Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Hot Injection Synthesis of $CuInS_2$ Nanocrystals using Metal Xanthates and Their Application in Hybrid Solar Cells

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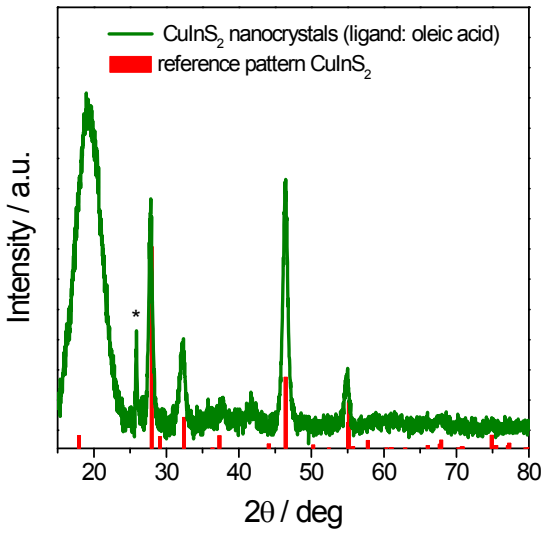

Fig. S1 X-ray diffraction pattern of the $CuInS_2$ nanocrystal sample prepared with oleic acid as capping ligand. The peak marked with an asterisk stems from a secondary phase. The broad peak around 20 ° 2θ can be ascribed to the capping ligand in the sample.

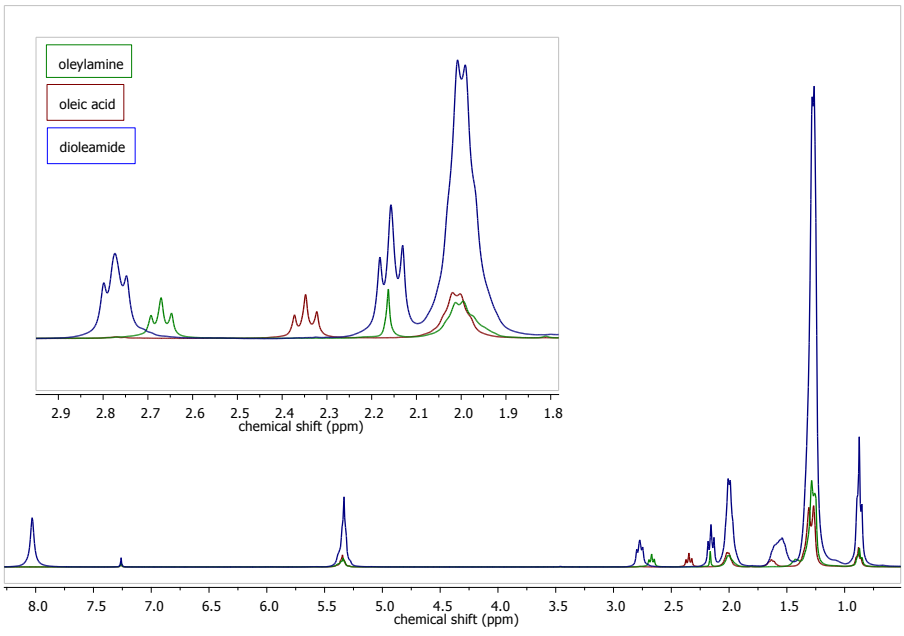

Fig. S2 ^{1}H-NMR pattern of oleylamine (green), oleic acid (red) and dioleamide (blue).

The ^{1}H-NMR spectra of oleylamine, oleic acid and dioleamide is shown in Fig. S1. The characteristic broad signal of the carboxylic acid group (11 ppm, not shown in this figure for a better visibility of the other peaks) has vanished in favor of a new peak (8.05 ppm) which can be assigned to the newly formed CO-NH functionality of dioleamide. The triplet of the CH_2 group next to the amino

functionality in oleylamine at around 2.65 ppm is shifted downfield (to 2.8 ppm) whereas the CH_2 group adjacent to the carbonyl functionality is shifted upfield (from 2.35 ppm to 2.15 ppm) as a consequence of amide formation.

