Supplementary information

Nanofabricated optical tuning and epitaxial overgrowth of In_2S_3 shell on CdSe core†

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† Electronic supplementary information (ESI) available: Lattice strain simulation, Electrophoretic mobility and zeta potential. See DOI:

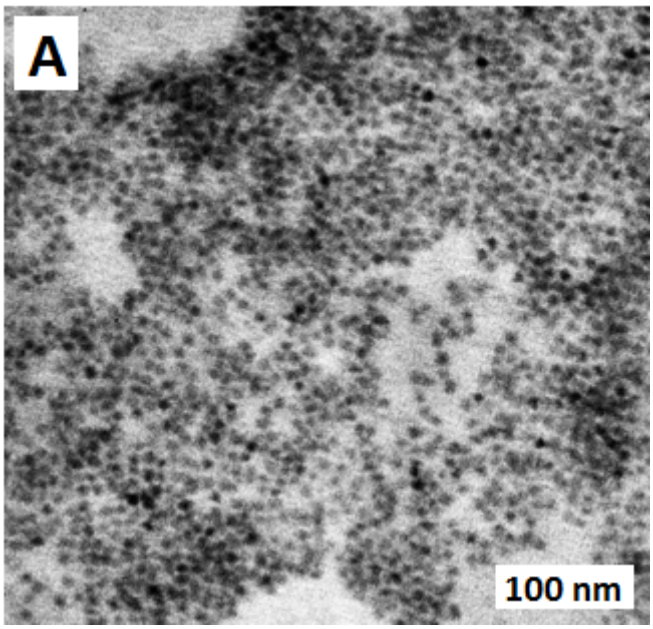

Fig. S-1 TEM image of GSH-CdSe QDs

Lattice strain simulation. The Halder-Wagner method[1,2] was used to determine the lattice strain (ε) of GSH-CdSe/In_2S_3 QD nanocrystals. An alternative equation proposed by Halder-Wagner contains the lattice-plane spacing (d^*) for the reciprocal cell and the integral breadth (β^*) of the reciprocal lattice point as described by:

$$\left(\frac{\beta^*}{d^*}\right)^2 = \frac{K}{D} \cdot \frac{\beta^*}{(D^*)^2} + (2\varepsilon)^2 \qquad (1)$$

$$\beta^* = \frac{\beta cos\theta}{\lambda} \qquad (2)$$

$$d^* = \frac{2cos\theta}{\lambda} \qquad (3)$$

This is based on the theory that the Gaussian and Lorentzian components of β^* are primarily due to the strain and size effects of the nanocrystals. Equation (1) can be rewritten with respect to direct space as:

$$\left(\frac{\beta}{tan\theta}\right)^2 = \frac{K\lambda}{D} \cdot \frac{\beta}{tan\theta sin\theta} + 16\varepsilon^2 \qquad (4)$$

Equation 4 has a straight line y = mx+c in which the Halder-Wagner plot, y = $(\beta/\tan\theta)^2$ is plotted against $\beta/(\tan\theta\sin\theta)$. The lattice strain (intercept) of the obtained straight line = $16\varepsilon^2$. Fig. S-1 shows the resulting Halder-Wagner plots for the size-dependent GSH-CdSe/In_2S_3 QD nanocrystals.

Electrophoretic mobility. During electrophoresis, the mobile phase of the colloidal core/shell nanocrystal scatters an incident laser. Therefore, due to the mobility of the colloidal nanocrystals, the frequency shift is proportional to the speed of the nanocrystal (Doppler shift), hence making the frequency of the original laser to be different from the scattered light. The negative or positive dimensions of ZP of the colloidal nanocrystals are determined by the electrode in which the nanocrystals are moving towards during electrophoresis.[3] Therefore, we have determined the electrophoretic mobility of the QD nanocrystals. Fig. S-2 displays the electrophoretic mobility curves of the size-dependent GSH-CdSe/In_2S_3 QD nanocrystals while their corresponding values are -4.8±0.6 μmcm/Vs for GSH-CdSe/In_2S_3-1, -4.4±0.5 μmcm/Vs for GSH-CdSe/In_2S_3-2, -4.4±0.4 μmcm/Vs for GSH-CdSe/In_2S_3-3 and -3.4±0.6 μmcm/Vs for GSH-CdSe/In_2S_3-4, respectively. The electrophoretic mobility values were in the range of -4.8 μmcm/Vs to -3.4 μmcm/Vs. GSH-CdSe/In_2S_3-2 and GSH-CdSe/In_2S_3-3 had the same electrophoretic mobility. We can deduce that the trend in electrophoretic mobility of the QDs were synonymous to the ZP charge. The more negative is the ZP charge of the QD, the more negative is the electrophoretic mobility and vice versa. The differences in electrophoretic mobility can be ascribed to the variation in the number of GSH thiol ligand anchored to the QDs surface and also its steric effect.

