Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

Electronic Supporting Information

Defect Rich Seed Mediated Growth: A Novel Synthesis Method to Enhance Defect Emission in Nanocrystals

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Experimental

Typical reaction profile for microwave synthesis are given below,

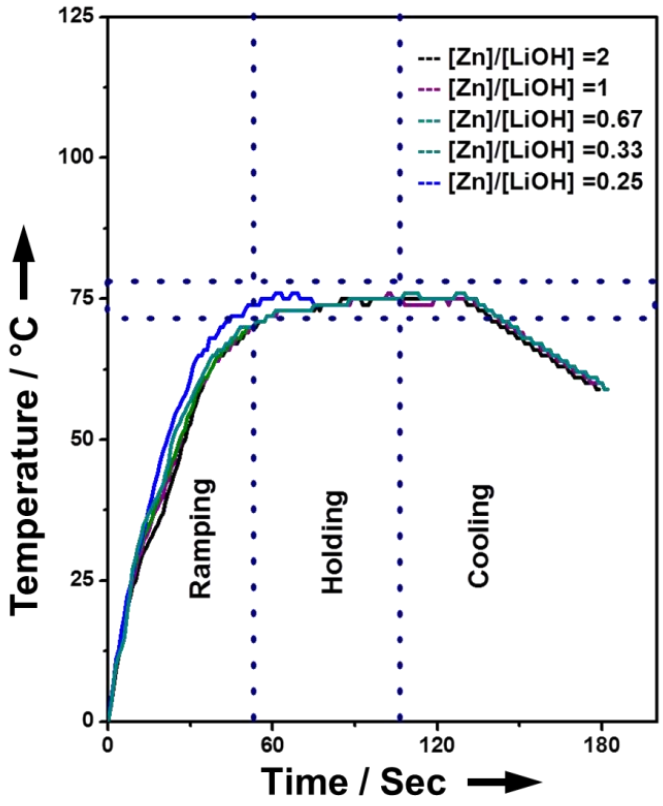

Fig. S1. A typical reaction profile showing effect of [LiOH) on microwave based dielectric heating.

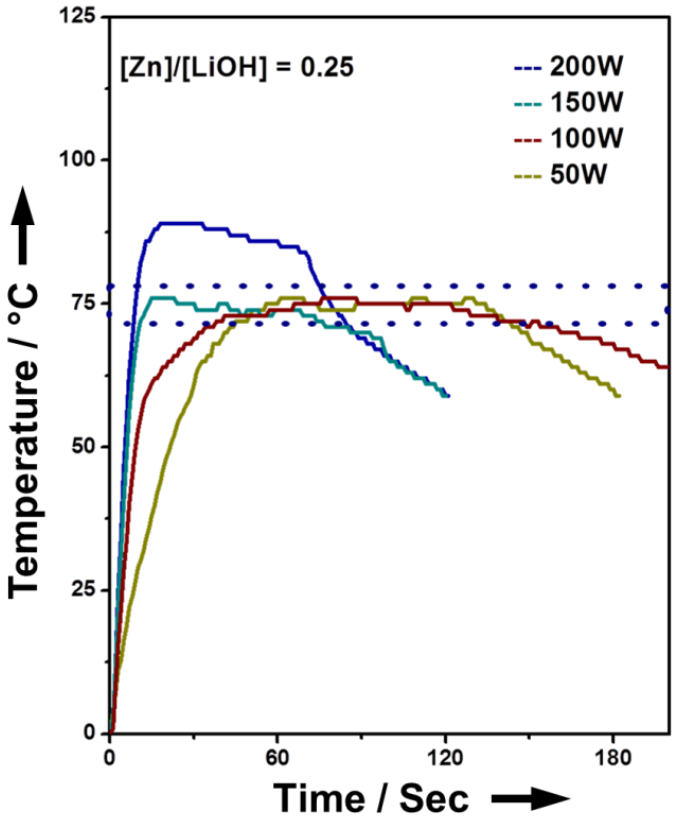

Fig. S2. A typical reaction profile showing effect of microwave power on dielectric heating for [Zn]/[LiOH] = 0.25.

Characterization

X-ray powder diffraction (XRD) data were collected using Philips (PANalytical) powder diffractometer PW3040/60 X'pert Pro with Cu Kα radiation. The photoluminescence (PL) spectra were acquired using HORIBA JobinYvon Fluorolog 3 model(quinine sulfate and rhodamine 6G were used as references for quantum yield(Q.Y.) calculation).

