Supporting Information

Water-dispersible Copper Sulfide Nanocrystals via Ligand Exchange of 1-dodecanethiol

*Christina H.M. van Oversteeg,[a,b] Freddy E. Oropeza,[c] Jan P. Hofmann,[c] Emiel J.M. Hensen,[c] Petra E. de Jongh [b] and Celso de Mello Donega[a]**

a. Condensed Matter and Interfaces, Debye Institute for Nanomaterials Science, Utrecht University, 3508 TA Utrecht, The Netherlands

b. Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, 3508 TA Utrecht, The Netherlands

c. Laboratory of Inorganic Materials Chemistry, Department of Chemical Engineering and Chemistry, Eindhoven University of Technology, Postbox 513, 5600 MB Eindhoven, The Netherlands

*Corresponding author: E-mail: c.demello-donega@uu.nl

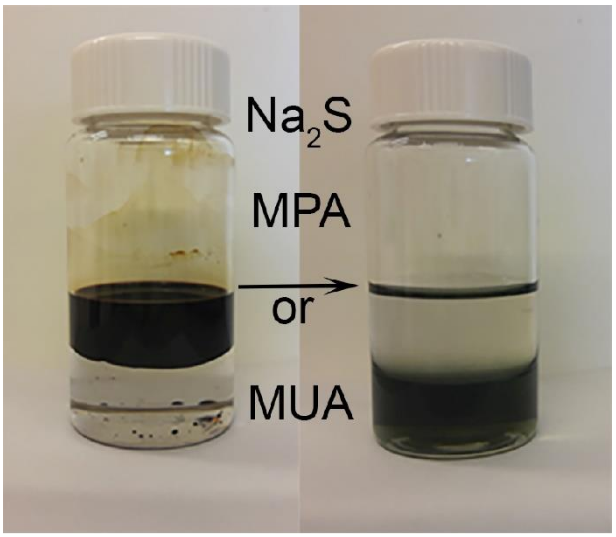

Figure S1. In a succesful ligand exchange using S^{2-}, MPA^{-} or MUA^{-}, the black colloidal $Cu_{2-x}S$ nanocrystals undergo a phase transfer from toluene to formamide upon exchange of the native 1-dodecanethiol ligand.

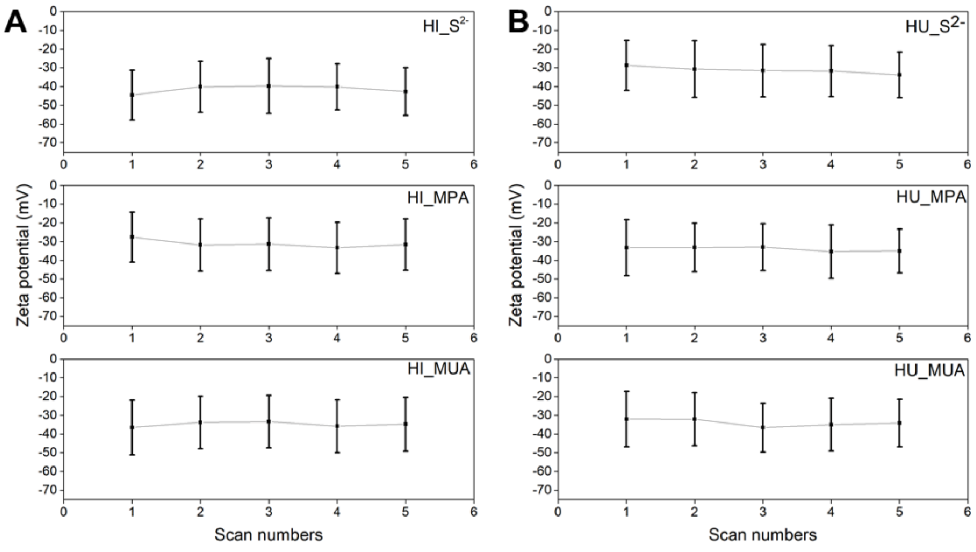

Figure S2. ζ-potential of $Cu_{2-x}S$ nanocrystals in formamide prepared by **A)** hot-injection synthesis or **B)** heating-up synthesis and capped with S^{2-}, MPA or MUA, respectively.

