

Supplementary Information

Single-Sized Colloidal CdTe Nanocrystals with Strong Bandgap Photoluminescence

Ruibing Wang,^a Jianying Ouyang,^a Steve Nikolaus,^a Luc Brestaz,^a Md. Badruz Zaman,^a
Xiaohua Wu,^b Donald Leek,^a Christopher I. Ratcliffe,^a and Kui Yu^{a,*}

Stacie Institute for Molecular Sciences,[†] and Institute for Microstructural Sciences,[‡]
National Research Council of Canada, Ottawa, Ontario K1A 0R6, Canada

1. Experimental Section

1.1. Synthesis of CdTe MSQD Family 427 (Batch (a) shown in manuscript Figure 2a):

two solutions were prepared separately. A $\text{Cd}(\text{OAc})_x(\text{OOC}-(\text{CH}_2)_n-\text{CH}_3)_{2-x}$ solution in ODE was made in a reaction flask by mixing $\text{Cd}(\text{OAc})_2 \cdot 2\text{H}_2\text{O}$ (0.4 mmol) and alkylcarboxylic acid (0.133 mmol) in 4 grams ODE at 120 °C for two hours under vacuum; the reaction flask was cooled down to 60 °C and protected under Argon. A TOPTe solution in TOP was prepared by mixing 0.05 mmol elemental Te powder with 0.1 mmol TOP in a small vial and sonicated for three hours. The freshly-prepared TOPTe solution was transferred into the reaction flask and rinsed with 1 gram ODE. The mixture was degassed, stirred and heated to 120 °C for one hour; then the temperature was kept at a constant temperature for a certain growth periods, or increased slowly to 240 °C under a flow of Argon. Aliquots were taken to monitor the temporal evolution of the optical properties of the growing nanocrystals with absorption and emission measurements.

1.2. Efforts on the development of larger MSQD ensembles. Figure S1 shows the emission spectra of the growing CdTe nanocrystals from one synthetic batch but sampled at different growth temperature during the increase of the reaction temperature from 120 °C to 240 °C; the nanocrystals sampled were dispersed in toluene.

