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Electronic Supplementary Information

for

Effect of Cu/In ratio and shell bhickness on photo-stability of CuInS₂/ZnS nanocrystals

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Fig. S1 TEM images of CIS/ZnS core/shell NCs (2MLs) with Cu/In molar ratios of 1/1 (a), 1/2 (b) and 1/8 (c).



Fig. S2 Size distribution of CIS/ZnS (2MLs) core/shell NCs with difference different Cu/In molar ratios.



Fig. S3 XPS spectra of (a) Zn 2p, (b) Cu 2p, (c) In 3d, and (d) S 2p of CIS/ZnS (2MLs) NCs with Cu/In ratio of 1/1 and 1/4 in the synthesis process. The Zn 2p are located at 1022.3 eV and 1045.3 eV (Fig. S3a), corresponding to $Zn^{2+.1}$ The binding energies of Cu $2p_{3/2}$ and Cu $2p_{1/2}$ are located at 932.5 eV and 952.4 eV, respectively, with a peak splitting of 19.9 eV (Fig. S3b), which is in agreement with the reported values for Cu^{+.2} The binding energies of In 3d are located at 445.0 eV and 452.6 eV with a peak splitting of 7.6 eV (Fig. S3c), corresponding to $In^{3+.2}$ The S 2p has doublet peaks of S $2p_{1/2}$ and $2p_{3/2}$ due to the spin-orbit coupling, and the S 2p peaks at 161.9 eV and 162.8 eV with a peak splitting of 0.9 eV in Fig. S3d match well with S^{2-.2}



Fig. S4 Absorption spectra of CIS/ZnS core/shell NCs (2MLs) with Cu/In ratios of 1/1, 1/2, 1/4, 1/8 during the strong light illumination.



Fig. S5 TEM image of CIS/ZnS NCs with a hexagonal plate shape.



Fig. S6 XRD patterns of CIS core and CIS/ZnS NCs.



Fig. S7 Absorption spectra of sample CS1, sample CS2 and sample CS3 during the strong light illumination.

 Table S1 Elements compositions of CIS/ZnS NCs determined by EDX measurement.

sample	CIS/ZnS NCs	CIS/ZnS NCs	CIS/ZnS NCs	CIS/ZnS NCs	CIS/ZnS NCs (CS2)	CIS/ZnS NCs (CS3)
	(2MLs)	(2MLs)	(2MLs)	(2MLs)		
Cu/ In ratio in						
the raw	1/1	1/2	1/4	1/8	1/4	1/4
Material						
solution						
Cu/ In ratio						
of product	0.91	0.56	0.45	0.36	0.40	0.33
Composition						
of product	1:1.1:3.3:3.6	1:1.8:6.0:5.5	1:2.2:8.2:7.2	1:2.8:12.0:10.5	1:2.5:12.4:10.8	1:3.0:24.3:19.3
(Cu:In:Zn:S)						

Time	CS1-0h	CS1-100h	CS2-0h	CS2-100h	CS3-0h	CS3-100h
range						
1	1.32	0.60	1.15	0.23	1.13	1.14
2	1.45	0.70	1.56	0.45	1.83	1.26
3	1.22	0.67	1.41	0.49	1.52	1.20
4	1.35	0.58	1.20	0.30	1.21	1.10
5	1.21	0.56	1.08	0.41	1.07	1.25
6	1.25	0.43	1.28	0.55	1.40	1.35
7	1.11	0.96	1.65	0.43	1.18	1.34

Table S2 Ratio of S1/S2 of sample CS1(CIS/ZnS 2MLs), CS2 and CS3 from range 1 to 7 before and
after the light illumination.

Reference

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