

Electronic Supplementary Information

One-pot Synthesis of CuInS₂ Nanocrystals Using Different Anions to Engineer Morphology and Crystal Phase

Aiwei Tang,^{*a,b} Zunlan Hu,^a Zhe Yin,^a Haihang Ye,^a Chunhe Yang,^a and Feng Teng^{*b}

^aDepartment of Chemistry, School of Science, Beijing JiaoTong University, Beijing 100044, P. R. China

E-mail: awtang@bjtu.edu.cn; Tel: +86-10-51683627

^bKey Laboratory of Luminescence and Optical Information, Ministry of Education, Beijing JiaoTong University, Beijing 100044, P. R. China

Email: fteng@bjtu.edu.cn

Fig. S1

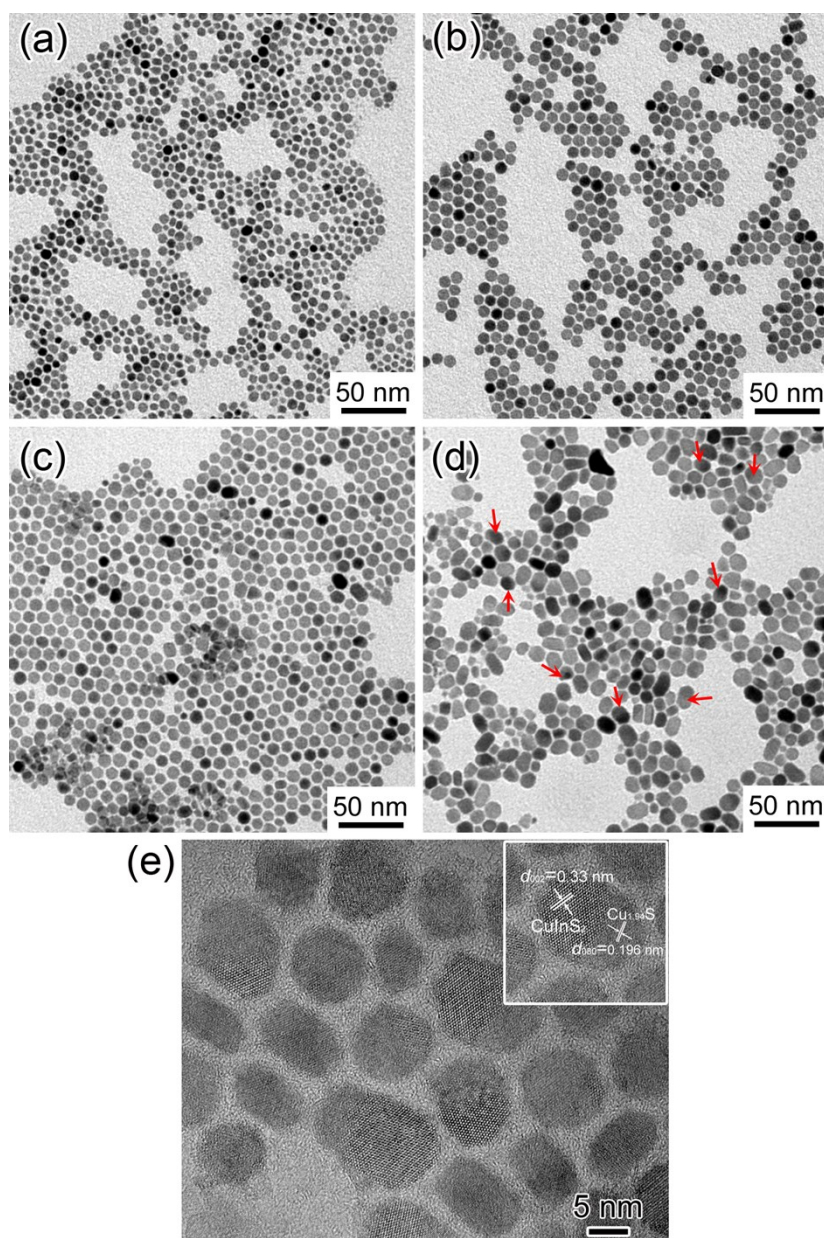


Fig. S1 TEM images of Sample A for different reaction time: (a) 0 min; (b) 10 min; (c) 30 min; (d) 60 min, and the heterostructured nanocrystals are labeled by the red arrows , and (e) the corresponding HRTEM image of Sample A obtained at 60 min, and the inset shows the enlarged image of the $\text{Cu}_{1.94}\text{S}$ - CuInS_2 heterostructured nanocrystals.

