

Supplementary Materials

Optimized Stoichiometry for CuCrO₂ Thin Films as Hole Transparent Layer in PBDD4T-2F:PC₇₀BM Organic Solar Cells

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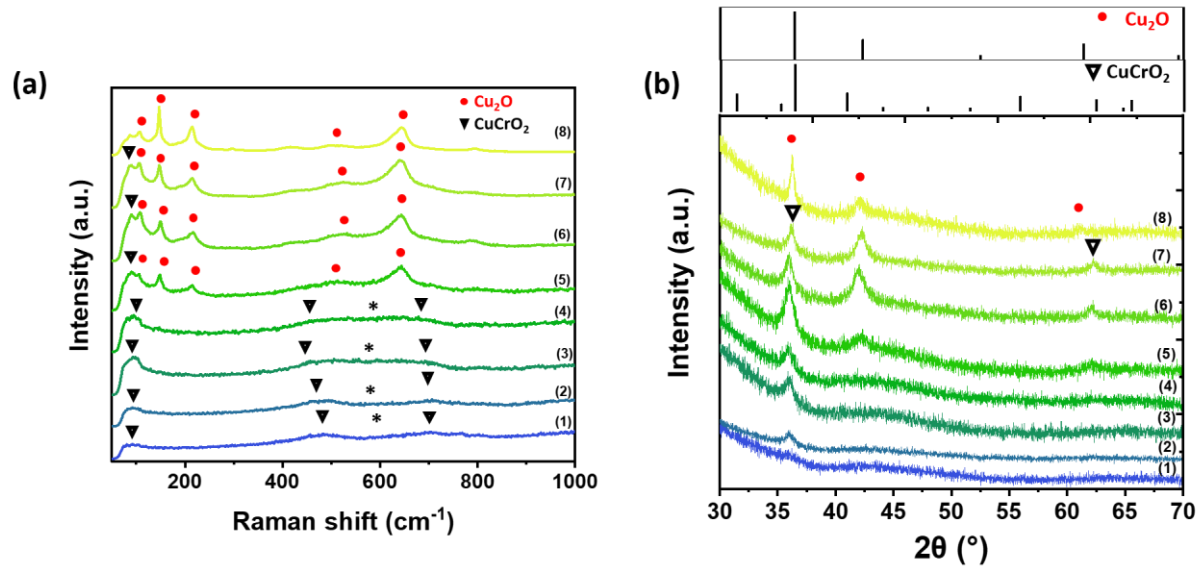


Figure S1. Structural properties of out of stoichiometry CuCrO_2 thin films. (a) Raman spectra of out of stoichiometry CuCrO_2 thin films with a Cu cationic ratio in the solution, X , of (1) 40%, (2) 50%, (3) 60%, (4) 65%, (5) 67%, (6) 70%, (7) 80%, (8) 100%. The red dots correspond to Cu_2O Raman modes, black triangles to CuCrO_2 ones. Defects related Raman modes are indicated with *. (b) XRD pattern of the same samples. The top windows show the ICDD references of rhombohedral CuCrO_2 delafossite structure (space group $R\bar{3}m$, ICDD 04-010-3330), and cubic Cu_2O (space group $Pn\bar{3}m$, ICDD 00-005-0667).

