Electronic Supplementary Material (ESI) for CrystEngComm.
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Supporting materials for:

Fine Tuning Crystal Structure of CdSe Quantum Dots by Varying Dynamic characteristics of Primary Alkylamine Ligands

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Synthesis of pure ZB- and WZ-CdSe QDs

Stock solutions for the Se precursors:

Stock solution Se-A: The precursor was prepared by adding 0.15 mmol of SeO_2 (16.5 mg) into 3 ml of 1-ODE. The mixture was stirred and heated to 100 °C under an Ar atmosphere. The reaction was continued until the SeO_2 powder dissolved completely. Subsequently, the reaction products were cooled to 60 °C.

Stock solution Se-B: According to the procedure in reference 1, 1 mmol of Se powder was fully dissolved in 0.236 g of TBP in a glovebox and further diluted with 0.69 g of 1-ODE.[1]

Synthesis of pure ZB-CdSe QDs:

ZB CdSe QDs were synthesized by a previously reported procedure with slight modification.[2] Typically, a mixture of 68 mg of (0.1 mmol) $Cd(St)_2$, 7.0 ml of 1-ODE

and 0.0025 mmol of OA was stirred and heated to 150 °C under nitrogen. After 60 min, the mixture was quickly heated to 250 °C. Subsequently, the Se-A stock solution was rapidly injected into the cadmium precursor solution. The reaction solution temperature dropped from 250 °C to 230 °C and remained at this value during CdSe QD growth. Needle-tip aliquots were taken to monitor the growth of the CdSe QDs by UV-vis and photoluminescence (PL) spectroscopies. The reaction was continued until CdSe QDs of the desired size were obtained. After precipitation and separation, the dots were suspended in hexane and stored in a cool place.

Synthesis of pure WZ-CdSe QDs:

The WZ-CdSe QDs were prepared according to published procedure.[1] Typically, $CdSt_2$ (0.0678 g, 0.1 mmol), OAm (0.75 g), trioctylphosphine oxide (TOPO, 0.25 g), and 1-ODE (4 ml) were loaded into a 25 ml three-neck flask. The mixed solution was bubbled with argon for 10 min at room temperature and then heated to 260 °C. Then, the Se-B stock solution was rapidly injected into the above mixed solution. The growth temperature of the CdSe QDs was maintained at approximately 240 °C. Needle-tip aliquots were taken to monitor the growth of the CdSe QDs by UV-vis and PL spectroscopies. The reaction was stopped when nanocrystals with the targeted size were produced. After precipitation and separation with acetone, the dots were dispersed in hexane and stored in a cool place.

