Electronic Supplementary Information

The Important Role of Surface Ligand on CdSe/CdS Core/Shell Nanocrystals for Affecting the Efficiency of H_2 Photogeneration from Water

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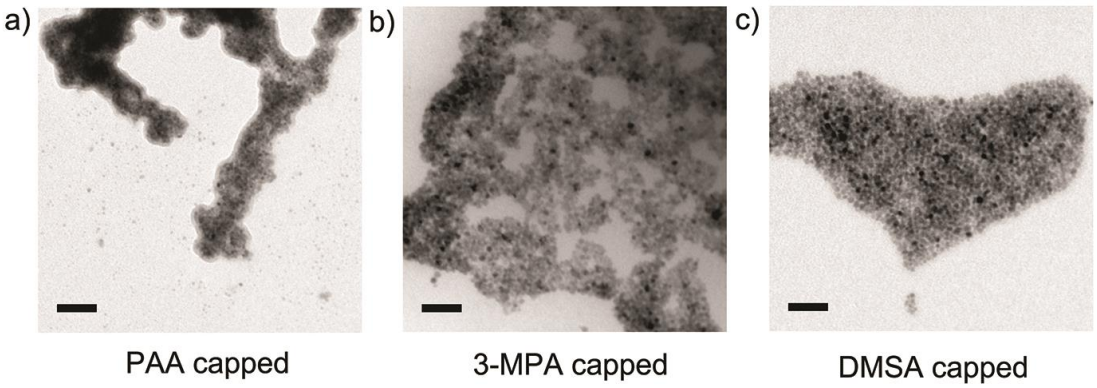

Fig. S1. TEM images of the (a) PAA capped QDs (***Note:*** *after the illumination the PAA capped QDs are still well dispersed in the solution, and cannot be precipitated to get the product. Thus, certain amount of HCl aqueous solution was required to introduce to precipitate of the product;*[1] *however, this will cause the partial dissolution for the case of CdSe/CdS core/shell NCs, which makes the PAA capped QDs much smaller than that capped with other two ligands*); (b) 3-MPA capped QDs and (c) DMSA capped QDs after the 5 h hydrogen evolution measurements that employing Pt as the catalyst, respectively. The scale bars: 50 nm.

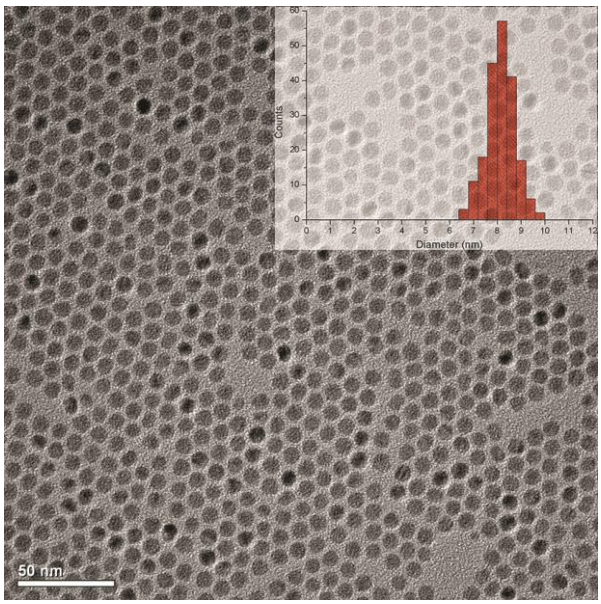

Fig. S2. Typical TEM image of the OA capped CdSe/CdS core/shell NCs, scale bar: 50 nm. The inset is the size histograms obtained from 200 particles in the image.

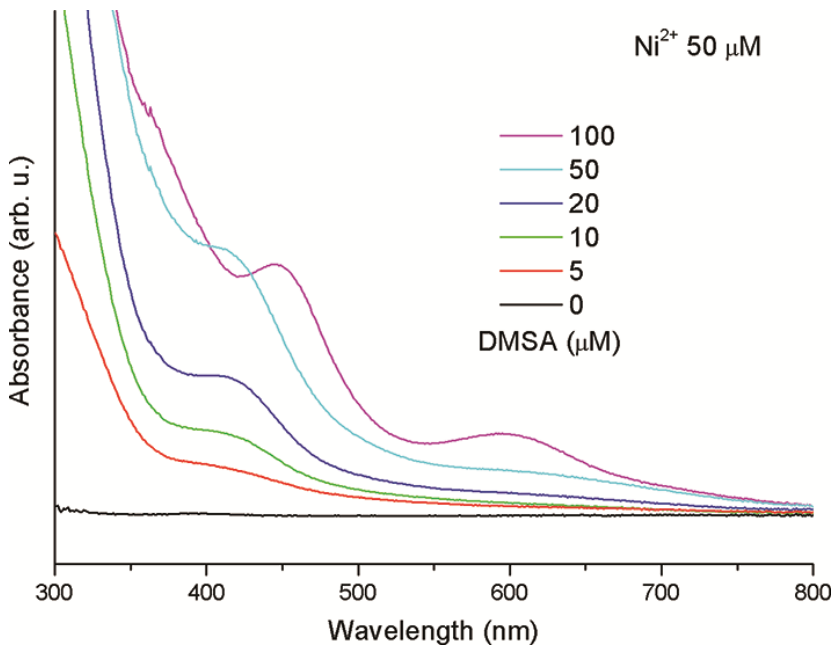

Fig. S3. UV-Vis spectra of the aqueous solution with 50 μM of Ni^{2+} ions by increasing the concentration of DMSA.

	OA capped	PAA capped	3-MPA capped	DMSA capped
sulfur/cadmium (At.)	0.63	0.72	1.48	1.31
PL QY (%)	64.8	35.7	26.5	4.6

Table S1. The atomic (At.) ratio of sulfur/cadmium obtained from the XPS results and PL QY of the NCs capped with different ligands.

CdSe/CdS core/shell	A_1	τ_1 (ns)	A_2	τ_2 (ns)
OA capped	1	33.0	N/A	N/A
PAA capped	0.17	8.9	0.83	31.7
3-MPA capped	0.24	7.2	0.76	29.3
DMSA capped	0.31	4.8	0.69	24.1

Table S2. PL decay fitting parameters of CdSe/CdS core/shell NCs capped with different ligands, fitting equation: $R(t) = A_1 e^{(-t/\tau_1)} + A_2 e^{(-t/\tau_2)}$.

Reference:

1. T. Zhang, J. Ge, Y. Hu and Y. Yin, *Nano lett.*, 2007, **7**, 3023-3027.