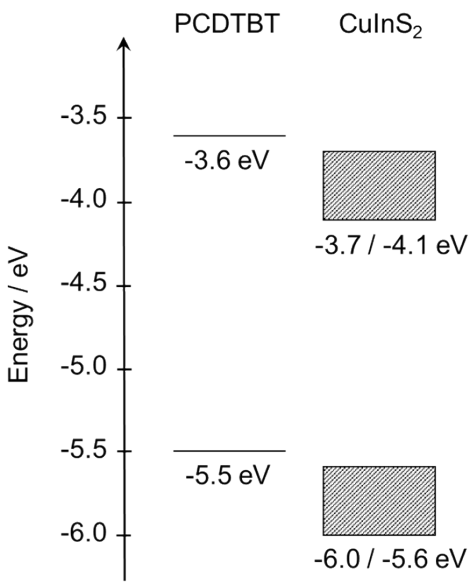

Fig. S3 Energy levels of the conjugated polymer PCDTBT[1] and $CuInS_2$ nanocrystals.[2,3]

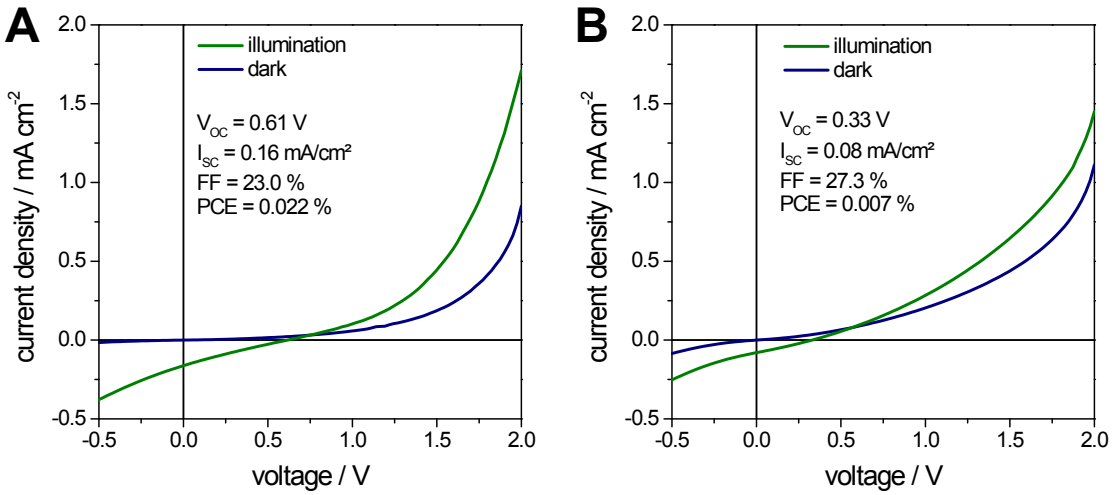

Fig. S4 JV curves of typical PCDTBT/$CuInS_2$ based solar cells with a polymer/$CuInS_2$ weight ratio of 1:5 (A) and 1:15 (B) in the dark and under 100 mW/cm² illumination.

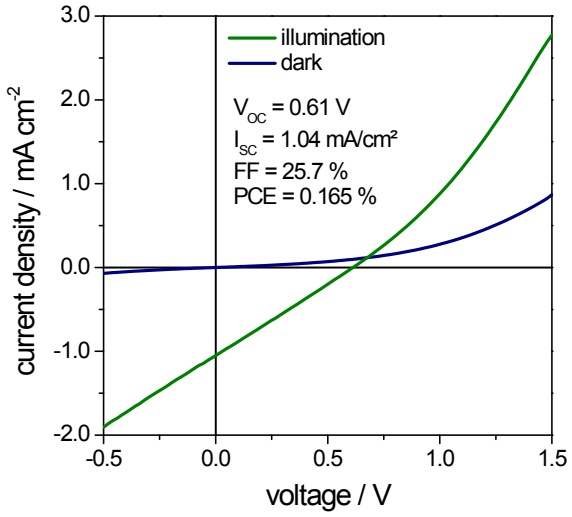

Fig. S5 JV curves of a typical PCDTBT/$CuInS_2$ based solar cell with a polymer/$CuInS_2$ weight ratio of 1:9 in the dark and under 100 mW/cm² illumination. The absorber layer was annealed at 140 °C for 10 min after spin coating.

References:

[1] N. Blouin, A. Michaud and M. Leclerc, *Adv. Mater*., 2007, **19**, 2295-2300.

[2] E. Arici, N. Sariciftci and D. Meissner, *Adv. Funct. Mater*., 2003, **13**, 165-171.

[3] H. Zhong, S. S. Lo, T. Mirkovic, Y. Li, Y. Ding, Y. Li and G. D. Scholes, *ACS Nano*, 2010, **4**, 5253-5262.