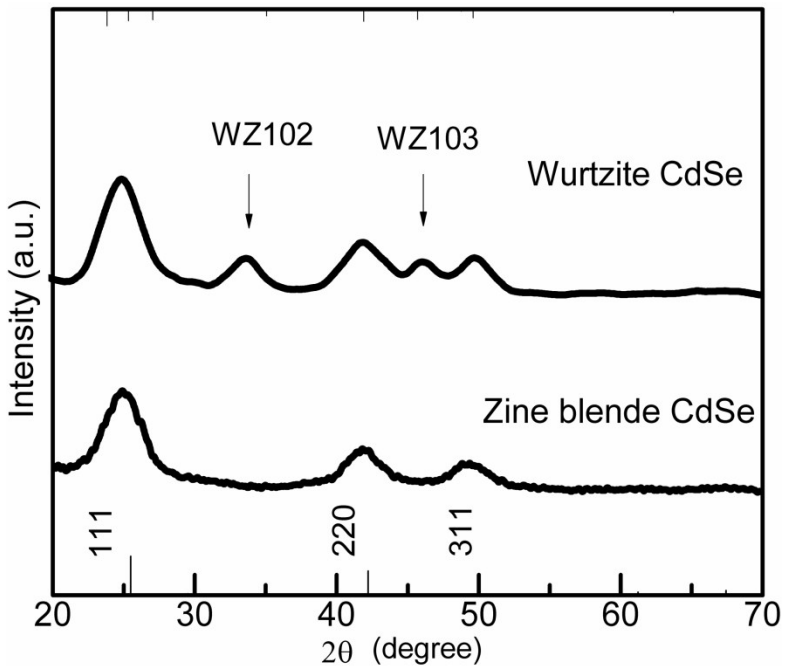

Figure S1. XRD patterns of pure ZB- and WZ-CdSe QDs

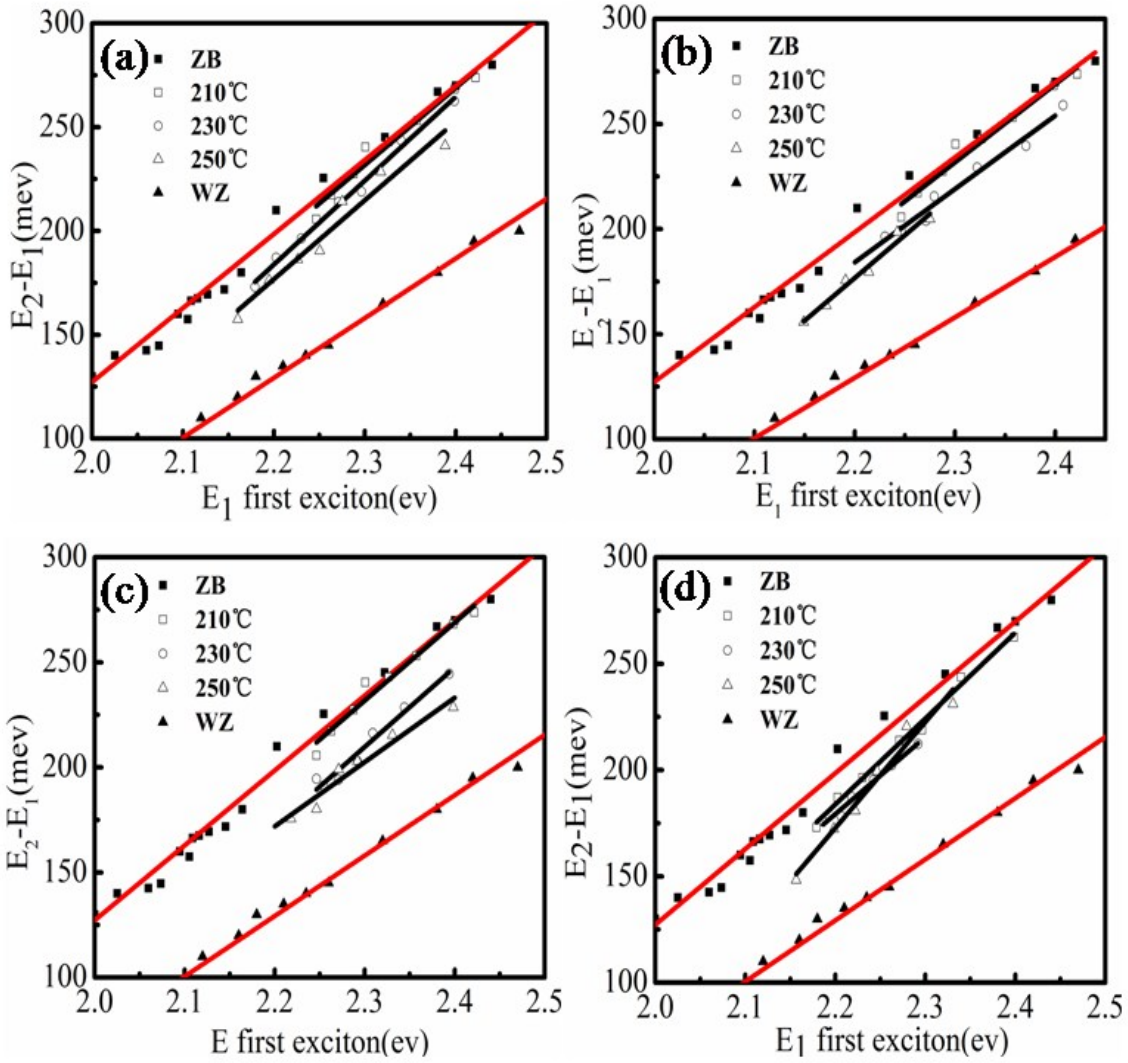

Figure S2. The $\Delta E_{2\text{-}1}$ vs E_1 fitting lines of CdSe QDs synthesized at 210 °C, 230 °C, and 250 °C with 0.25 mmol of OAm (a), HDA (b), TDA (c), and DDA (d).

