Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Supplementary Information

Organic-Inorganic doped Nickel Oxide Nanocrystals for Hole Transport Layers in Inverted Polymer Solar Cells with Color Tuning

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Samples	Feeding molar % of dopant for synthesis	Atom	Experimental molar (%at.)
Cu-$NiO_{x(1.9\%)}$	**2%**	**Ni**	**98.1**
		Cu	**1.9**
Cu-$NiO_{x(2.4\%)}$	**3%**	**Ni**	**97.6**
		Cu	**2.4**
Cu-$NiO_{x(4.5\%)}$	**5%**	**Ni**	**95.5**
		Cu	**4.5**
Cu-$NiO_{x(8.4\%)}$	**10%**	**Ni**	**91.6**
		Cu	**8.4**
Cu-$NiO_{x(12.2\%)}$	**15%**	**Ni**	**87.8**
		Cu	**12.2**
Cu-$NiO_{x(15.5\%)}$	**20%**	**Ni**	**84.5**
		Cu	**15.5**

Table S-1. Atomic percentage of the experimental doping levels of Cu-doped NiO_x NPs as determined by AAS.

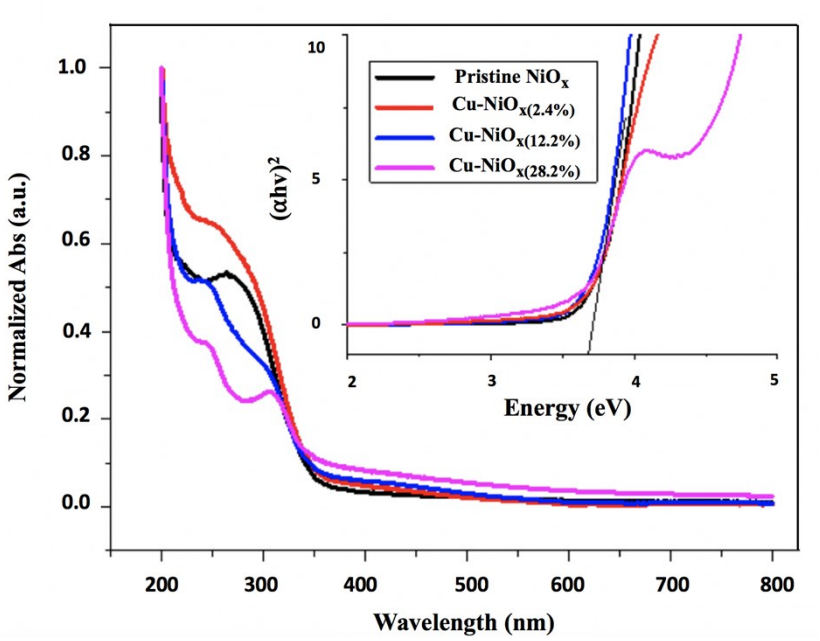


Figure S-1. Absorption spectra of IPA-based solutions of pristine NiO_x and different doping levels of Cu-NiO_x. Insert are Tauc plots of the corresponding solutions.

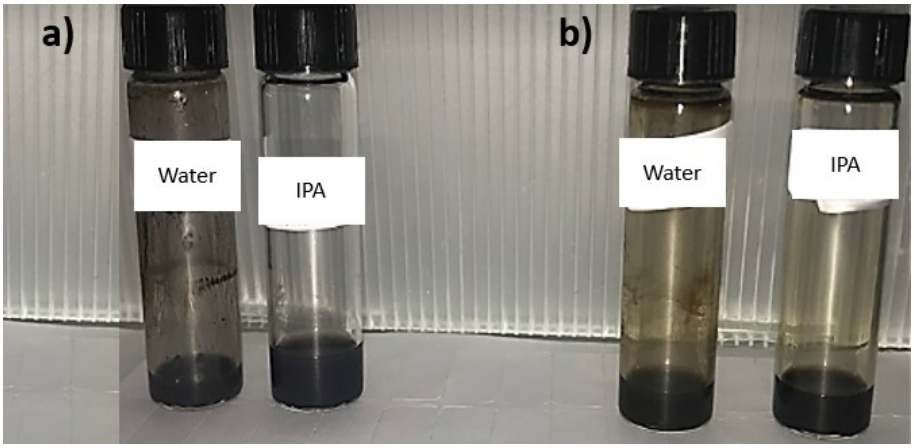
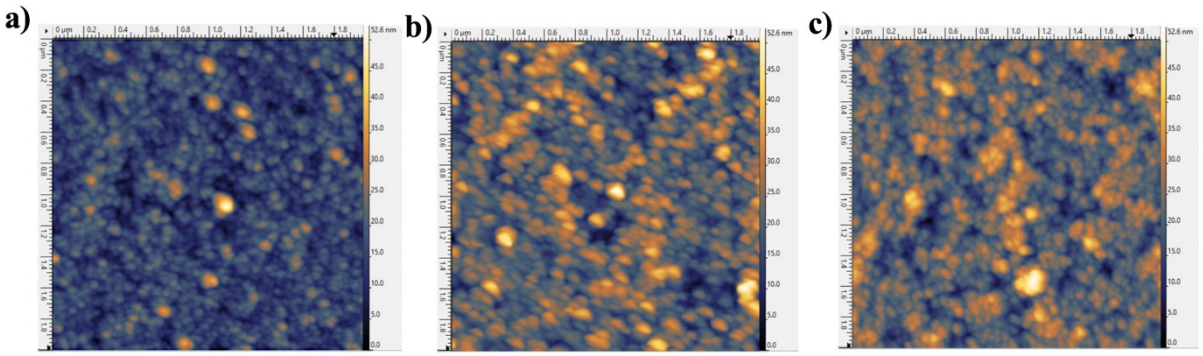


