

Supporting Information for

Synthesis of Quantum-sized Cubic ZnS Nanorods by the Oriented Attachment Mechanism

*Jung Ho Yu, Jin Joo, Hyun Min Park, Sung-Il Baik, Young Woon Kim, Sung Chul Kim, and Taeghwan Hyeon**

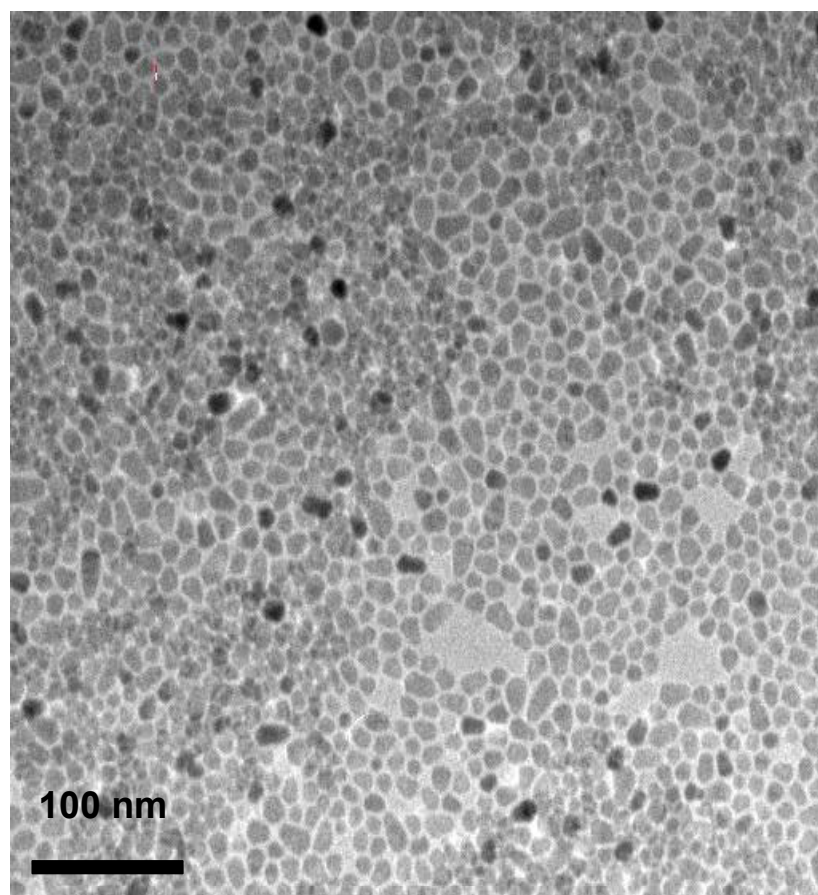


Figure S1. TEM image of ZnS nanocrystals synthesized by adding 0.15 g of TOPO in the reaction mixture.

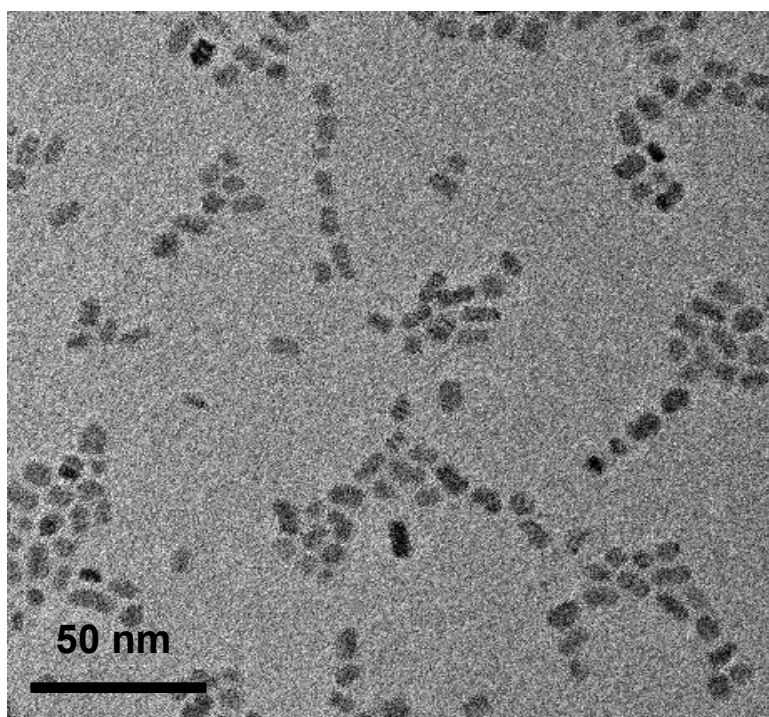


Figure S2. ZnS nanocrystals after the secondary aging in oleylamine at 300 °C.