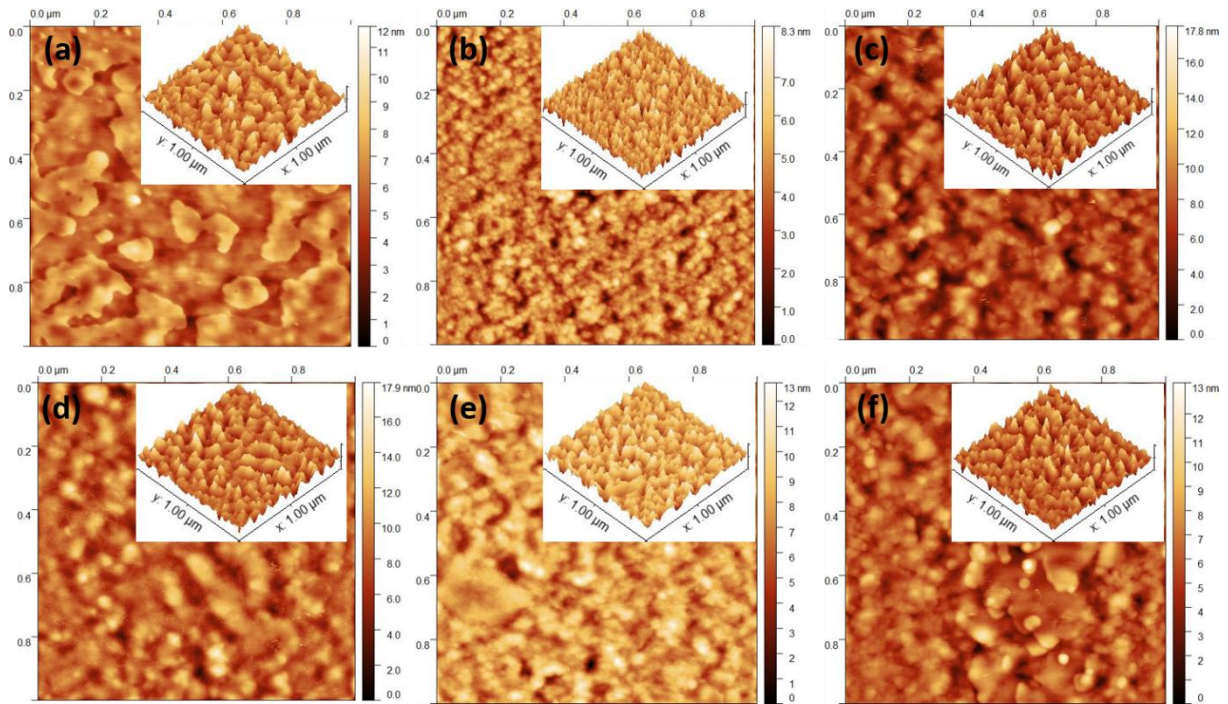


Figure S2. AFM measurement for out of stoichiometry CuCrO_2 thin films. Top view of samples synthesized from a solution with a Cu cationic ratio, X , of (a) 40%, (b) 50%, (c) 60%, (d) 65%, (e) 70%, and (f) 100%. Each inset represents the corresponding 3D mapping of each sample. The measured values of root mean square (RMS) roughness values are 1.3 nm, 1.0 nm, 2.1 nm, 2.0 nm, 1.4 nm, 1.5 nm for X of 40%, 50%, 60%, 65%, 70%, and 100%, respectively.

