Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A

Supporting Information

Zinc Alloyed Iron Pyrite Ternary Nanocrystals for Band Gap Broadening

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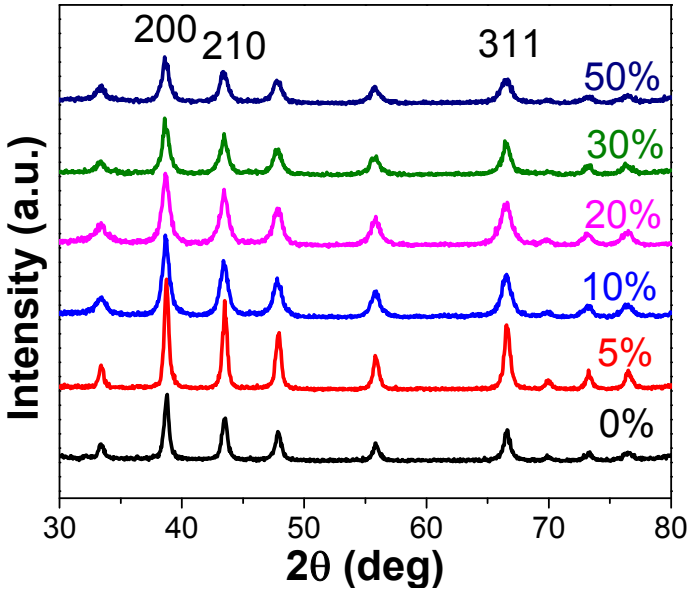

Fig. S1 Full range XRD patterns of the $Zn_xFe_{1-x}S_2$ NCs synthesized with different starting ratio of zinc in the precursors.

Table S1. Summarized diffraction angles (*2θ*), crystal plane distances (*d*), and lattice parameters (a_0).

Zn_s	$(2\theta)_{200}$/°	$(2\theta)_{210}$/°	$(2\theta)_{311}$/°	d_{200}/Å	d_{210}/Å	d_{311}/Å	a_0/Å
0%	38.8	43.55	66.6	2.695	2.413	1.631	5.399
5%	38.75	43.5	66.55	2.699	2.416	1.632	5.404
10%	38.65	43.45	66.55	2.705	2.419	1.632	5.410
20%	38.65	43.45	66.60	2.705	2.419	1.631	5.409
30%	38.6	43.45	66.40	2.709	2.419	1.635	5.416
50%	38.6	43.4	66.35	2.709	2.421	1.636	5.419