Fig. S2

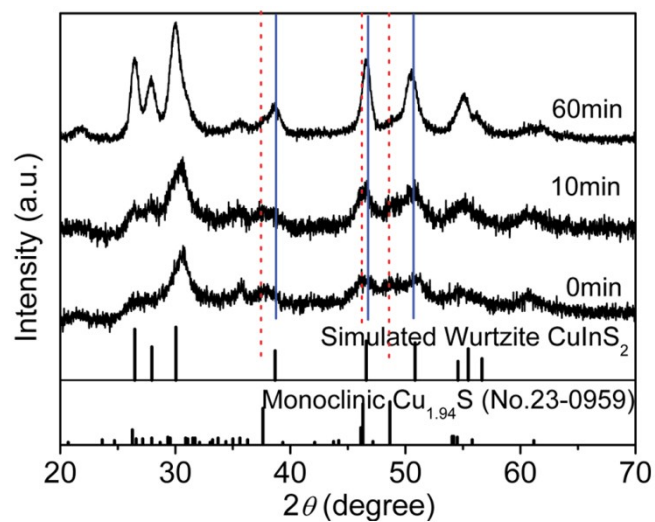


Fig. S2 XRD patterns of Sample A obtained at different reaction time, and the bottom lines are the simulated wurtzite CuInS_2 and the standard lines of monoclinic $\text{Cu}_{1.94}\text{S}$ (JCPDS No. 23-0959). The solid and dashed vertical lines represent the main diffraction peaks of wurtzite CuInS_2 and monoclinic $\text{Cu}_{1.94}\text{S}$.

Fig.S3

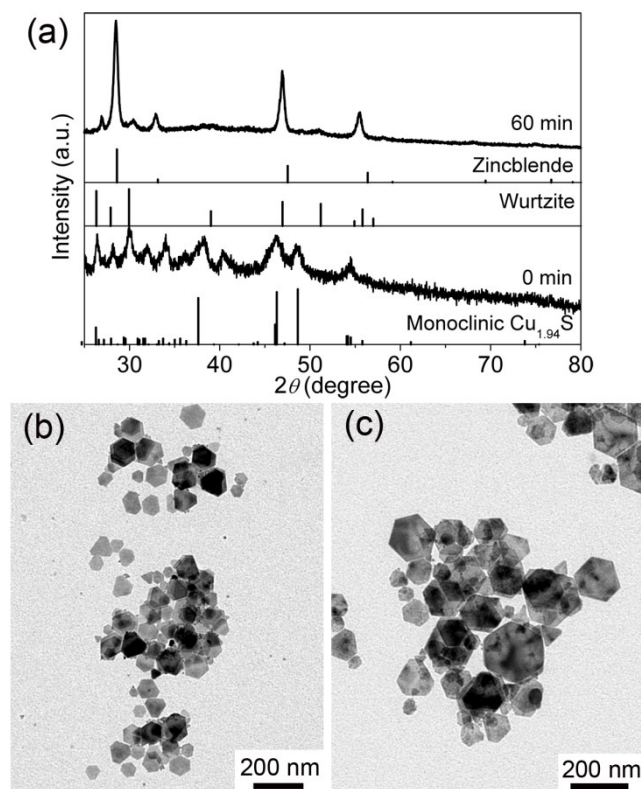


Fig.S3 (a) XRD patterns of Sample B obtained at 0 min and 60 min, and the bottom lines represent the standard diffraction peaks of monoclinic $\text{Cu}_{1.94}\text{S}$ and the simulated diffraction lines of zincblende and wurtzite CuInS_2 ; TEM images of Sample B obtained at (b) 0 min and (c) 10 min.

