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## **Supplementary Information**

The Structure-Dependent Quantum Yield of Zn<sub>x</sub>Cd<sub>1-x</sub>S

## Nanocrystals

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Table S1. The XRD results of Znx NCs.

NCs	Index	2θ (°)	$\Delta 2\theta(^{o})$	D (nm)	d (Å)	ε (%)
Zn0.2	CdS (111)	26.80	4.87	1.68	3.32	-1.54
	CdS (220)	43.90	4.84	1.77	2.06	
	CdS (311)	52.56	3.53	2.51	1.74	
Zn0.3	CdS (111)	27.25	4.12	1.98	3.27	-3.08
	CdS (220)	44.54	3.18	2.70	2.03	
	CdS (311)	52.94	4.10	2.16	1.73	
Zn0.4	CdS (111)	27.42	4.24	1.93	3.25	-3.60
	CdS (220)	45.00	4.82	1.78	2.01	
	CdS (311)	53.68	4.10	2.17	1.71	
Zn0.5	CdS (111)	27.14	3.34	2.45	3.28	-2.74
	CdS (220)	45.10	3.17	2.71	2.01	
	CdS (311)	53.00	3.03	2.93	1.73	

NCs	Index	<i>d</i> (Å)	<i>a</i> (Å)	Particle Size (nm)
Zn0.2	CdS{111}/ZnS{111}	3.36	5.82	3.6±0.4
Zn0.3		3.29	5.70	3.1±0.4
Zn0.4		3.15	5.46	3.1±0.3
Zn0.5		3.32	5.75	2.7±0.4

Table S2. HRTEM results of  $Zn_x NCs$ 

Zn K-edge						
Sampla	Dath	CN[a]	<b>R</b> <sup>[b]</sup>	σ <sup>2</sup> (×10 <sup>-3</sup> ) <sup>[c]</sup>	$\Delta E_0^{[d]}$	
Sample	Path		(Å)	(Ų)	(eV)	
ZnO	Zn-O	4.8	1.99	0.006	-0.2	
	Zn-Zn	9.6	3.21	0.000		
	Zn-O	2.1	1.95			
Zn0.2	Zn-S	0.4	2.29	0.003	-0.9	
	Zn-Zn	0.3	3.08			
	Zn-O	2.3	1.96		-0.9	
Zn0.3	Zn-S	0.3	2.33	0.003		
	Zn-Zn	0.3	3.18			
	Zn-O	2.6	1.97			
Zn0.4	Zn-S	0.2	2.33	0.003	3.0	
	Zn-Zn	0.3	3.09			
	Zn-O	2.8	1.97			
Zn0.5	Zn-S	0.2	2.42	0.003	3.6	
	Zn-Zn	1.4	3.20			
d K-edge						
Sample			<b>p</b> <sup>b</sup>	$\sigma^{2}(\times 10^{-3})^{c}$	AE d	
	Path	<b>CN</b> <sup>a</sup>	K (Å)	$(\mathring{A}^2)$	(eV)	
G 10	Cd-O	4.4	2.28	0.000	1.5	
CdO	Cd-Cd	7.1	3.33	0.008	1.7	
	Cd-O	1.1	2.20			
CdS	Cd-S	2.2	2.50	0.003	2.5	
	Cd-Cd	0.1	3.55			
	Cd-O	0.9	2.16			
Zn0.2	Cd-S	2.0	2.46	0.003	2.9	
	Cd-Cd	0.2	3.55			
	Cd-O	0.8	2.13			
Zn0.3	Cd-S	2.3	2.50	0.003	0.7	
	Cd-Cd	0.2	3.55			
	Cd-O	0.6	2.21			
Zn0.4	Cd-S	2.1	2.52	0.003	3.7	
	Cd-Cd	0.6	3.55			

Table S3. XAS fitting results of Znx NCs in Zn and Cd K-edges.

	Cd-O	1.2	2.21		
Zn0.5	Cd-S	2.1	2.51	0.003	2.5
	Cd-Cd	0.2	3.56		

[a] CN: coordination number, [b] R: bond distance, [c]  $\sigma^2$ : Debye-Waller factor, [d]  $\Delta E_0$ : inner potential correction.



Figure S1 Fourier transformed EXAFS spectra with the fitting curves for Znx NCs in (a)Zn and (b)Cd K-edge.