Supporting information for

Shape and Property Control of Mn Doped ZnSe Quantum Dots: From Branched to Spherical

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Figure 1S Determination of Photoluminescence Quantum Yield

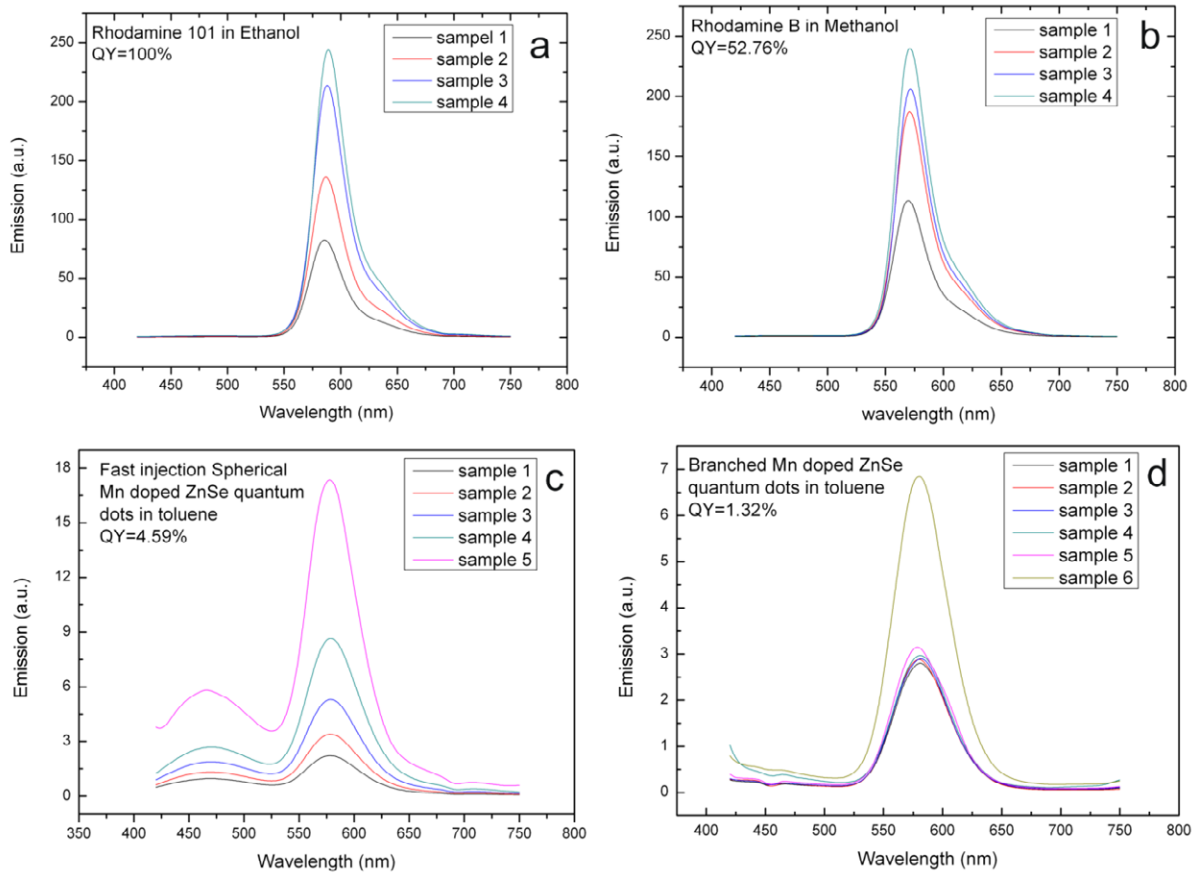

Figure 1S. Determination of photoluminescence quantum yield: (a) Rhodamine 101 in ethanol, QY=100%. (b) Rhodamine B in ethanol, QY=52.76%. (c) Fast injection spherical Mn doped ZnSe quantum dots in toluene, QY=4.59%. (d) Branched Mn doped ZnSe quantum dots in toluene, QY=1.32%.