Fig.S4

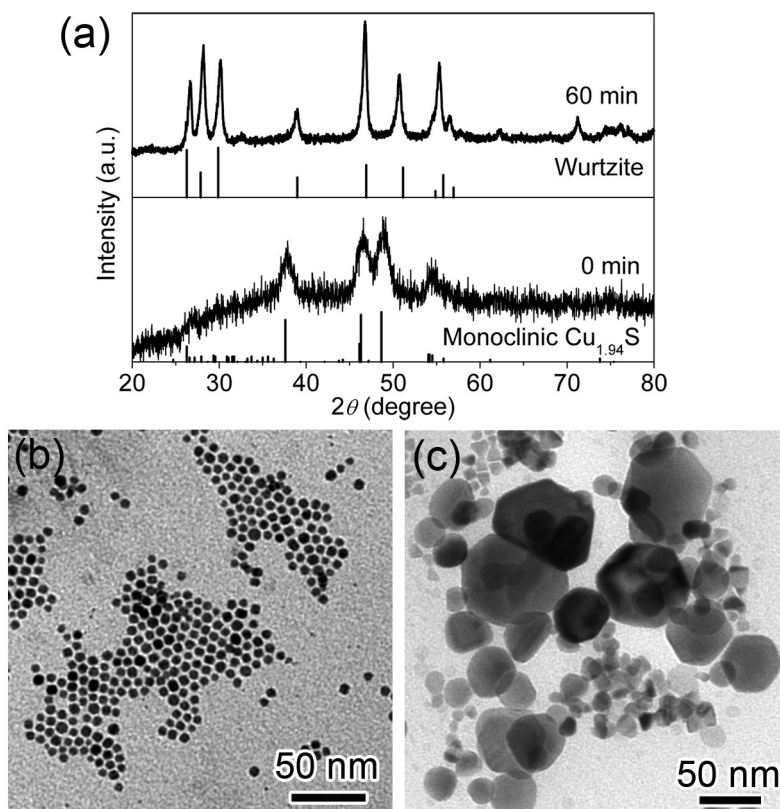


Fig.S4 (a) XRD patterns of the products synthesized by using hot-injection method, in which 2.5 mmol of $\text{Cu}(\text{acac})_2$ was mixed with ODE and DDT and was heated to 240 °C, and the aliquot was extracted, and then 2.5 mmol of InCl_3 in ODE was quickly injected into the hot mixture, and kept for 60 min at 240 °C; TEM images of the products obtained at (b) 0 min and (c) 60 min.

Fig. S5

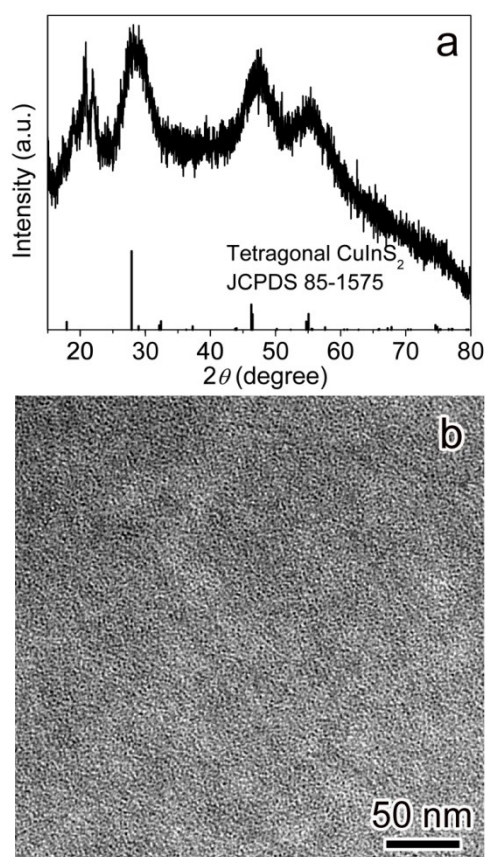


Fig. S5 (a) XRD pattern and (b) TEM images of Sample C obtained at the initial stage (0 min), and the bottom lines of (a) represent the standard diffraction peaks of tetragonal chalcopyrite CuInS_2 phase (JCPDS No. 85-1575).