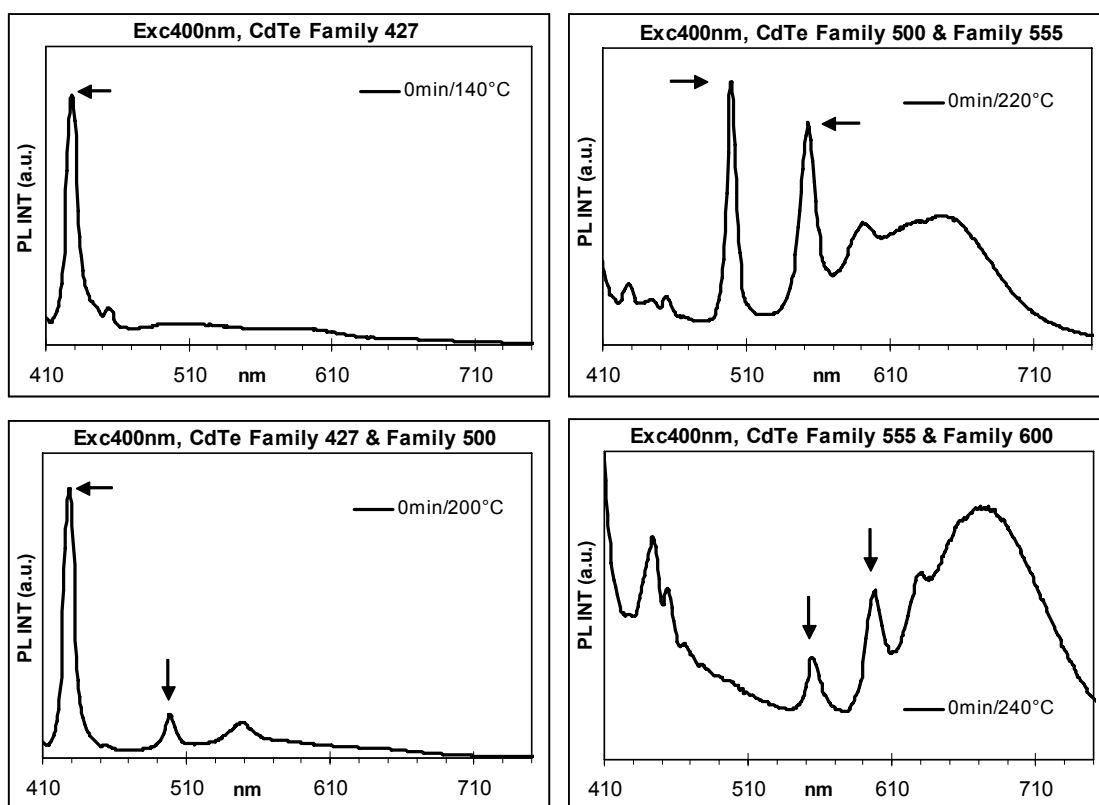


Figure S1. Emission spectra (with the excitation wavelength of 400 nm) of the growing CdTe nanocrystals from one synthetic batch but sampled at different growth temperature during the increase of the reaction temperature from 120 °C to 240 °C; the nanocrystals sampled were dispersed in toluene.

1.3. Purifications for TEM/XRD/NMR characterization: Sample/Toluene/MeOH = 1:3:4 (volume ratio) or around 1:2:3, to get a miscible suspension; afterwards, the suspension was centrifuged to get precipitate and washed with Toluene/MeOH (\sim 1:2). Such purification was carried out twice.