Figure S-2. Aspect of water and IPA-based solutions stored for 6 months at ambient conditions for (a) pristine NiO_x and (b) Cu-$NiO_{x(12.2\%)}$.



[Cu-$NiO_{x(12.2\%)}$] (mg/mL)	Thickness (±5 nm)	Roughness (±1 nm)
10	15	4
20	40	6
30	45	7

Figure S-3. AFM images of the Cu-$NiO_{x(12.2\%)}$ films deposited on ITO substrates from (a) 10 mg/mL, (b) 20 mg/mL, and (c) 30 mg/mL IPA solutions with a table summarizing the thicknesses and the roughness of the corresponding layers.

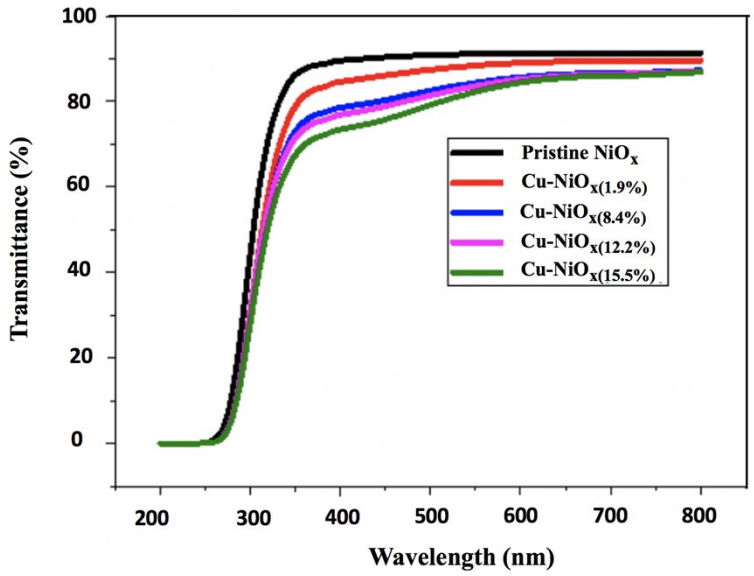
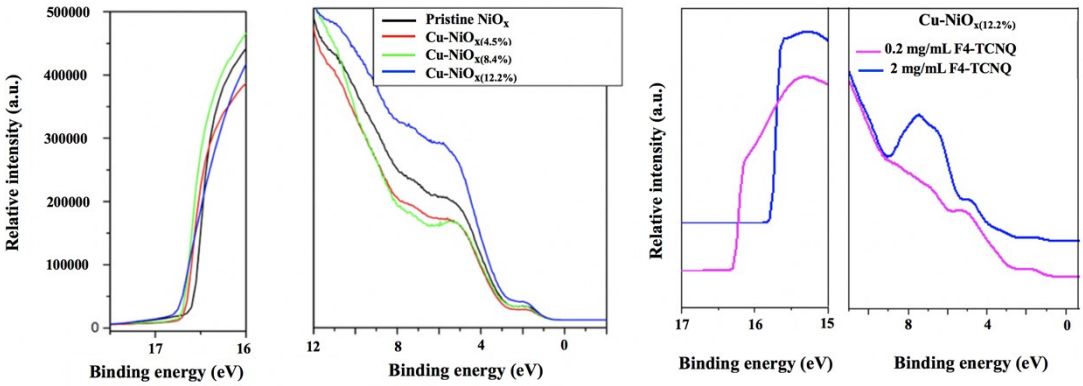
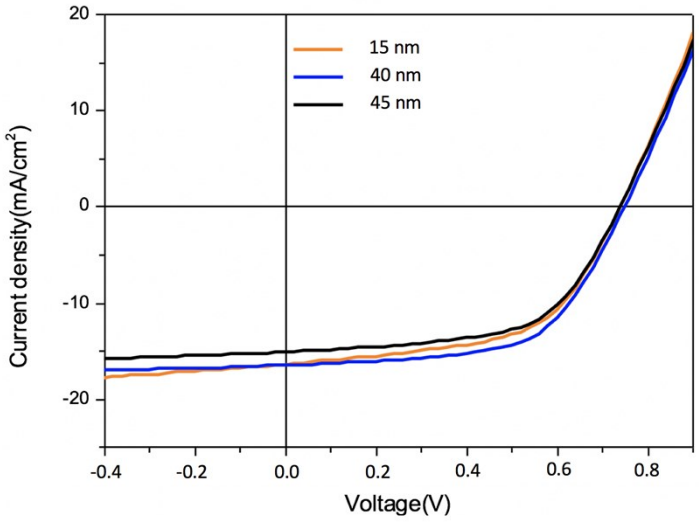