Fig. S6

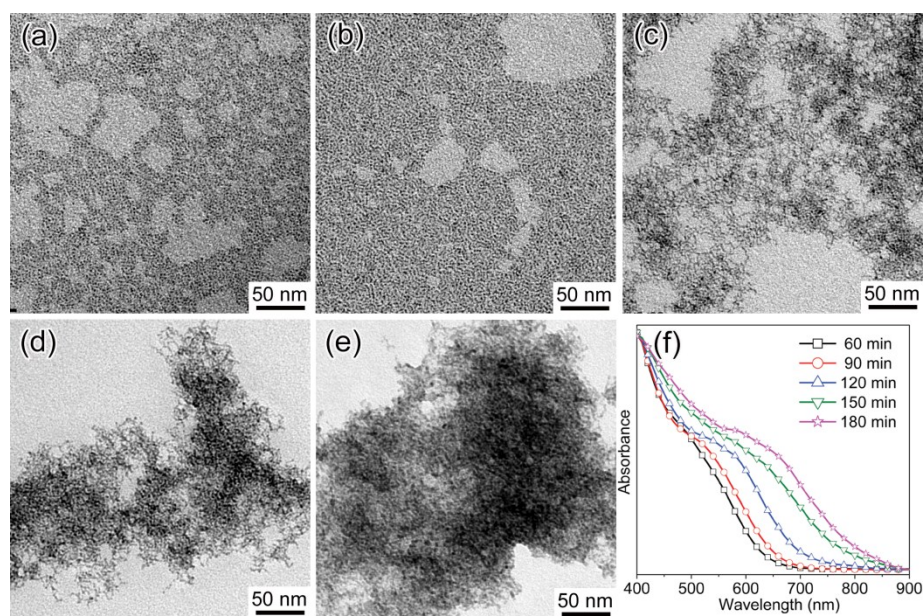


Fig. S6 TEM images of Sample C obtained at different reaction time: (a) 60 min; (b) 90 min; (c) 120 min; (d) 150 min; (e) 180 min; (f) the corresponding UV-Vis absorption spectra measured in chloroform.