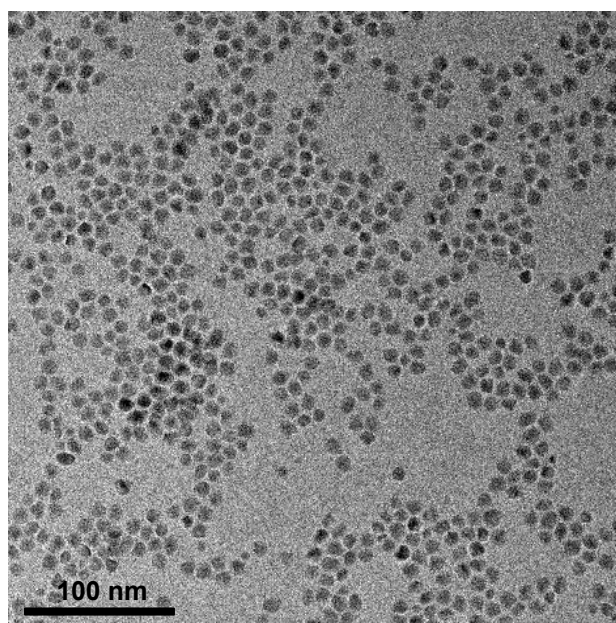


Figure S3. 10 nm quasi-spherical ZnS nanocrystals after one cycle of size selection process.

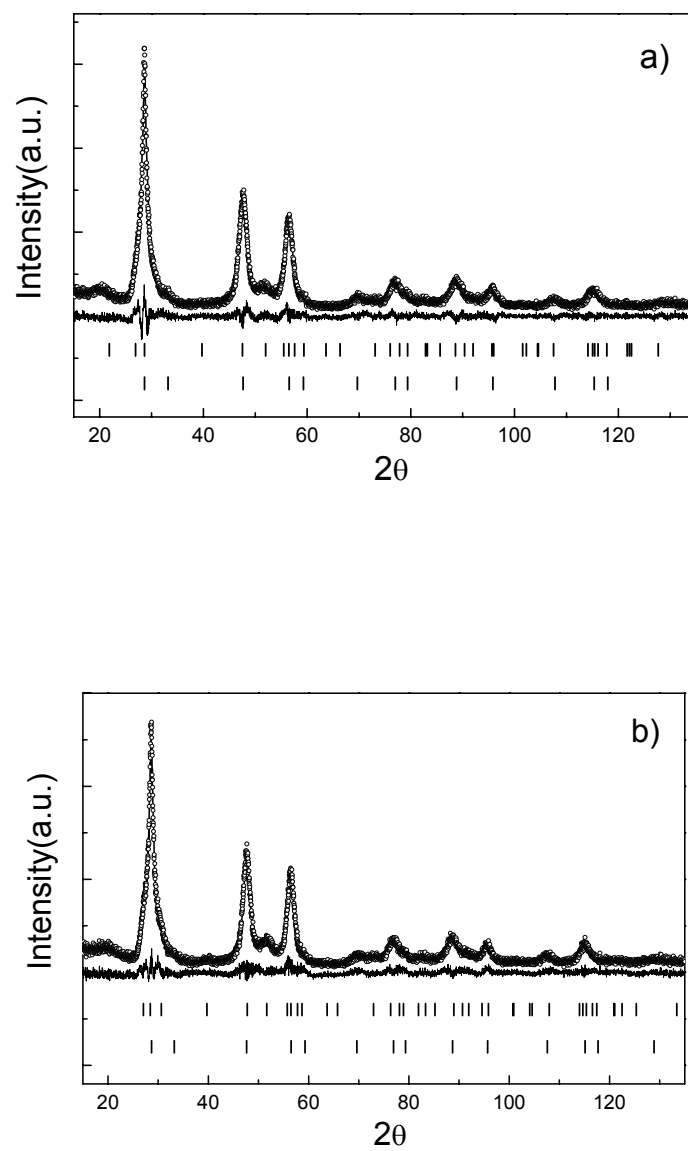


Figure S4. Observed, calculated, and difference profiles for the ZnS nanorods and 5 nm quasi-spherical ZnS nanocrystals using a Rietveld refinement.