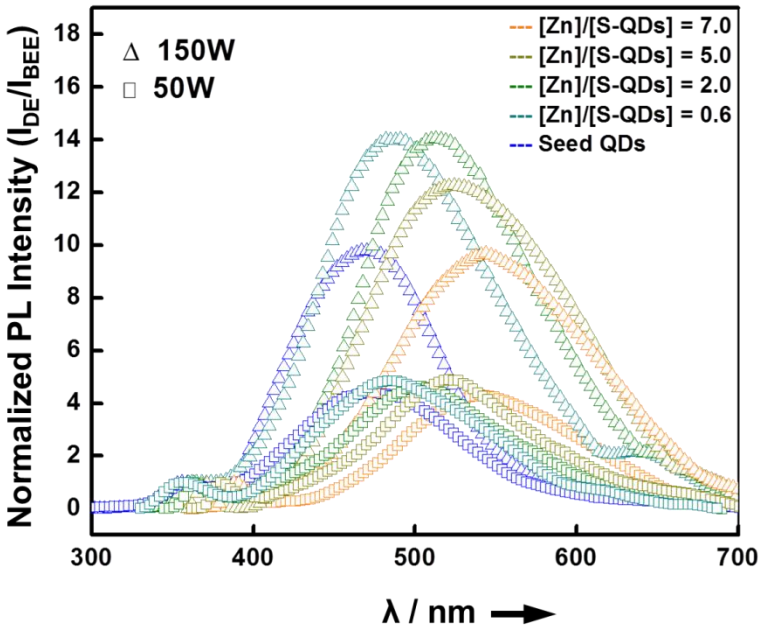

Fig. S3. PL spectra of different size D-ZnO QDs grown from S_{HD}-ZnO and S_{LD}-ZnO QDs. ([S-QDs] = concentration of seed QDs)

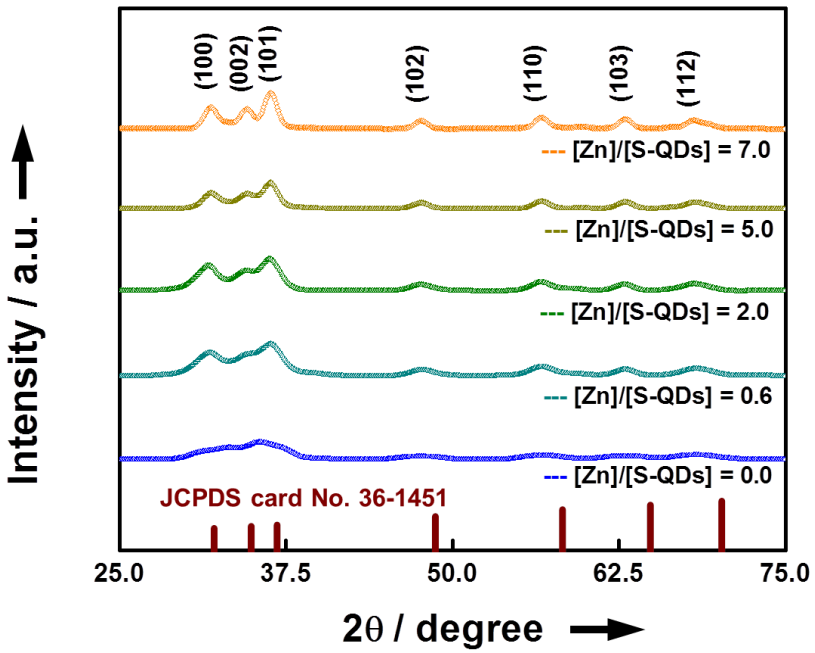

Fig. S4. XRD pattern of different size D-ZnO QDs grown from S_{HD}-ZnO and S_{HD}-ZnO QDs. ([S-QDs] = concentration of seed QDs)