Fig.S7

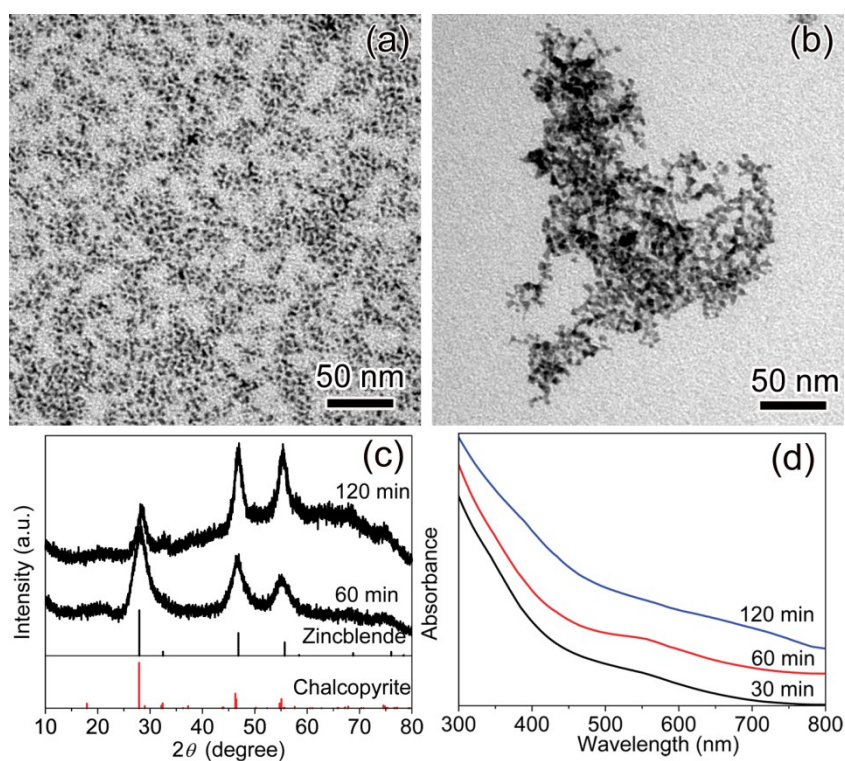


Fig. S7 TEM images of Sample D obtained at (a) 30 min and (b) 120 min; (c) XRD patterns of Sample D obtained at different reaction time, and the bottom lines represent the standard diffraction peaks of the tetragonal chalcopyrite CuInS_2 (JCPDS No.85-1575) and stimulated zincblende CuInS_2 phase, and (d) the corresponding UV-Vis absorption spectra.

Fig. S8

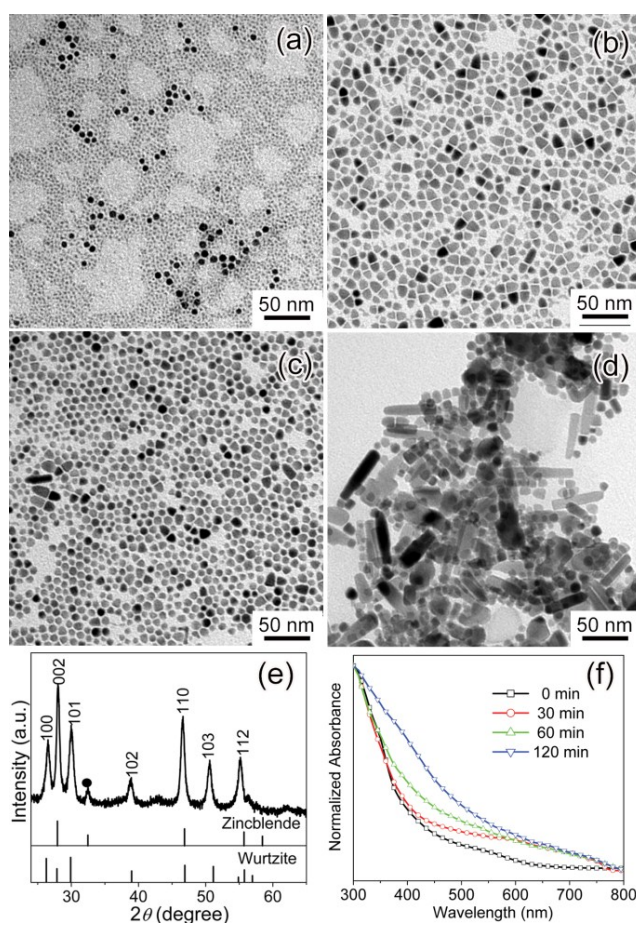


Fig. S8 TEM images of Sample E obtained at different reaction time: (a) 0 min; (b) 60 min; (c) 60 min; (d) 120 min; (e) XRD pattern of Sample E obtained at 120 min, and the bottom lines represent the simulated zincblende and wurtzite CuInS_2 ; (f) UV-Vis absorption spectra of sample E obtained at different reaction time.