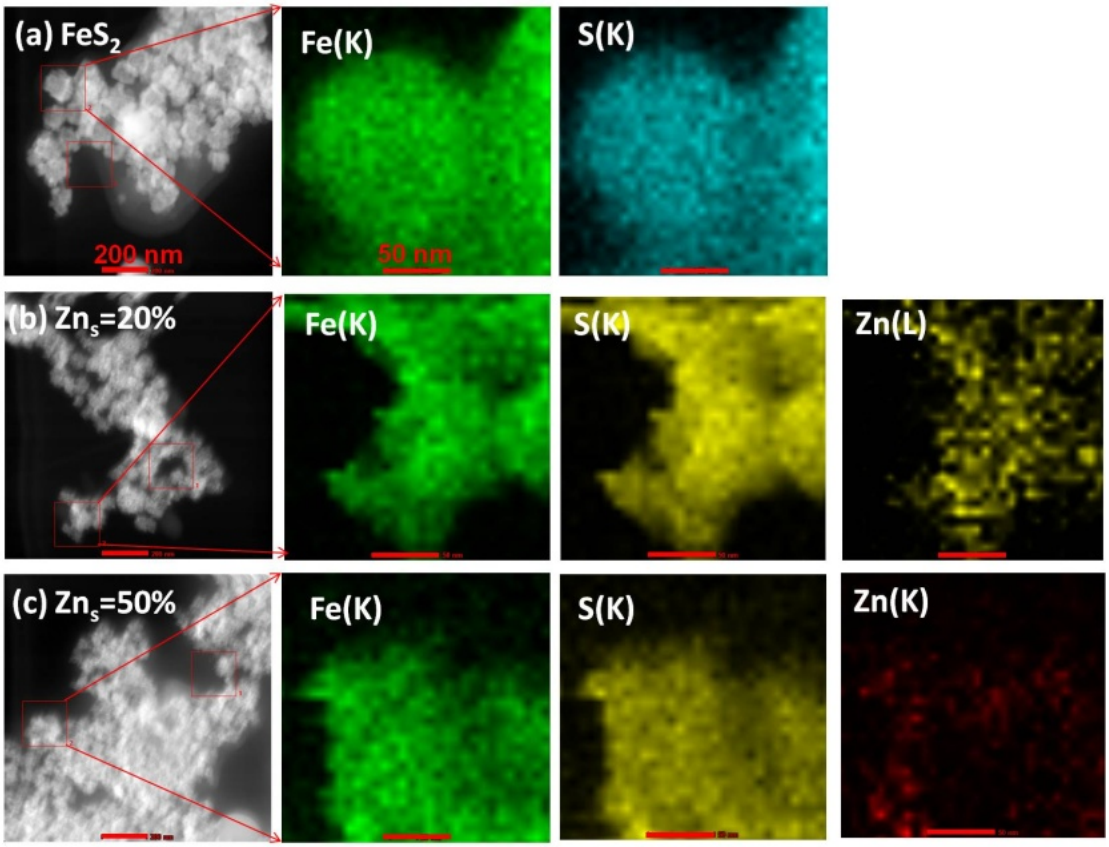

Fig. S2 STEM images and elemental mapping of the $Zn_xFe_{1-x}S_2$ NCs synthesized with starting zinc ration Zn_s=0% (a), 20% (b) and 50% (c). The scale bars are 200 nm for the STEM images and 50 nm for the mapping, respectively.

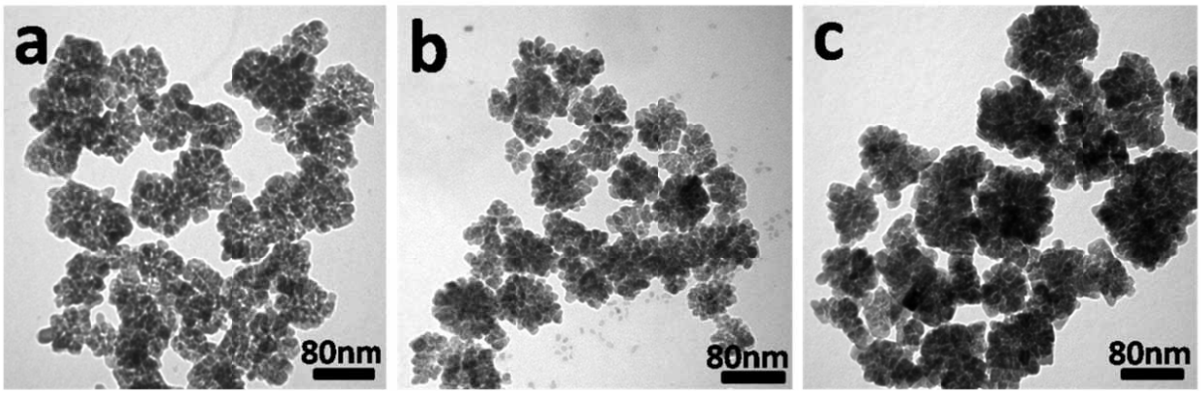

Fig. S3 TEM images of the $Zn_xFe_{1-x}S_2$ NCs synthesized using zinc acetate and 1 mmol of (Fe+Zn): (a) Zn_s=0%, (b) Zn_s=10%, and (c) Zn_s=20%.

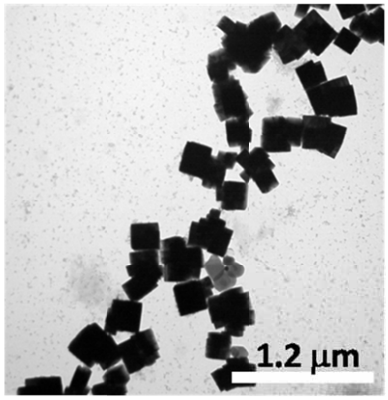

Fig. S4 TEM image of the $Zn_xFe_{1-x}S_2$ NCs synthesized with S injected at 170 °C and 10 at% zinc stearate.