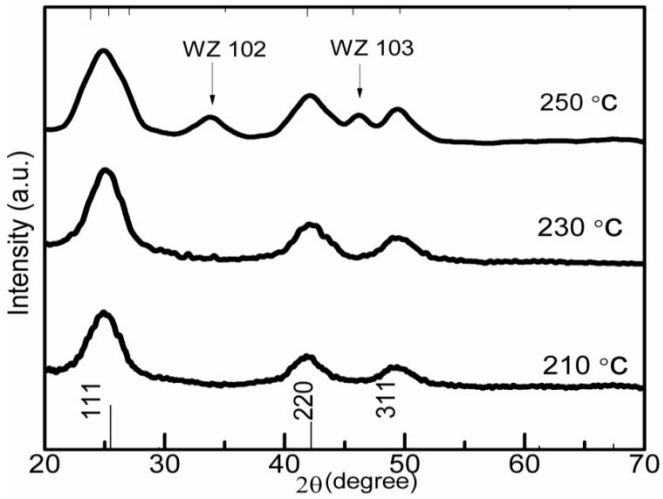

Figure S3. XRD patterns of CdSe QDs (approximately 4 nm) synthesized with 0.25 mmol of OAm at 210 °C, 230 °C, and 250 °C.

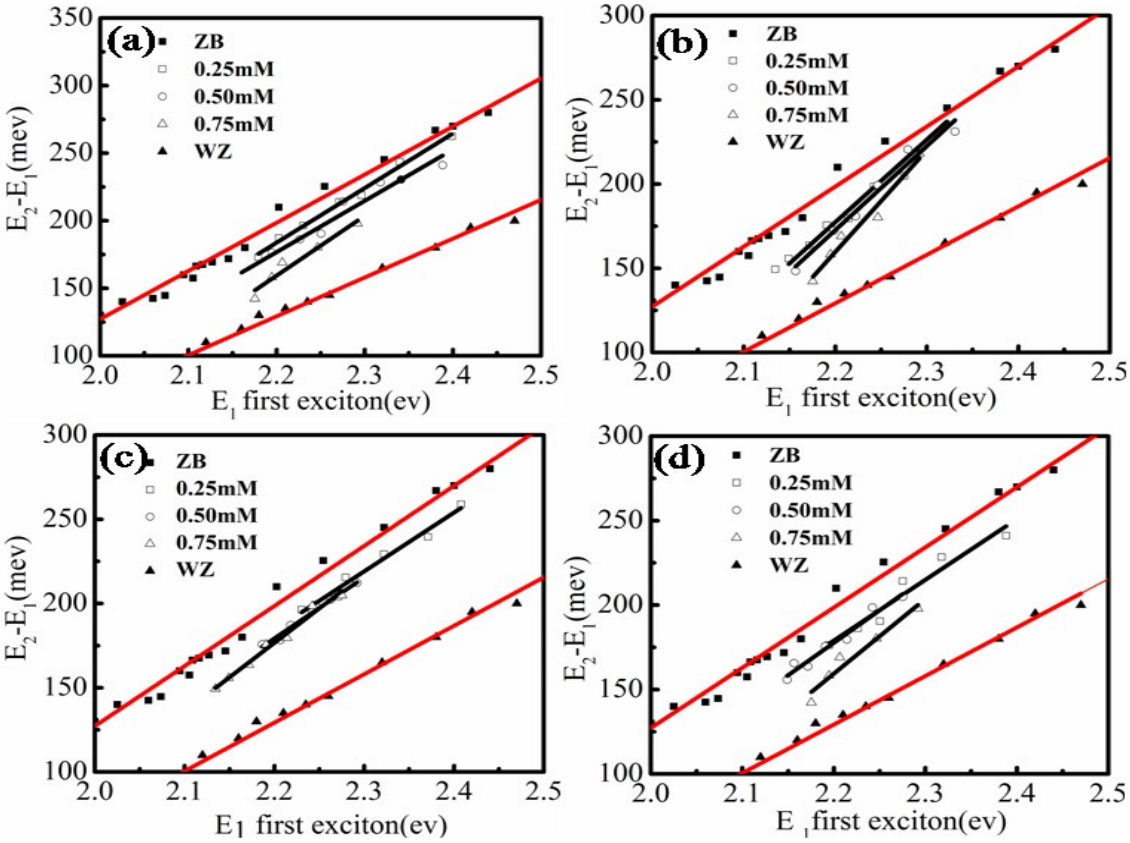

Figure S4. The $\Delta E_{2\text{-}1}$ vs E_1 fitting lines of CdSe QDs synthesized at 230 °C with 0.25 mmol, 0.5 mmol, and 0.75 mmol of OAm (a), HAD (b), TDA (c), and DDA (d).

1. Y. Gao and X. G. Peng, *J. Am. Chem. Soc.*, 2014, **136**, 6724-6732.
2. H. Duan, Y. Jiang, Y. Zhang, D. Sun, C. Liu, J. Huang, X. Lan, H. Zhou, L. Chen and H. Zhong, *Nanotechnology*, 2013, **24**, 285201-.