Fig. S9

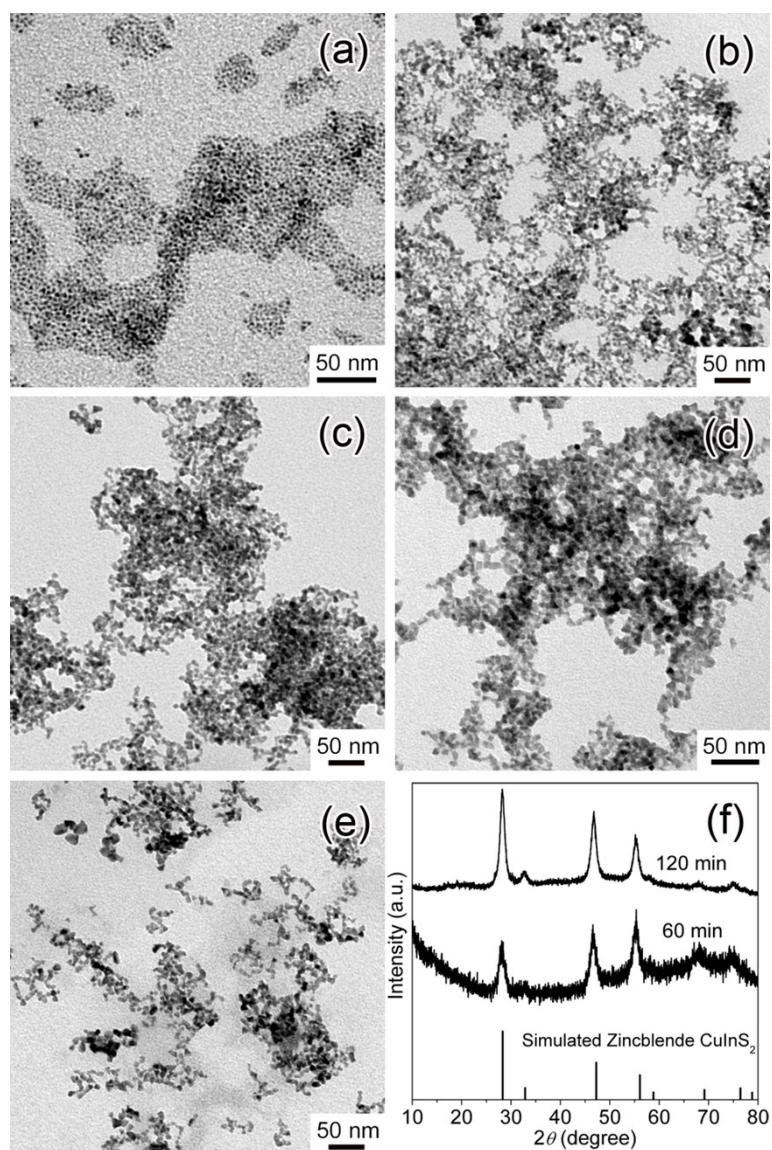


Fig. S9 TEM images of Sample F obtained at different reaction time: (a) 0 min; (b) 30 min; (c) 60 min; (d) 90 min; (e) 120 min; (f) XRD patterns of Sample F obtained at 60 min and 120 min, and the bottom lines represent simulated zincblende CuInS₂ phase.