2. Characterization

2.1. TEM:

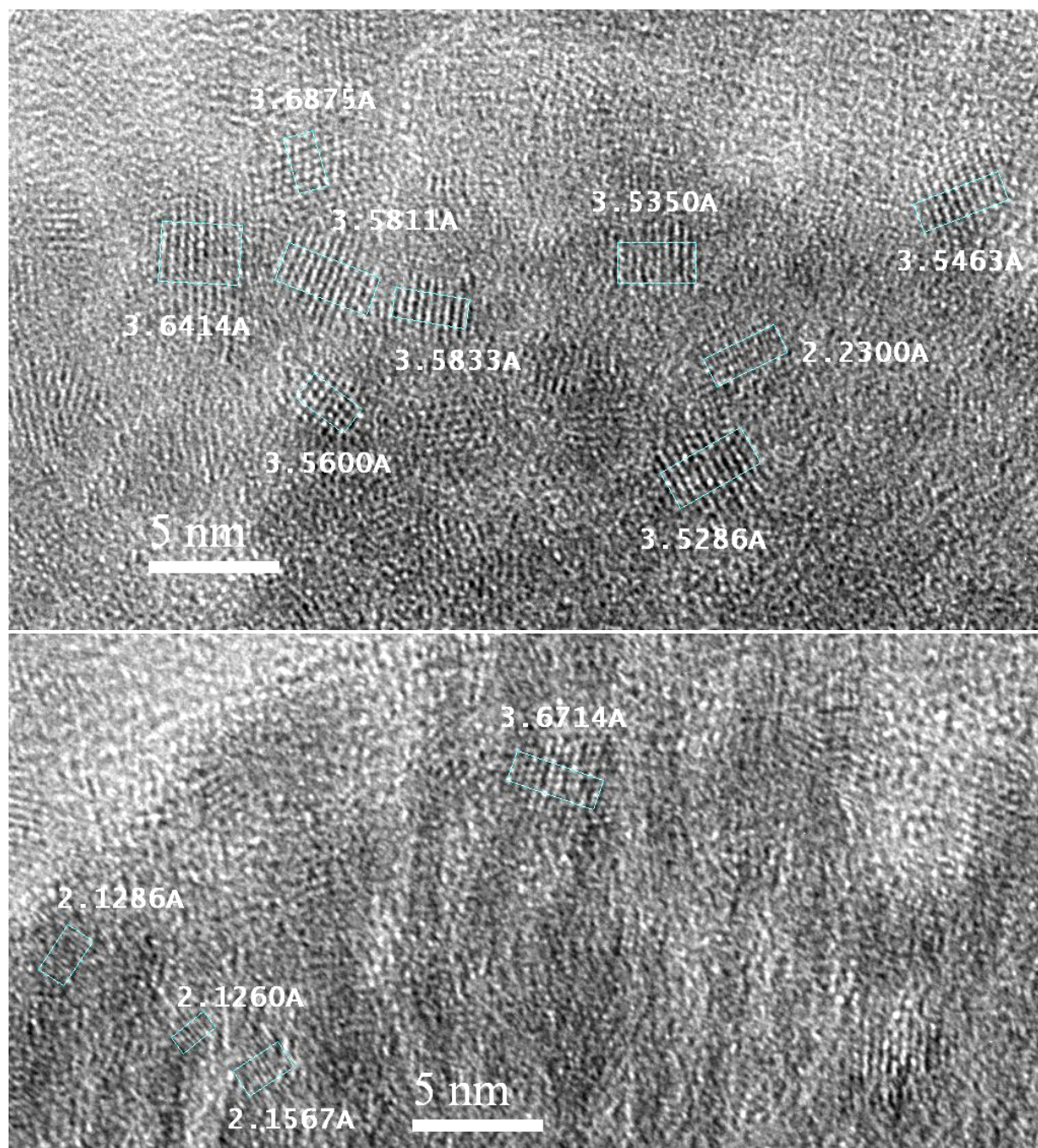


Figure S2-a. Two HRTEM images showing the d spacing measured, indicating a wurtzite crystal structure; the scale bar is 5 nm. For wurtzite CdTe, two d spacings of (101) and (103) are

characteristic; the two measured d spacing values are close to 3.52 Å and 2.11 Å, which are the standard values of the d spacing of (101) and (103) planes, respectively. (See Refs (a) Sandeep Kumar and Thomas Nann *Chem. Commun.* “Hexagonal CdTe nanoparticles of various morphologies” **2003**, 2478-2479; (b) JCPDS 19-0193)