The PL quantum yield (QY) measurement of d-dots. The PL QY of the Mn doped ZnSe was determined by using Rhodamine 101 dye as reference and Rhodamine B dye for cross calibration. All the samples are excited at 400 nm wavelength and their emission varies from 420 nm to 750 nm, with dominate peaks at around 580 nm. In the first step, absorption of the sample spectrum was measured with subtraction of spectrum of solvent. The optical density of the samples was determined at 400 nm wavelength, which was used later as excitation wavelength for PL measurement. Then, emission spectrum were taken with only solvent and varies concentration of the samples by drop by drop techniques. The optical density of both dyes at 400 nm is less than 0.05 for avoiding detector saturation. The optical density of Mn

doped ZnSe quantum dots at 400 nm is less than 0.1 for avoiding self quenching and no-linear effect. The PL spectrums of samples were corrected by subtracting emission spectrum of solvent from the emission spectrum of samples. The solvent-corrected PL spectrums were presented in Figure 1S (a)-(d). The graph of integrated fluorescence intensity verse absorbance at 400 nm excitation wavelength was plot and fitted linearly, shown in the content figure 5 (e)-(f). The gradients were determined by analysing the slope of the fitted line. The PL QY of both standard dyes and quantum dots samples were calculated with the following equation, which is suggested by IUPAC.[1]

$$\phi_{dot} = \phi_{REF}\left(\frac{Grad_{dot}}{Grad_{REF}}\right)\left(\frac{\eta_{dot}^2}{\eta_{REF}^2}\right)$$

Dot=nanocrystals, REF=Reference, η=refractive index of a solvent. The Quantum yield of Rhodamine 101 in ethanol is 100% [2] and Rhodamine B in methonal at 298k is 52% [3]. The measured value for standard dye fits the literature well, which gives cross calibration.

Reference:

[1] IUPAC, Reference materials for fluorescence measurement, *Pure & Appl. Chem.*1988, vol 60, No,7, pp. 1107-1114

