
| 52.75 | $MoO_3$ | [1 0 -4], [2 1 1], [0 8 0] |
| | $Mo_9O_{26}$ | [ 3 2 3] |
| | $Mo_4O_{11}$ | [2 3 1] |
| 55.16 | $MoO_3$ | [1 2 0], [0 2 2], [1 1 2] |
| | $Mo_9O_{23}$ | [3 1 6] |
| | $Mo_4O_{11}$ | [11 2 1] |
| 61.71 | $MoO_3$ | [2 6 0], [4 3 0] |

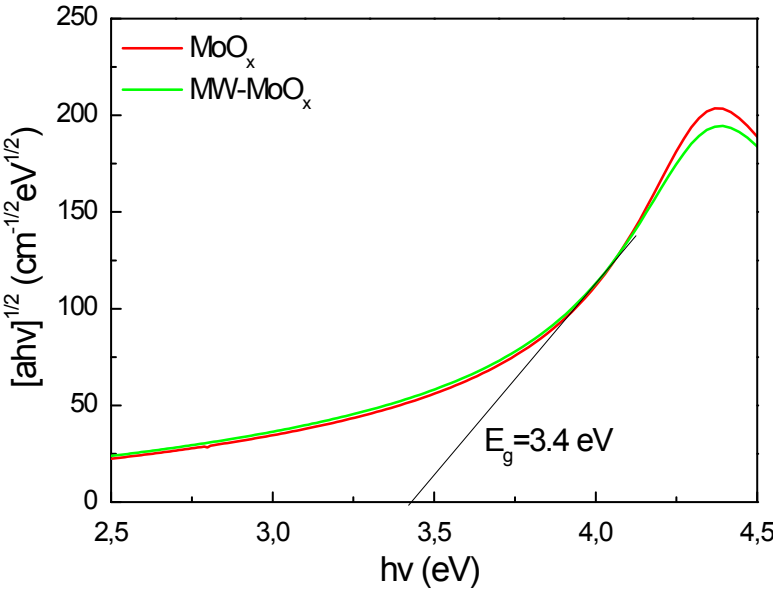



**Figure S1** Tauc plot, as derived from absorption measurements, of 30 nm thick as-deposited hydrogenated under-stoichiometric and the microwave annealed Mo oxide films for the estimation of optical energy band gap.

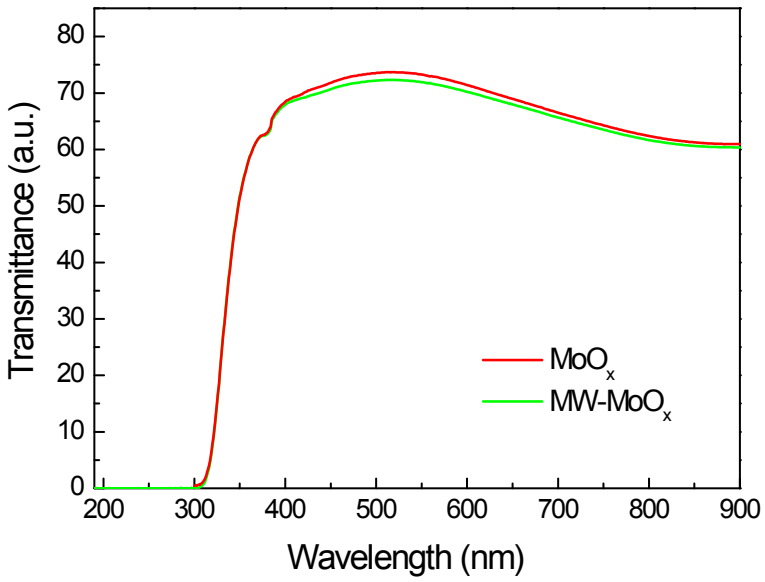



**Figure S2** Transmittance spectra of the as-deposited Mo oxide film and the MW-annealed one deposited on glass/FTO substrates.