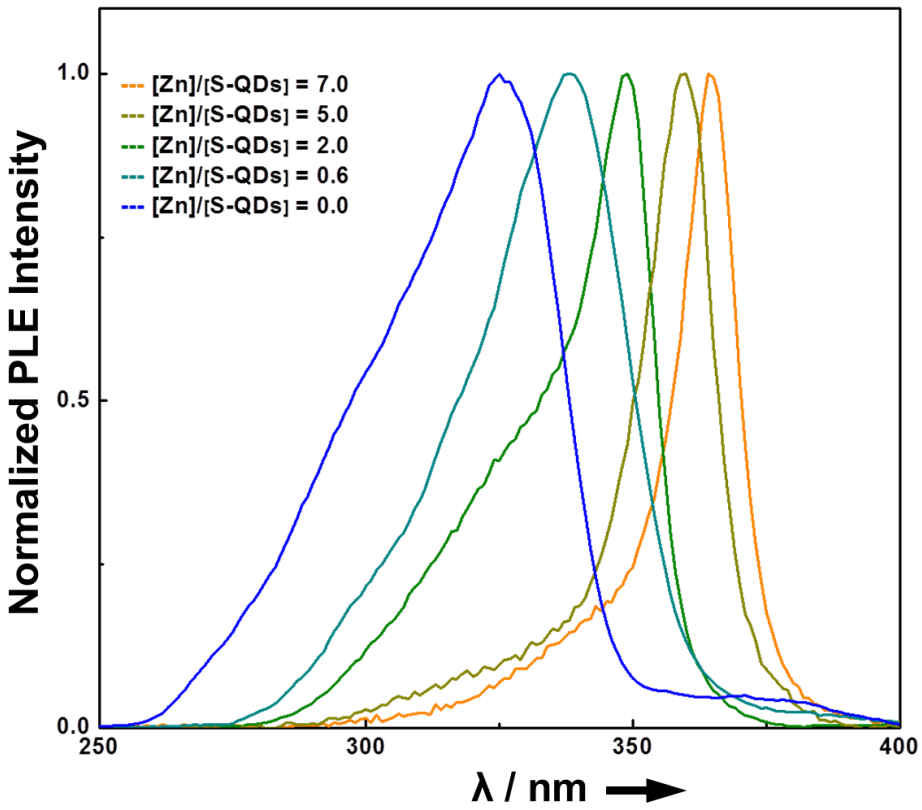

Fig. S5. PLE of different size D-ZnO QDs grown from S_{HD}-ZnO QDs and S_{HD}-ZnO QDs. ([S-QDs] = concentration of seed QDs)

The particle size of QDs can be obtained from the PLE spectra, λ_{max} of the PLE spectra is taken as the band gap value for each sample. The band gap values (E_g) obtained from PLE was inserted into to an approximation (eq. 1) reported by Schoenhalz et al. [1] to obtain corresponding diameter 'd 'of the D-ZnO QDs and the results are shown in main text (Table 1).

