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Inorganic Ligands Mediated Synthesis of $CuInS_2$ Nanocrystals with Tunable Properties

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Contents:

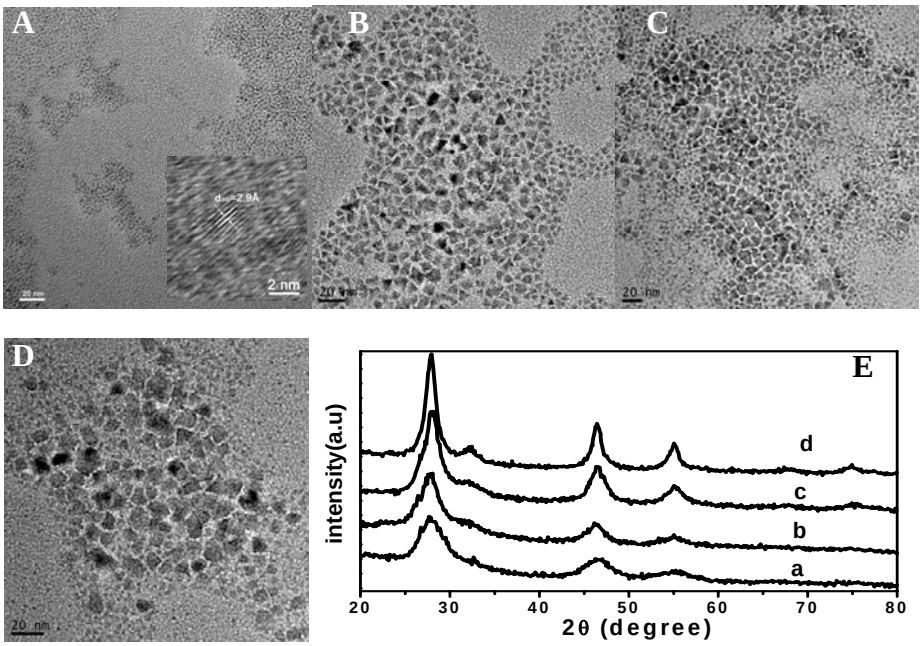

Fig.S1 TEM images and XRD of the $CuInS_2$ NCs synthesized at different reaction temperatures for 60 min, (A, a) 180 ^oC, (B, b) 200 ^oC, (C, c) 220 ^oC and (D, d) 240 ^oC, respectively.

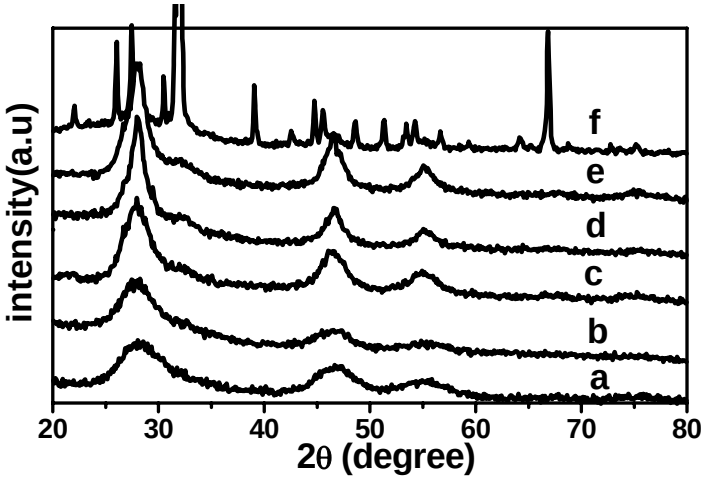

Fig.S2 XRD patterns of $CuInS_2$ NCs synthesized at 200 ^oC by changing the reaction factors; (a) 0.00 mmol $Sn(acac)_2Cl_2$ for 120 min; (b) 0.05 mmol $Sn(acac)_2Cl_2$ for 60 min; (c) 0.1 mmol $Sn(acac)_2Cl_2$ for 30 min, (d) 60 min and (e) 90 min, respectively; (f) 0.2 mmol $Sn(acac)_2Cl_2$ for 120 min.

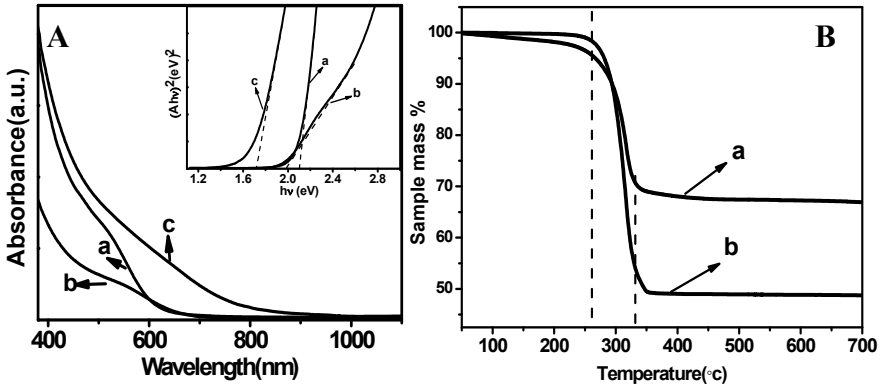

Fig.S3 (A)The UV-Vis absorption spectra and corresponding band gap of $CuInS_2$ NCs obtained with different concentration of $Sn(acac)_2Cl_2$. (a) 0.00 mmol (b) 0.05 mmol and (c) 0.1 mmol $Sn(acac)_2Cl_2$, respectively. (B) TGA spectra of the $CuInS_2$ NCs with (a) and without (b) the participation of $Sn(acac)_2Cl_2$ for 120 min.