Fig. S10

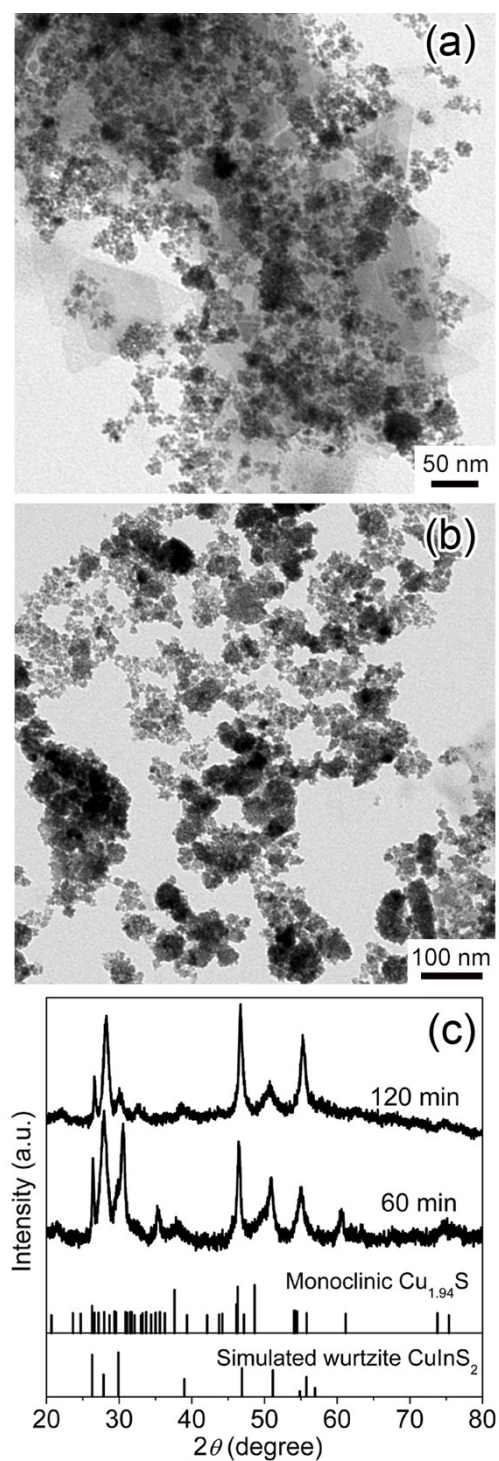


Fig. S10 TEM images of Sample H obtained at different reaction time: (a) 0 min; (b) 30 min; (c) XRD patterns of the products obtained at 60 min and 120 min, and the vertical lines represent the standard diffraction peaks of monoclinic $\text{Cu}_{1.94}\text{S}$ and the simulated diffraction lines of wurtzite CuInS_2 .

Fig. S11

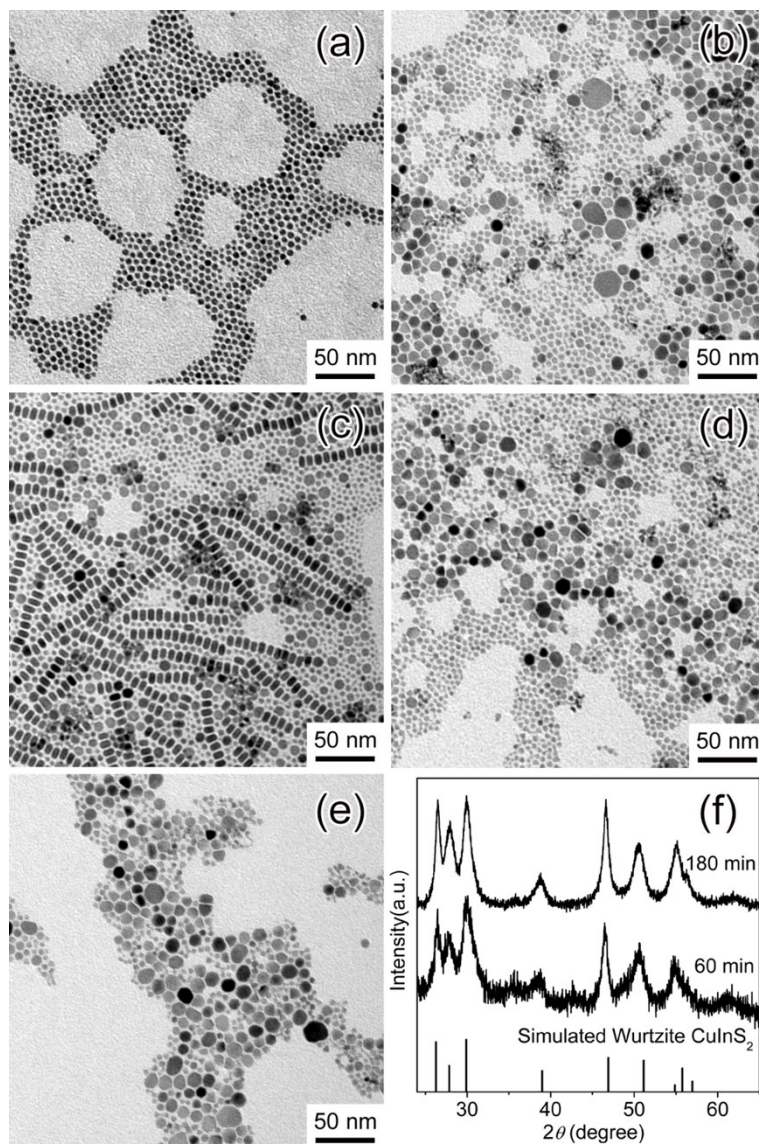


Fig. S11 TEM images of Sample I obtained at different reaction time: (a) 0 min; (b) 30 min; (c) 60 min; (d) 90 min; (e) 120 min; (f) the corresponding XRD pattern of the product obtained at 60 and 120 min, together with the simulated diffraction lines of wurtzite CuInS_2 shown in the bottom.