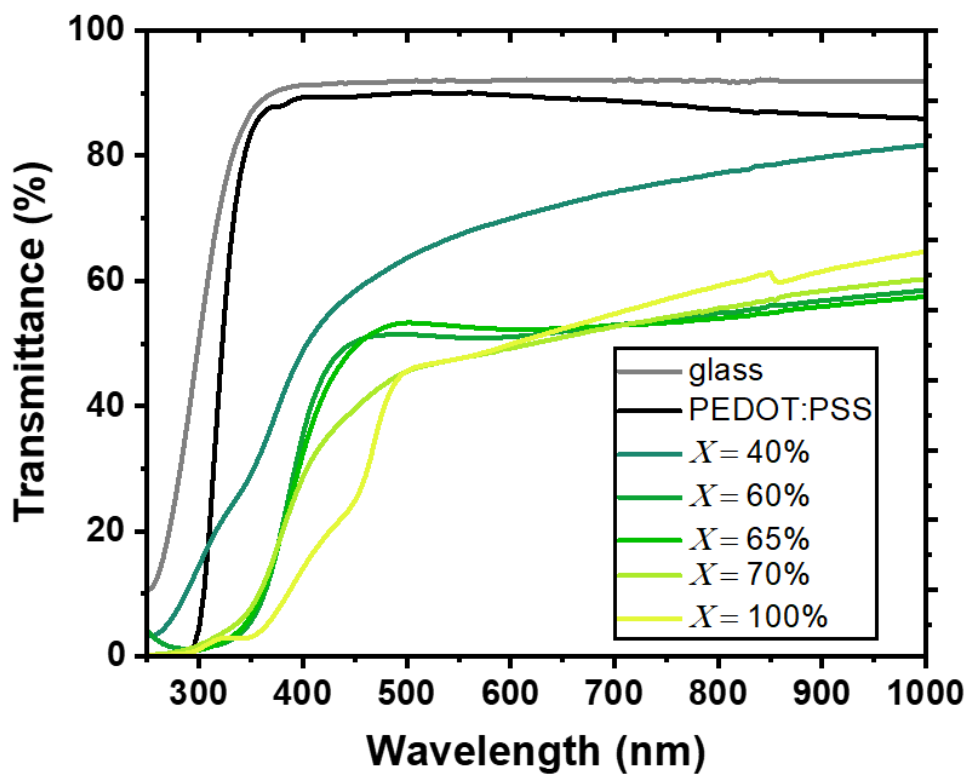


Figure S3. Transmittance spectra of the CuCrO_2 reference for various Cu cationic ratio in the solution, X , deposited on corning glass. The substrate, as well as the spin-coated PEDOT:PSS are shown as comparison.

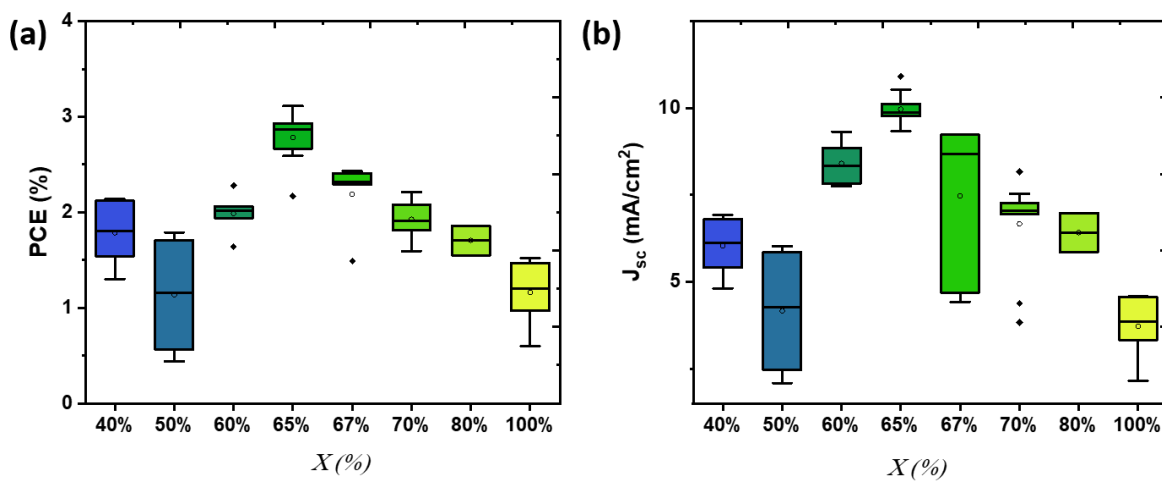


Figure S4. Statistical dispersion of the performances for OSC with out of stoichiometry CuCrO_2 thin films as HTL. a) box chart of the PCE calculated from the J-V characteristic under AM 1.5 illumination as a function of the Cu cationic ratio in the solution, X . b) box plot of the variation of the J_{sc} with X . The percentiles are set to 95% whisker top, 75% box top, 25% box bottom, and 5% whisker bottom for each data set.