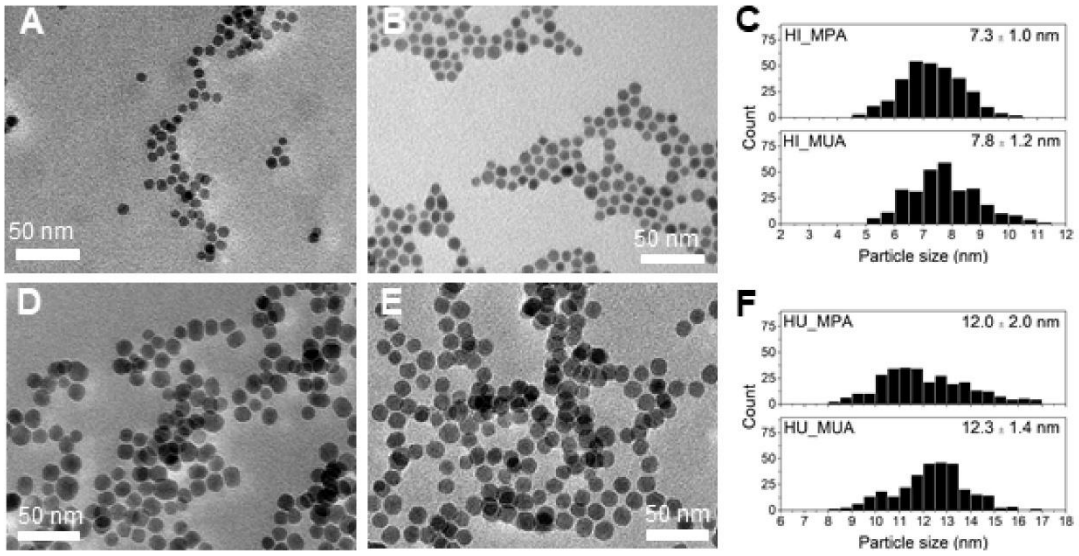

Figure S3. TEM images of $Cu_{2-x}S$ nanocrystals prepared by hot-injection synthesis and capped by **A)** MPA and **B)** MUA and **C)** corresponding particle size histograms. TEM images of $Cu_{2-x}S$ nanocrystals prepared by heating-up synthesis and capped by **D)** MPA and **E)** MUA and **F)** corresponding particle size histograms.

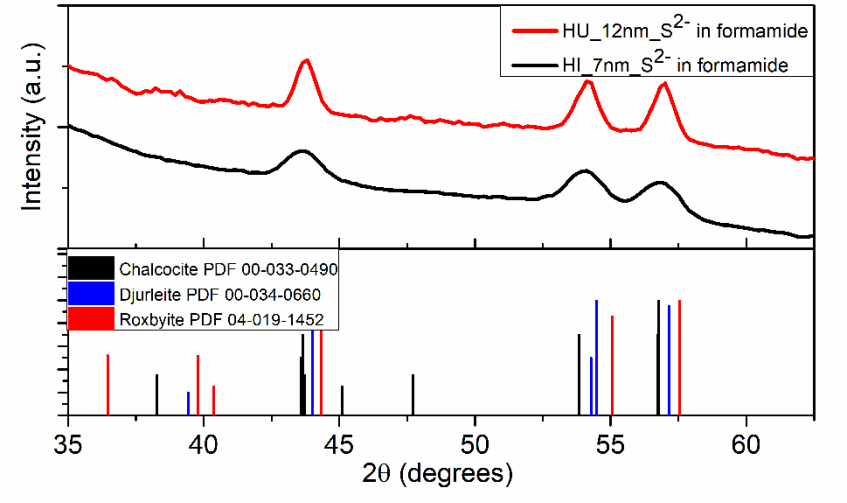

Figure S4. X-ray diffractograms of the $Cu_{2-x}S$ nanocrystals after ligand exchange with S^{2-} and phase transfer to formamide. Measurements were done using a sample holder with air-tight dome to minimize exposure to air.