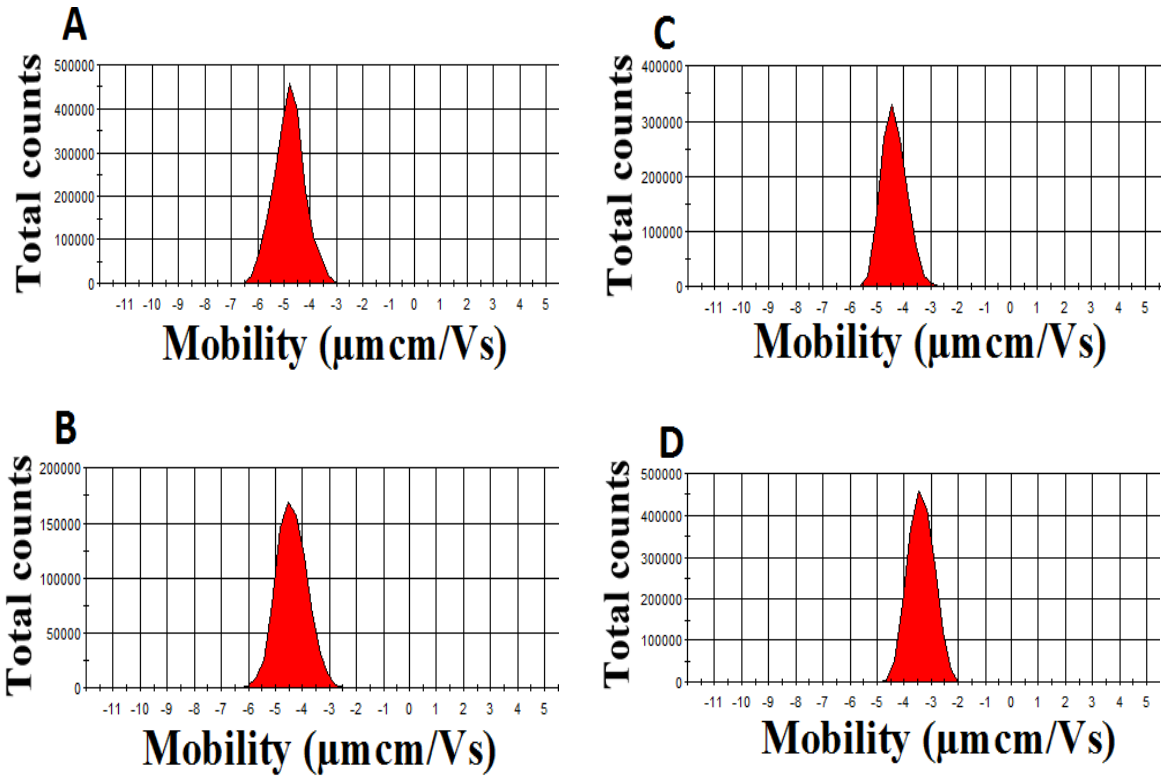

Fig. S-2 Electrophoretic mobility curves for (A) GSH-CdSe/ In2S3-1, (B) GSH-CdSe/ In2S3-2, (C) GSH-CdSe/ In2S3-3 and (D) GSH-CdSe/ In2S3-4 QDs.

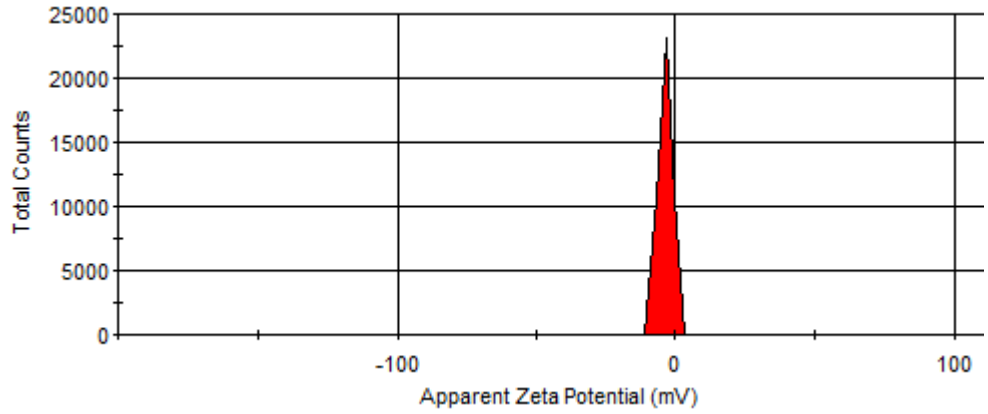

Fig. S-3 Zeta potential curve for ultrapure Millipore water.

References

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2. N. C. Halder, C. N. J. Wagner, *Adv. X-Ray Anal.,* 1966, **9**, 91–102

3. T. Ito, L. Sun, M. A. Bevan, R. M. Crooks, *Langmuir,* 2004, **20**, 6940-6945.