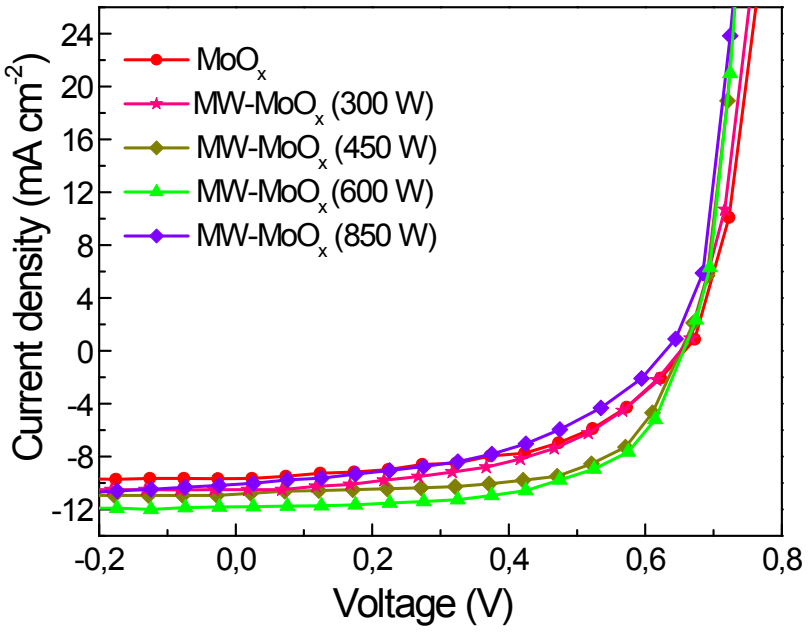



**Figure S3** J-V curves of devices with $MoO_x$ interlayers for different heating powers.

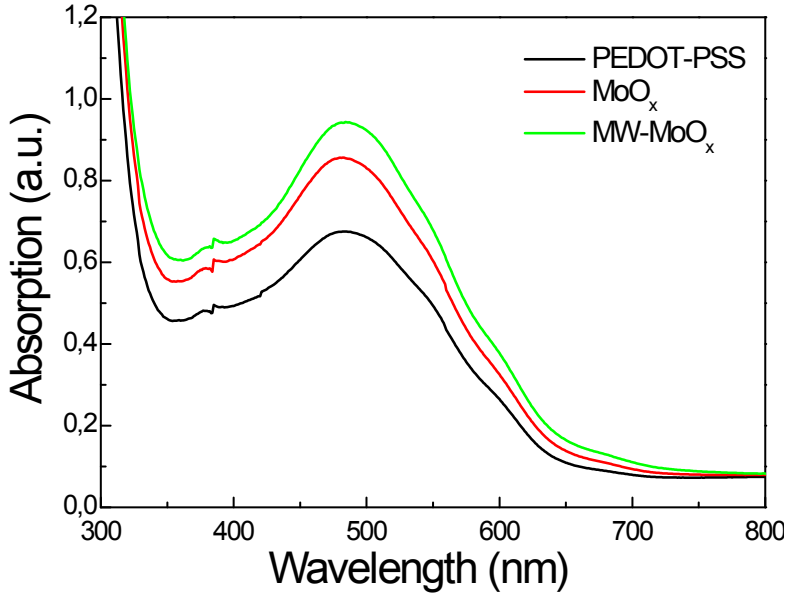
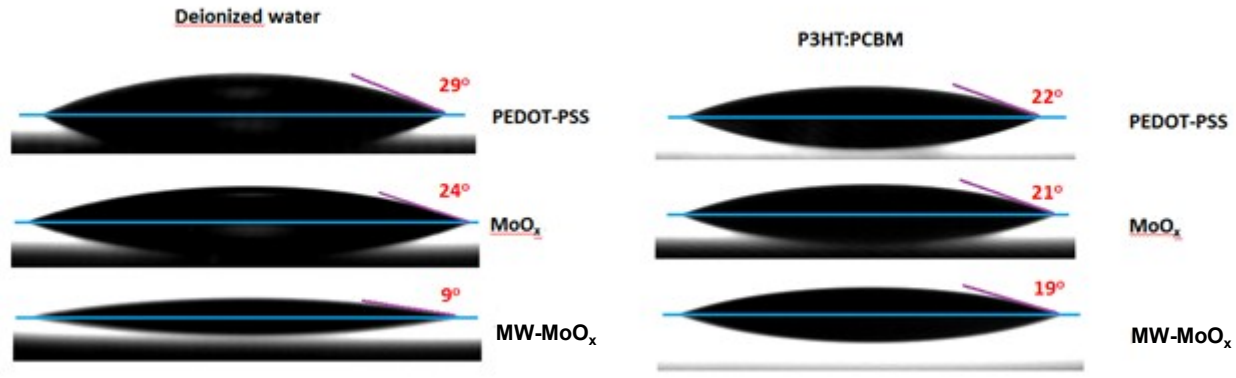



**Figure S4** Absorption spectra of the P3HT:$PC_{71}$BM blend films spin-coated on Mo oxide layers subjected (or not) to microwave annealing after deposition.




**(a)** **(b)**

**Figure S5** Measured contact angle between a drop of (a) deionized water and (b) P3HT:$PC_{71}BM$ blend and Mo oxide films as deposited or being subjected to microwave annealing.