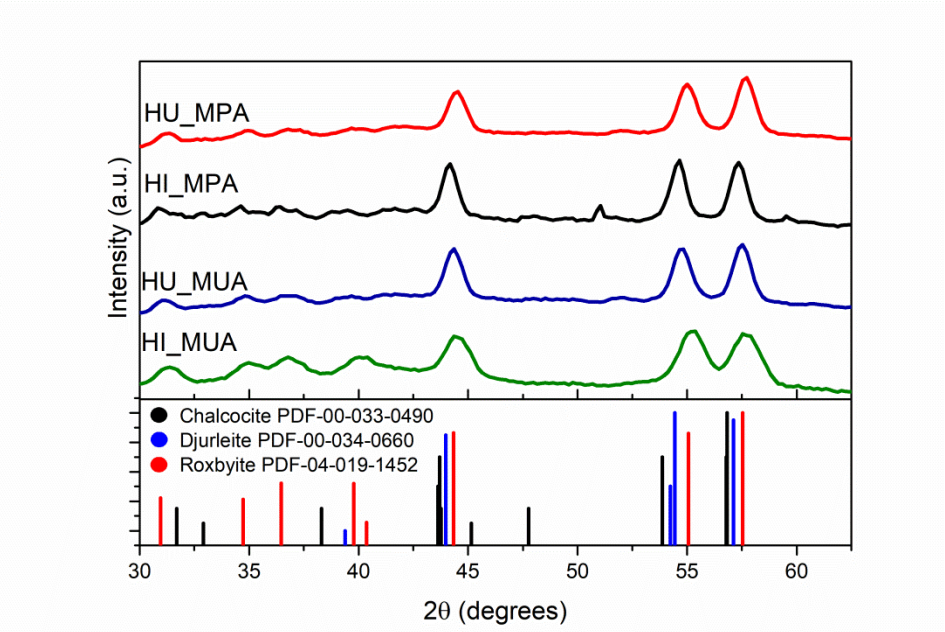

Figure S5. X-ray diffractograms of the $Cu_{2-x}S$ nanocrystals after ligand exchange with MPA (HU_MPA and HI_MPA) and MUA (HU_MUA and HI_MUA) and subsequent phase transfer to water in air. The $Cu_{2-x}S$ nanocrystals are slightly oxidized to a roxbyite phase, as evidenced by the shift of the peak positions.

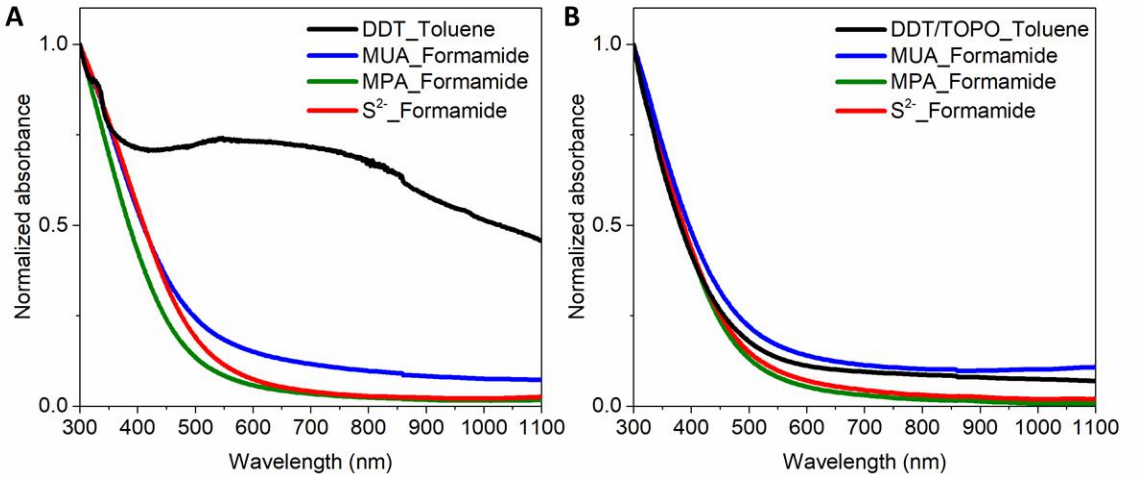

Figure S6 Absorption spectra before and after ligand exchange with MUA, MPA and S^{2-} of the $Cu_{2-x}S$ nanocrystals prepared by **A)** heating-up synthesis and **B)** hot-injection synthesis.