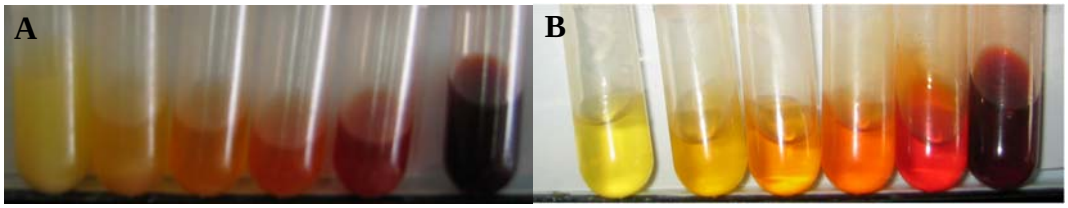

Fig.S4 The color changes of the mixture solution (A) with and (B) without the participation of $Sn(acac)_2Cl_2$ at 200 ^oC, as time prolonged.

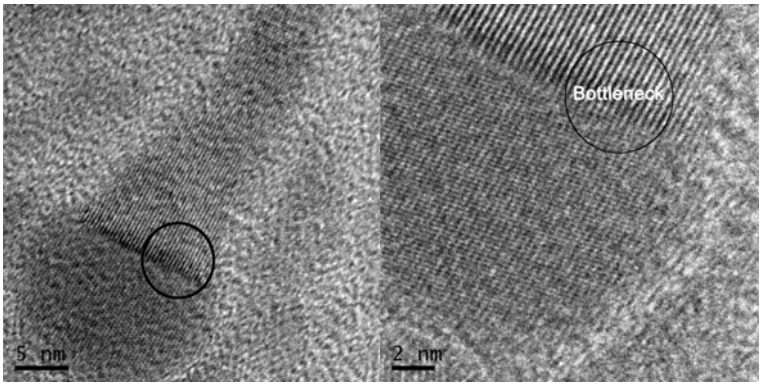

Fig.S5 The HRTEM image of a single lute-like nanocrystal of $CuInS_2$ NCs obtained without the participation of $Sn(acac)_2Cl_2$.

Tab.S1 Elemental composition values of $CuInS_2$ NCs obtained by changed the reaction concentration of $Sn(acac)_2Cl_2$ according to the EDS measurement.

Area	0.00	0.05	0.10
Area1(At %)Cu/ In/ S	28.37/19.63/51.99	20.68/22.6/56.72	27.44/22.28/50.28
Area2(At %)Cu/ In/ S	22.55/21.70/53.52	26.84/25.50/47.66	22.36/22.71/54.93
Area3(At %)Cu/ In/ S	25.27/16.46/53.89	29.89/17.88/52.24	23.92/22.51/53.57
Average(At%)Cu/ In/ S	25.23/20.56/53.61	25.80/21.99/52.21	24.57/22.50/52.93
Cu/ In/ S	0.93/0.71/2.00	0.99/0.84/2.00	0.93/0.85/2.00
Cu/In	1/0.81	1/0.85	1/0.92

Tab.S2 Elemental composition values of $CuInS_2$ NCs obtained by changed the reaction temperatures according to the EDS measurement.

Area	180 °C	200 °C	220 °C	240 °C
Area1(At %)Cu/ In/ S	32.03/19.01/48.96	27.44/22.28/50.28	24.51/25.86/49.32	26.08/23.38/51.54
Area2(At %)Cu/ In/ S	27.11/19.85/53.04	22.36/22.71/54.93	24.32/23.95/51.73	25.61/20.12/54.27
Area3 (At %)Cu/ In/ S	27.16/19.36/53.48	23.92/22.51/53.57	26.65/21.20/52.14	21.97/21.88/56.15
Average (At%)Cu/ In/ S	28.77/19.41/51.83	24.57/22.50/52.93	25.26/23.67/51.06	24.91/21.62/53.47
Cu/ In/ S	1.11/0.75/2.00	0.93/0.85/2.00	0.99/0.93/2.00	0.93/0.81/2.00
Cu/In	1/0.67	1/0.92	1/0.94	1/0.87/2.15

Tab.S3 Elemental composition values of $CuInS_2$ NCs obtained by changed the reaction times according to the EDS measurement.

Area	30 min	90 min	120 min
Area1(At %)Cu/ In/ S	**24.20/20.53/55.27**	**23.87/24.88/51.26**	**21.49/22.13/53.50/(2.89※)**
Area2(At %)Cu/ In/ S	**28.86/21.67/49.67**	**25.93/18.39/55.69**	**23.85/24.89/51.25(1.47※)**
Area3(At %)Cu/ In/ S	**25.86/18.46/55.68**	**18.80/24.00/57.20**	**23.37/21.7/52.48(2.44※)**
Average(At%)Cu/ In/ S	**26.31/20.22/53.54**	**22.87/22.41/54.72**	**22.80/23.06/52.41(2.67※)**
Cu/ In/ S	**0.98/0.76/2.00**	**0.84/0.82/2.00**	**0.87/0.88/2.00(0.08※)**
Cu/In	**1/0.77**	**1/0.98**	**1/1.01**

* indicates a percentage value of Sn elemental, ※≤ 2 sigma.