[2] Karstens, T. and Kobs. K., *J. Phys. Chem.* 1980, 84, 1871-1872

[3] Chang, T.-L., Cheung, H.C. *J. Phys. Chem.* 1982, 96, 4874-487

Figure 2S An in-situ TEM study of morphology dynamics

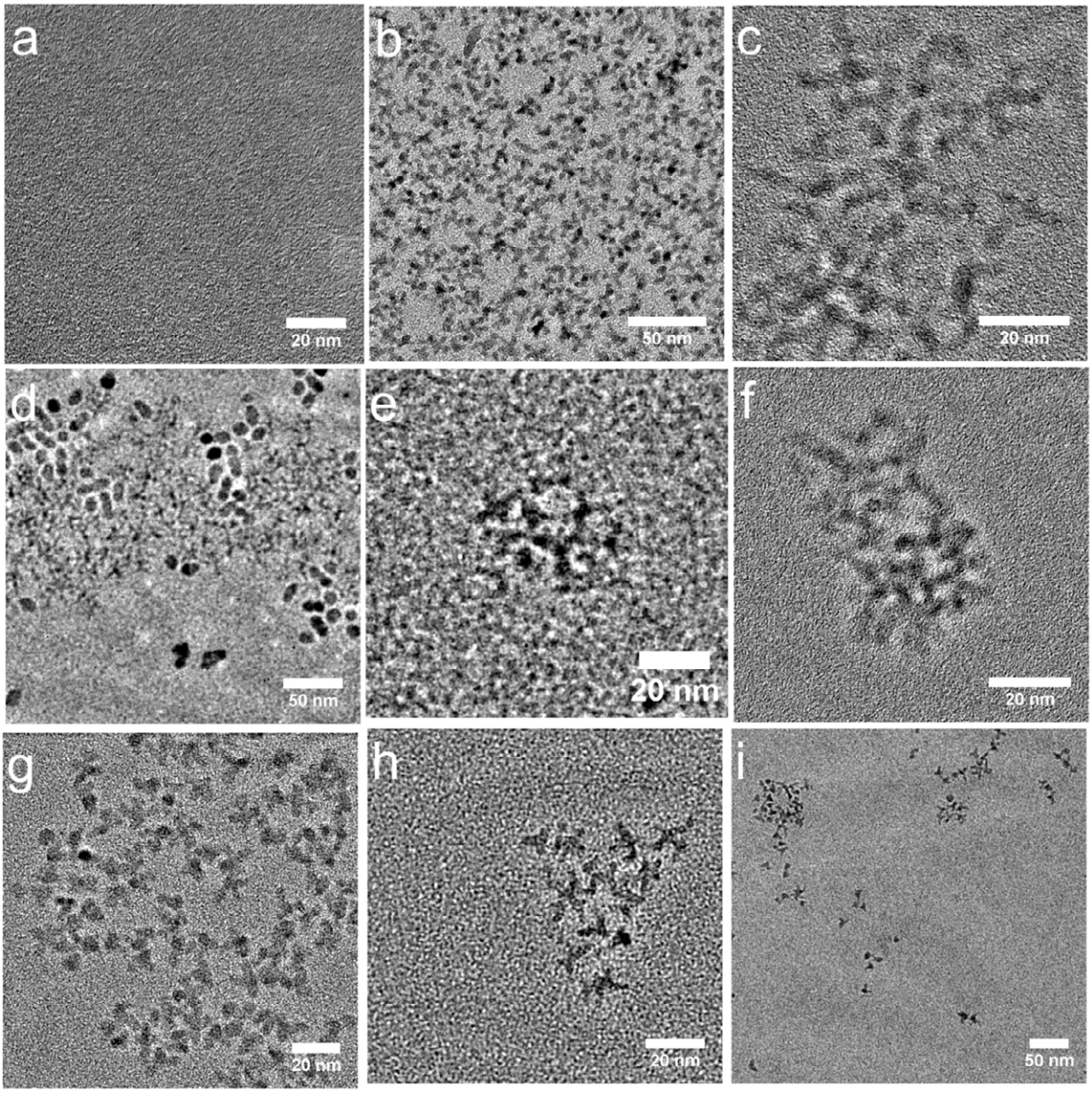

Figure 2S. TEM images of morphology dynamics of branched Mn doped ZnSe quantum dots during and after reaction: (a) MnSe small nanoclusters annealed after one hour. (b) Immediately after the 1st injection of Zinc precursor at 290 °C. (c) Immediately after the 2nd injection of zinc precursor. (d) Immediately after the 3rd injection of zinc precursor. (e) Immediately after the 4th injection of zinc precursor. (f) Cooling down the reaction to 180 °C. (g) Cooling down to room temperature. (h) One day after the reaction. (i) One months after the reaction.

In order to understand the growth mechanism and morphology dynamics of branched Mn doped ZnSe quantum dots during the reaction, a series in situ TEM study was performed.

Figure 2S (a) shows the stages of MnSe small nanoclusters annealed after one hour, just before the first injection of zinc precursor. It is very hard to pick up this MnSe nanoclusters due to its relatively small size and invisible in the condition of TEM performance. Figure 2S (b) shows the branched structure forms immediately after the first injection of zinc precursor. Morphology doesn't change very much after the first injection of zinc precursor. The morphology is quite stable without aggregation over one month.