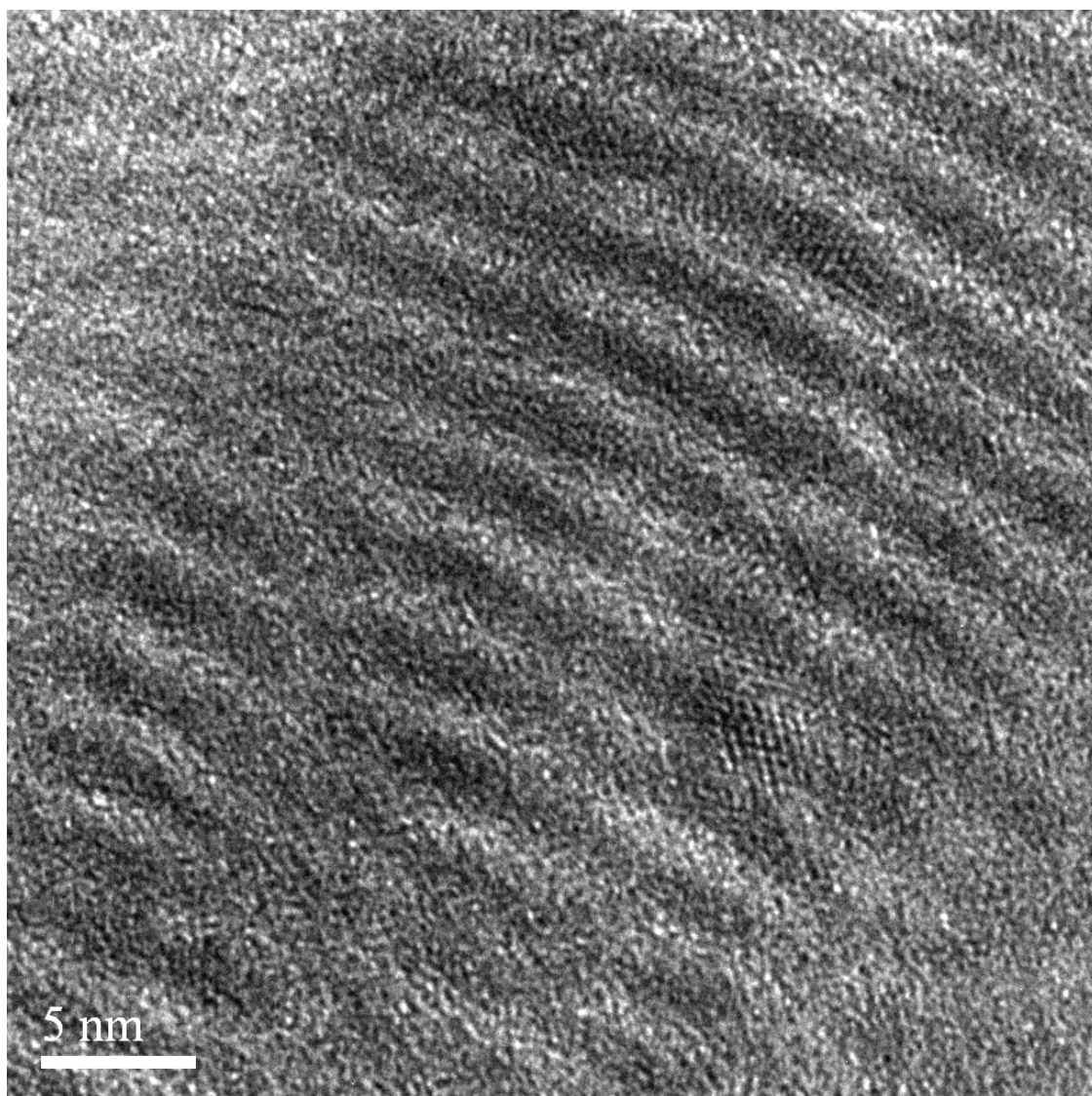


Figure S2-b. A HRTEM image showing the aggregation/coalescence of CdTe MSQD Family 427; the scale bar is 5 nm. One magic-sized QD ensemble consists of the nanocrystals which are highly uniform in size (from its synthetic batch and afterwards dispersed in solvents such as toluene). Meanwhile, they have a strong tendency to aggregate (during post-treatment). One of frequently occurred aggregations is called oriented attachment leading to the formation of nanowires (Ref 1, 2); it was acknowledged that the self-assembly of MSQDs results in the formation of long wires in some preferred direction(s), with the diameter close to or slightly

larger than their original size. What is shown in Figure S2-**b** is the self-assembled nanowires formed during the solvent evaporation, with the diameter of ~ 2.5 nm, the value of which is slightly larger than the original size of 1.5 nm (which was determined by our DOSY-NMR); the edge-to-edge distance of the two nearest wires is caused by the existence of surface ligands (long-chain fatty acids).

Ref. 1 Zhiyong Tang, Nicholas A. Kotov and Michael Giersig, *Science*, 2002, **297**, 237.

Ref. 2 Narayan Pradhan, Huifang Xu and Xiaogang Peng, *Nano Lett.*, 2006, **6**, 720.

2.2. High-resolution NMR:

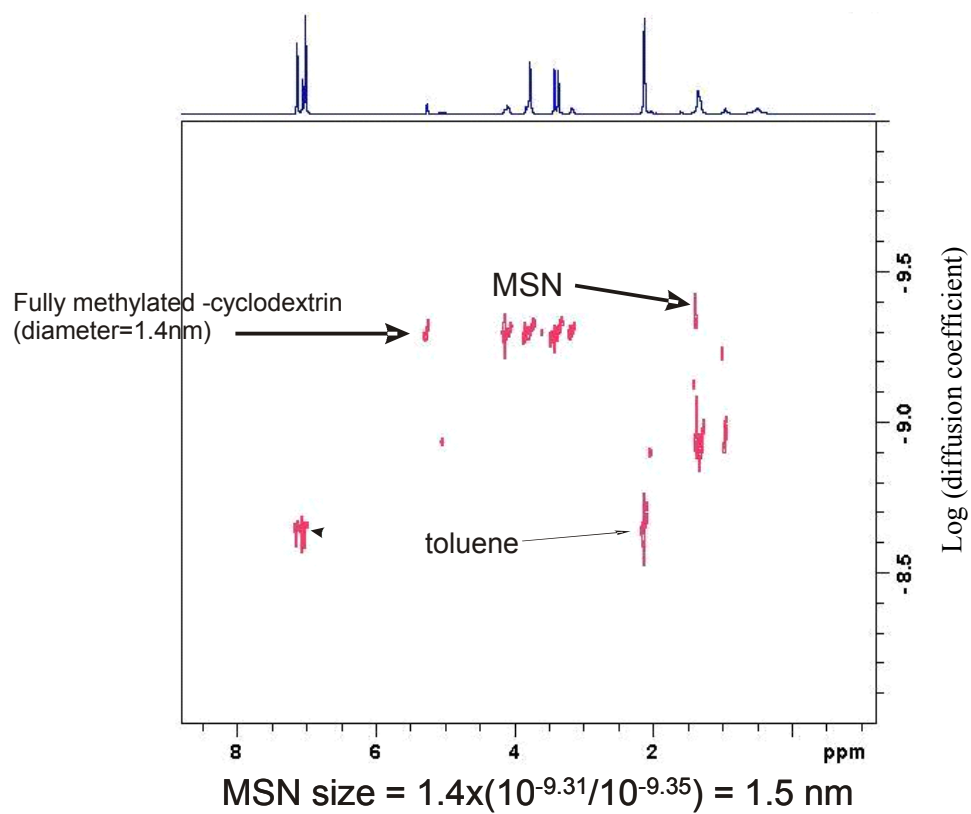


Figure S3. DOSY NMR determines the size of CdTe MSQD Family 427, suggesting the size of ca. 1.5 nm in diameter with methylated β -cyclodextrin as a reference.