$$E_g = 3.41 + 3.87 \times d^{-1.83} \quad (1)$$

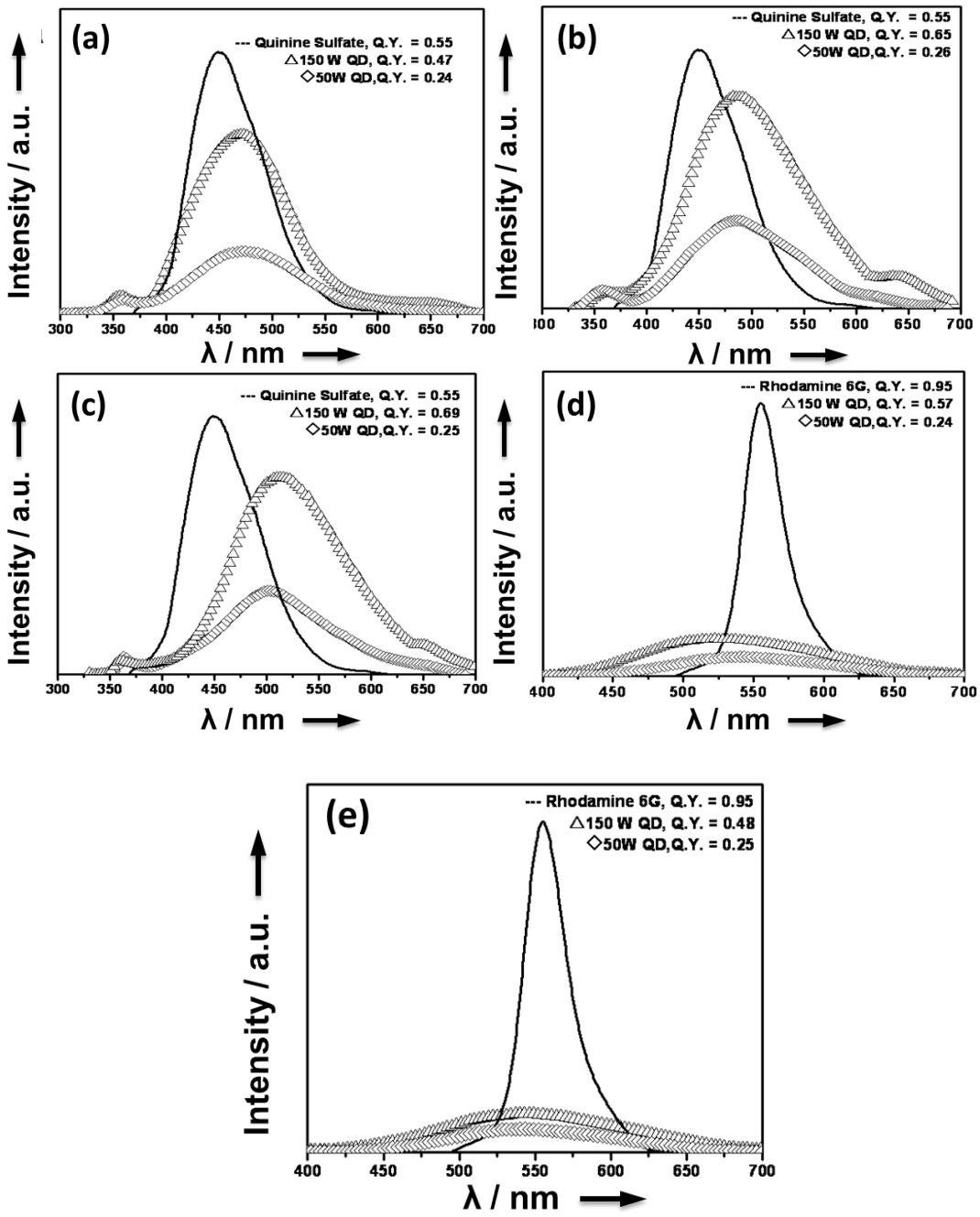

Fig. S6. Quantum yield comparison of different size D-ZnO QDs grown from S_{HD}-ZnO QDs and S_{LD}-ZnO QDs with standard dyes (Quinine sulfate and Rhodamine 6G). a) Seed QDs (S_{HD}-ZnO QDs and S_{LD}-ZnO QDs) b)[Zn]/[Seed QDs] = 0.6 c) [Zn]/[Seed QDs] = 2.0 d) [Zn]/[Seed QDs] = 5.0 and e) [Zn]/[Seed QDs] = 7.0

In Quantum yield (QY) estimation[2], typically D-ZnO QDs and the standards (quinine sulfate in 0.1 N H_2SO_4 and rhodamine 6G) are irradiated by the same excitation wavelength for samples

(i.e., λ_{max} of PLE (Fig. S5) for different D-ZnO QDs). The quantum yields of D-ZnO QDs were calculated using equation 2.

$$\Phi = \Phi_S [(I \cdot A_S \cdot n^2)/(I_S \cdot A \cdot n_S^2)] \quad (2)$$

where Φ is the quantum yield, I is the integrated intensity, A is the optical density and n is the refractive index of the solvent. The subscript S refers to the standard reference of known quantum yield. The excitation wavelength of both the sample and the standard should have similar optical density. Here the optical density of sample and standard are fixed at an absorbance of 0.08 at 340 nm. Then the integrated emissions of both PL spectra were compared to calculate the QY of the sample, taking into account the QY value of the standard as 0.95 for Rhodamine 6G and 0.55 for Quinine sulfate. The refractive indexes of ethanol and water are 1.3614 and 1.333 respectively.

References

1. A. L. Schoenhalz, J. T. Arantes, A. Fazzio, G. M. Dalpian, *J. Phys. Chem. C* 2010, **114**, 18293-18297.
2. D. F. Eaton, *Pure &Appl. Chem.*1988, **60**, 1107-1 114.