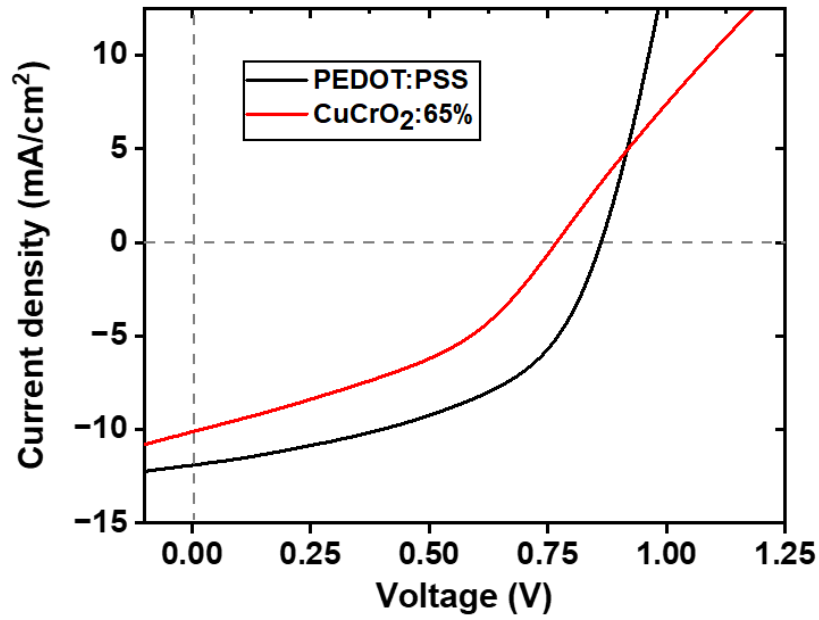


Figure S5. Comparison of J-V characteristic under A.M. 1.5 illumination of OSC with a HTL of PEDOT:PSS and of CuCrO₂: 65%.

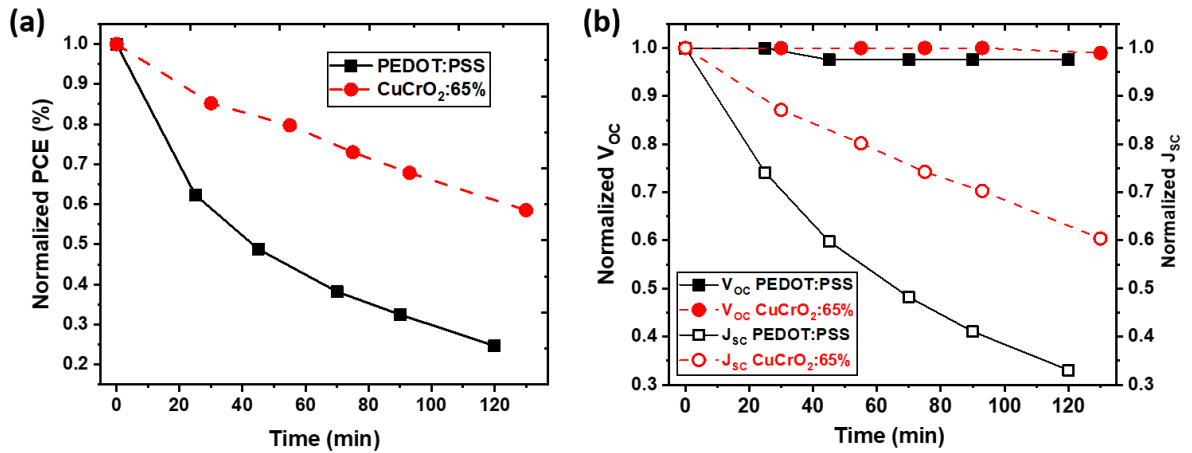


Figure S6. Evolution as function of the time under atmospheric conditions of the performances of the OSC. a) Normalized PCE of PEDOT:PSS-based device (black squares) and CuCrO₂: 65% OSC (red circles). b) Normalized open circuit voltage, V_{oc} (left axis and full symbols) and normalized short circuit current density, J_{sc} (right axis and empty symbols) for the same devices. These values are normalized respect the value measured prior exposure to air.