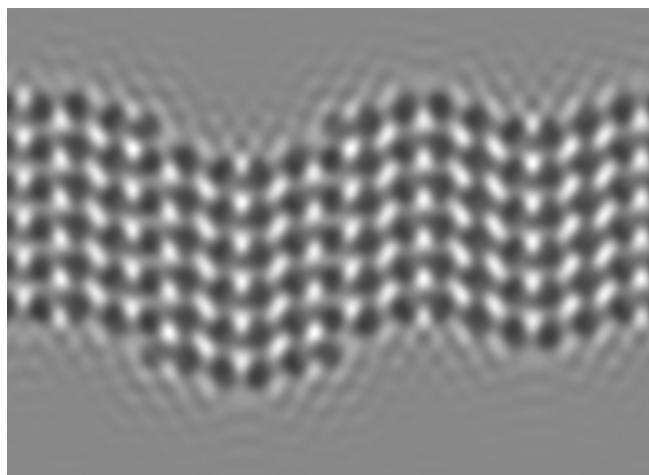
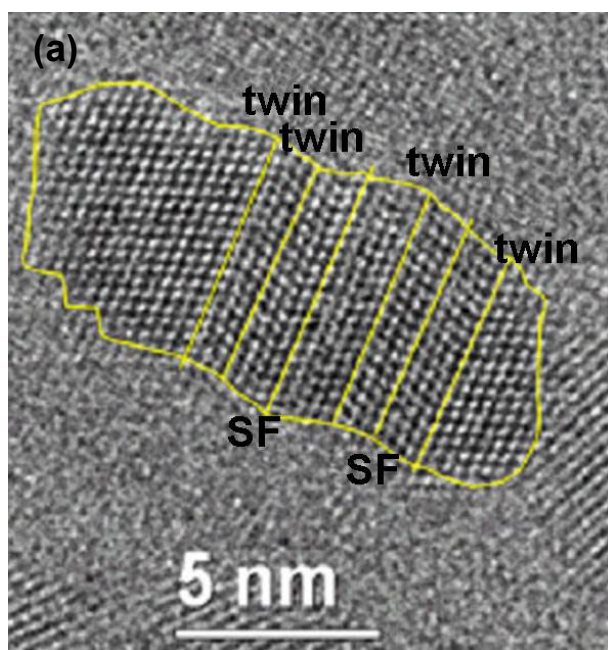


Figure S5. HRTEM image (a) and the corresponding simulated image (b) of a single ZnS nanorod. “Twin” means twinning defects, “SF” means stacking faults.

Table S1. Results of the crystal structure refinement data for ZnS nanocrystals refined by Rietveld method.

	Nano rod		5 nm ZnS	
	Spherite	Zinc Blende	Spherite	Zinc Blende
2 θ range($^{\circ}$)	20 ~ 135		20~ 135	
Number of data	5,001		5,001	
Refined parameters	16		16	
Wavelength(\AA)	1.5425		1.5425	
R _p	9.02		10.05	
R _{wp}	11.6		14.1	
χ^2 (Goodness of fit)	1.72		2.08	
Space group	F-43m	P6 ₃ mc	F-43m	P6 ₃ mc
Reflections collected	14	39	14	39
a(\AA)	5.394(1)	3.820(1)	5.403(1)	3.817(2)
c(\AA)		6.289(2)		6.297(3)
Volume (\AA^3)	156.94(5)	79.10(4)	158.18(4)	79.40(10)
Z	4	2	4	2
B(S) (\AA^2)	2.11	4.89	2.44	2.80
B(Zn) (\AA^2)	5.45	2.22	6.45	2.33
Weight %	17.9	82.1	21.0	79.0

$$\chi^2 \text{ (Goodness of fit)} = (R_{wp}/R_e)^2$$

$$R_p = \frac{\sum |y_i(obs) - y_i(calc)|}{\sum y_i(obs)} \quad R_{wp} = \left\{ \frac{\sum w_i (y_i(obs) - y_i(calc))^2}{\sum w_i (y_i(obs))^2} \right\}^{1/2}$$

$y_i(obs)$ and $y_i(calc)$ are the observed and calculated intensities at the i th step respectively, w_i is the weight factor.