Figure 3S. Selective area electron diffraction (SAED) measurements

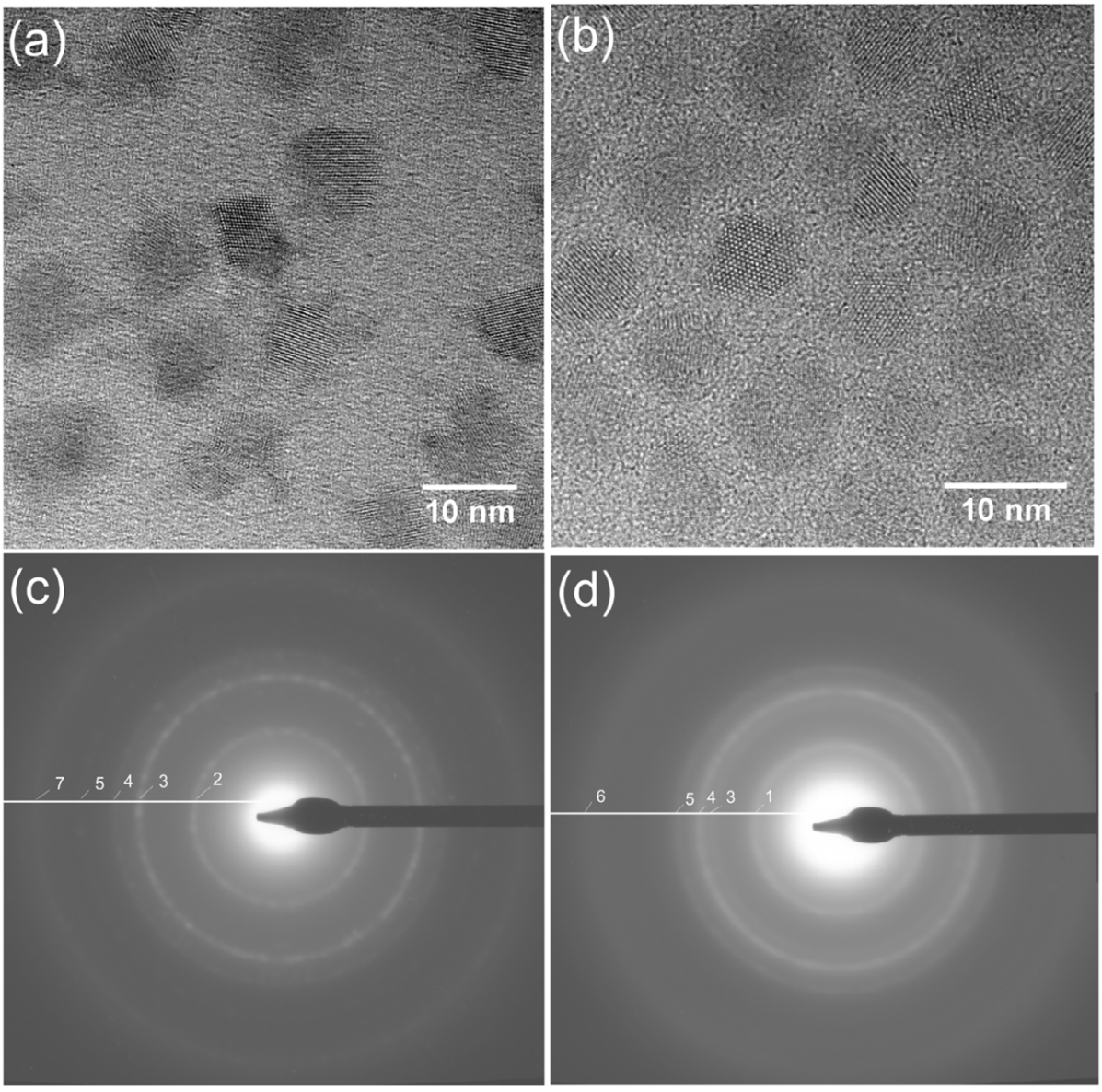

Figure 3S. (a) HETEM image of slow injection Mn doped ZnSe quantum dots with injection temperature at 220 °C. (b) HRTEM image of fast injection Mn doped ZnSe quantum dots with injection temperature at 220 °C. (c) SAED of slow injection Mn doped ZnSe quantum dots. (d) SAED of fast injection Mn doped ZnSe quantum dots.

Ring	hkil (hexagonal)	hkl (cubic)	d [Å]
1	100	None	3.519
2	Not shown	111	3.302
3	110	220	2.032
4	200	311	1.759
5	210	331	1.330
6	300	Not shown	1.173
7	Not shown	511	1.109

Table 1: Assignment of SAED rings to Mn doped ZnSe crystal structures; d: lattice spacing

SAED patterns of both slow and fast injection Mn doped ZnSe quantum dots with injection temperature at 220 ℃ was obtained from a field of Mn doped ZnSe nanocrystals shown in Figure 3S (a) and (b). At least five separation diffraction rings are observed, and this are assigned in table 1. In Figure 3S (d) ring 1 is unique to (100) plane of hexagonal (wurtize) structure. This confirms fast injection sample is wurtize structure while slow injection sample is zinc blende crystal phase. This is consistent with FFT analysis of HRTEM image of a few nanocrystals in Figure 3S (a) and (b).