Figure S-4. Optical transmission spectra of the 40 nm thick-pristine and Cu-NiO_x films deposited from IPA solutions on glass substrates.



F4-TCNQ concentration	WF
w/o	4.47 eV
0.2 mg/mL	4.94 eV
2 mg/mL	5.45 eV

Figure S-5. UPS spectra of the IPA-based NiO_x films with and without molecular doping.



$Cu\text{-}NiO_{x(12.2\%)}$ thickness	V_{OC} (mV)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
15 nm	741	16.4	56.3	6.9
40 nm	751	16.6	60	7.4
45 nm	741	15.2	59	6.6

Figure S-6. Typical J-V curves of the PTB7:$PC_{70}BM$ regular-based devices using different thicknesses of Cu-$NiO_{x(12.2\%)}$ HTLs with a summary of the photovoltaic parameters.

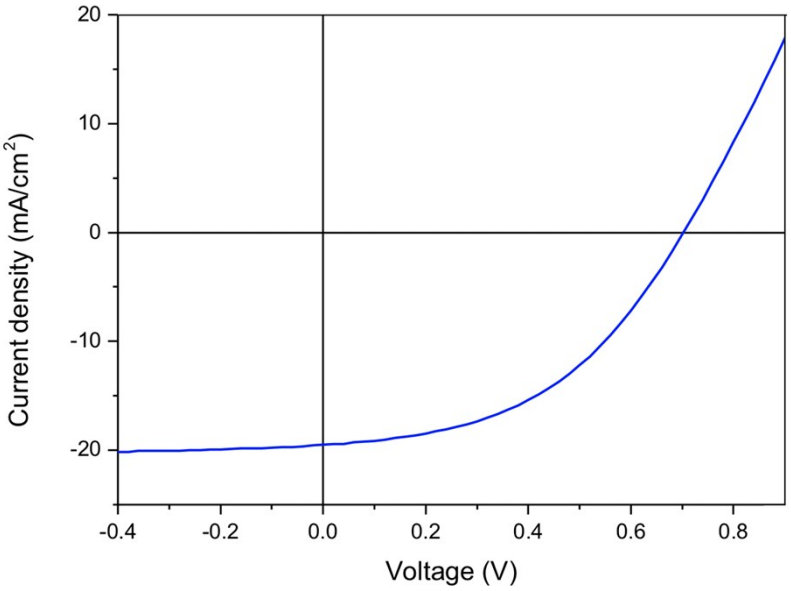


Figure S-7. J-V curve of the device: ITO/ZnO/80 nm-thick PBDB-T-2F:IT-4F/PEDOT:PSS/Ag

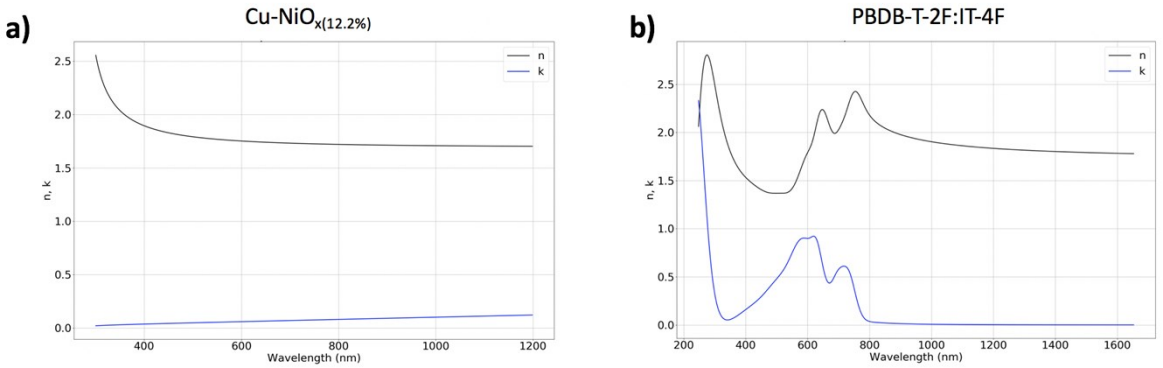


Figure S-8. Optical indices (n and k) as function of wavelength for (a) Cu-$NiO_{x(12.2\%)}$ and (b) PBDB-T-2F:IT-4F.