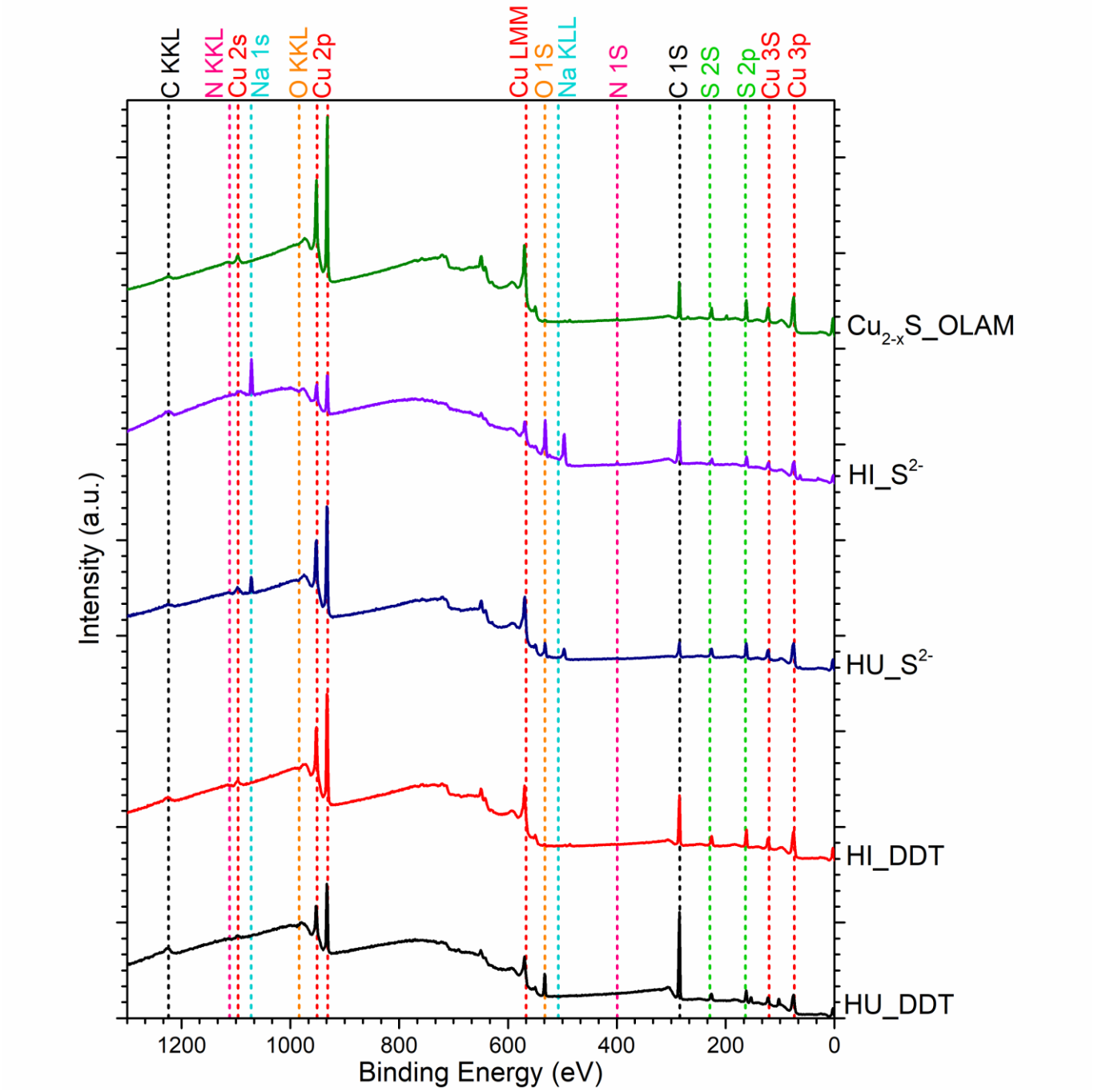

Figure S7. XPS Survey scans of all relevant samples.

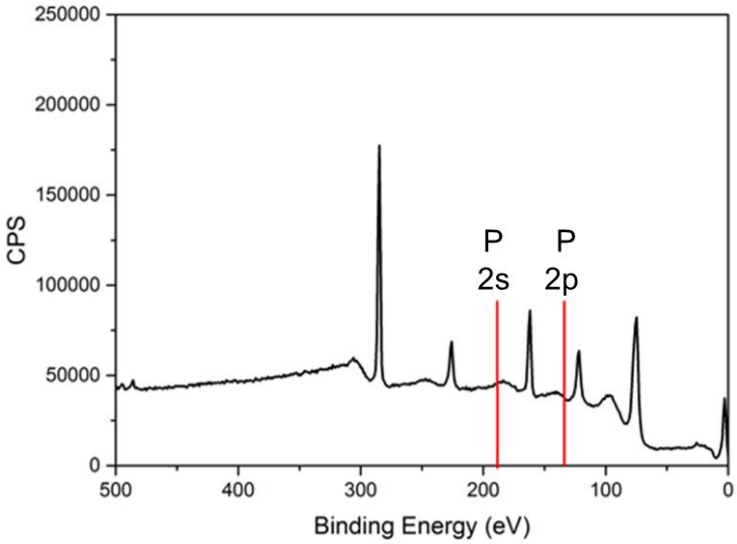

Figure S8. XPS Survey scan of the as-synthesized $Cu_{2-x}S$ nanocrystals prepared by hot-injection. The red lines indicate the binding energy at which a phosphorus signal would be observed (left: P2s, right: P2p). The absence of peaks in this region indicates the absence of phosphorus in this sample.