**Table S2** Polar and non-polar components of surface energies of the PEDOT:SS, Mo oxide and MW-annealed Mo oxide substrates as calculated from contact angle measurements results.

| **Substrate** | **$\theta_w$ (°)** | **$\theta_i$ (°)** | **$\gamma_s^p$ (mJ/m$^2$)** | **$\gamma_s^d$ (mJ/m$^2$)** | **$\gamma$ (mJ/m$^2$)** |
|---|---|---|---|---|---|
| **PEDOT:PSS** | 29.0 | 35.4 | 34.5 | 31.4 | 65.9 |
| **$MoO_x$** | 24.0 | 14.2 | 32.5 | 38.3 | 70.8 |
| **MW-$MoO_x$** | 9.0 | 12 | 37.5 | 37.9 | 75.4 |

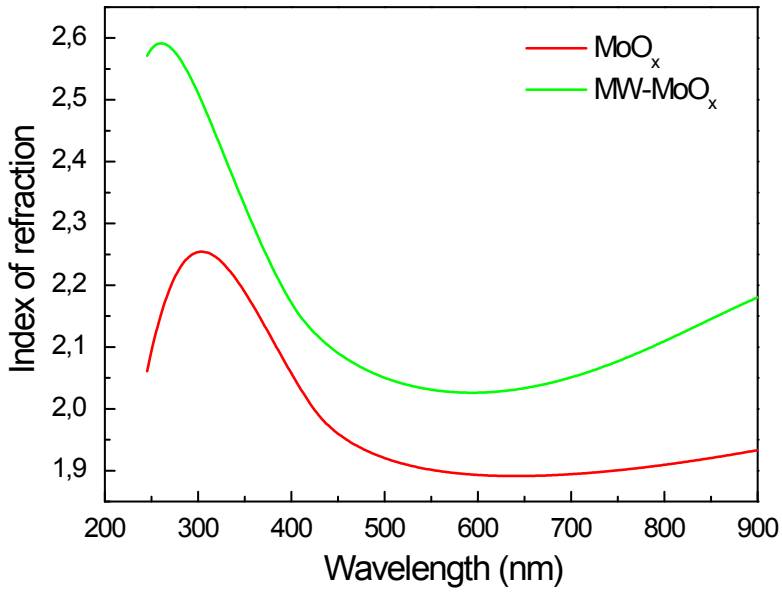



**Figure S6** Variation of the refractive index of $MoO_x$ and MW-annealed $MoO_x$ films.

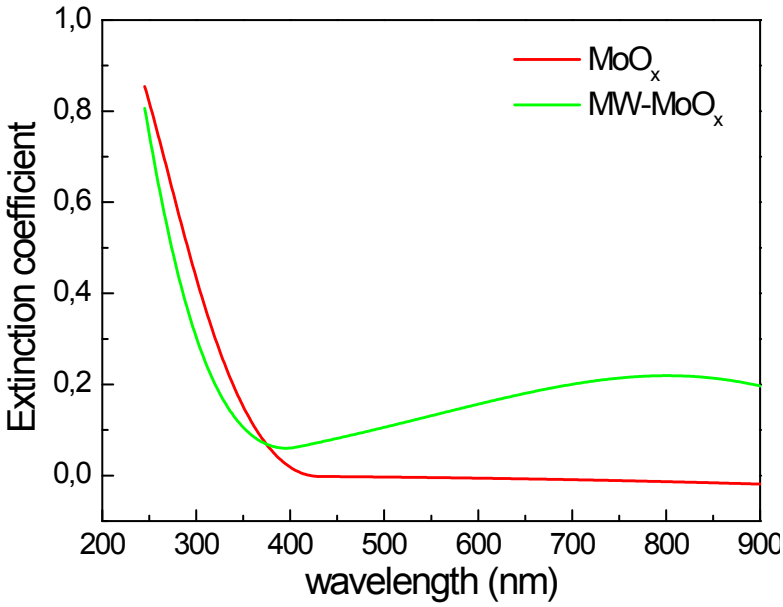



**Figure S7** Variation of the extinction coefficient of $MoO_x$ and MW-annealed $MoO_x$ films.

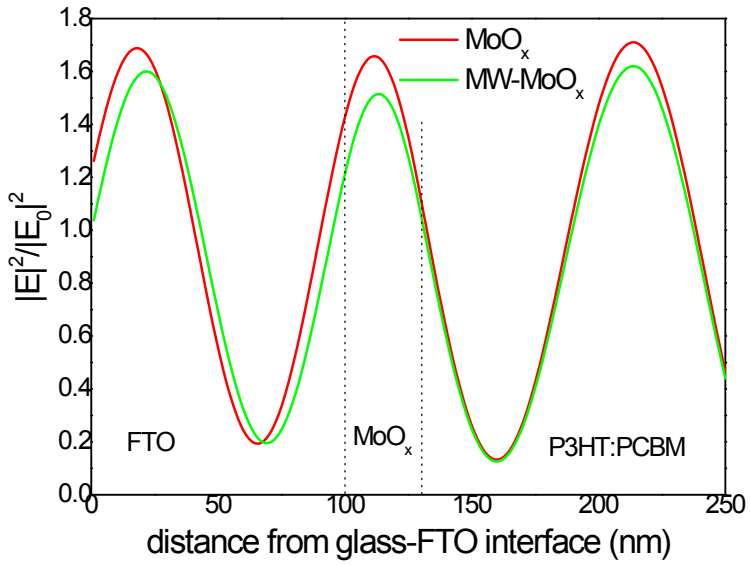



**Figure S8** Distribution of the normalized optical intensity of incident light within the device (estimated for an incident light with a wavelength of 530 nm where the maximum of the photoactive blend absorption occurs).