# Electronic Supplementary Information (ESI)

## Wurtzite or Zinc Blende? Surface decides the crystal structure of nanocrystals

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**Optimization of annealing temperature:**

Four sets of CdSe/Se samples were annealed at different temperatures (200 °C, 240 °C, 250 °C and 270 °C). **Fig. S1** shows the diffraction patterns of the starting material and four samples annealed at 200 °C, 240 °C, 250 °C and 270 °C, respectively. Below 240 °C, the nanoparticles showed only the wurtzite phase. The samples annealed above 240 °C showed mixed phases of the zinc blende and wurtzite structures. It can be seen from the diffraction pattern that annealing for 24 hours at 200 °C did not change the structure of the nanoparticles from that obtained in the as synthesized condition. The absence of diffraction peak corresponding to ZB indicated that any detectable WZ to ZB transformation had not occurred. The average particle size and standard deviation of the size distribution for particles annealed at 200 °C for 24 h were 3.5 nm and 0.5 nm, respectively, as determined from TEM (Fig. S1).

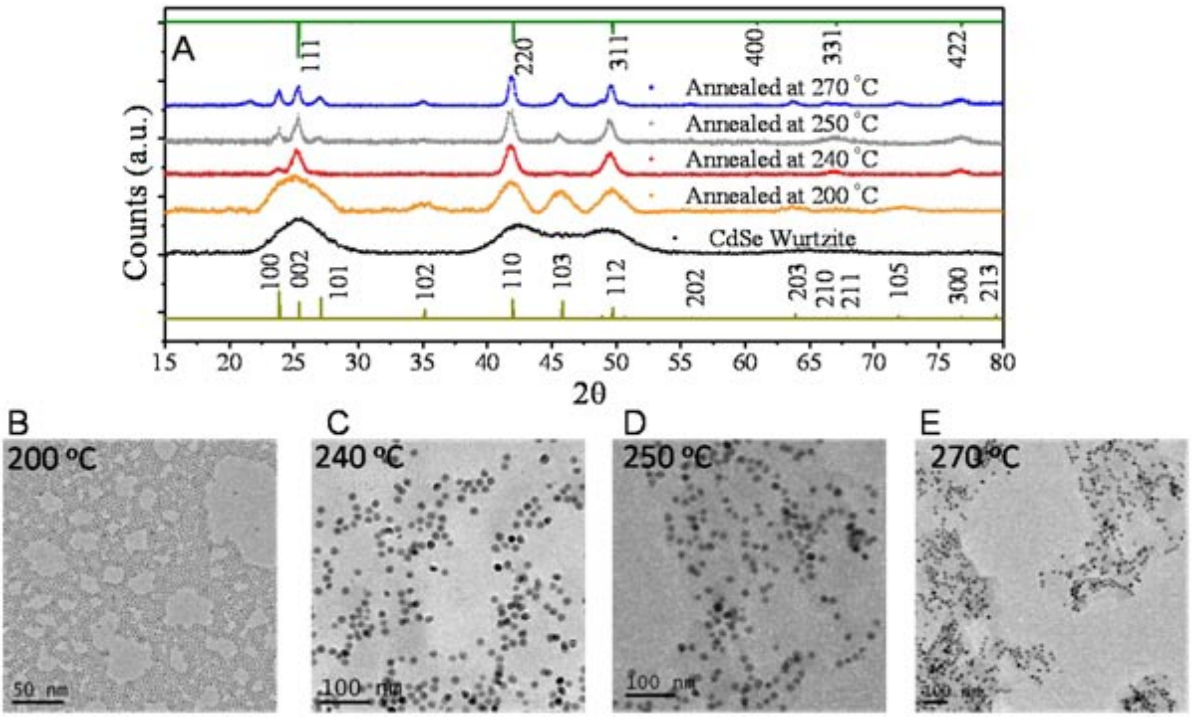


**Fig. S1.** A) X-ray diffraction pattern for CdSe wurtzite seed and annealed CdSe/Cd at 200 °C, 240 °C, 250 °C, and 270 °C. B, C, D and E are tem images of nanocrystals annealed at 200 °C, 240 °C, 250 °C, and 270 °C respectively.

These numbers indicated a very small change in the average size and size distribution when compared to those of the as-synthesized particles shown in Fig. S1C. Unlike with the annealing action at 200 °C, a WZ to ZB phase transformation was recorded at annealing temperature of 240 °C after 24 h. The 3.1 nm particles in the WZ phase were observed to undergo gradual WZ-to-ZB transition as they were placed for annealing at 240 °C. The ZB (111) peak is merged with the WZ (002) peak so that only one peak is visible. At a temperature of 240 °C, peaks corresponding to the ZB phase begin to appear in the spectrum as indicated by the relative increase of the merged WZ (002) and ZB (111) peak with respect to the WZ (100), (101), (102) and (103) peaks. The WZ and ZB phases coexist, with a continuous shift towards the ZB phase as the temperature increases, until approximately 240 °C, where all non-overlapping WZ peaks finally disappear. Further increase of temperature (270 °C) resulted in the increase of the nanoparticles

size, but with a subsequent increase in the intensities of WZ peaks due to higher stability of WZ phase at high temperature4.

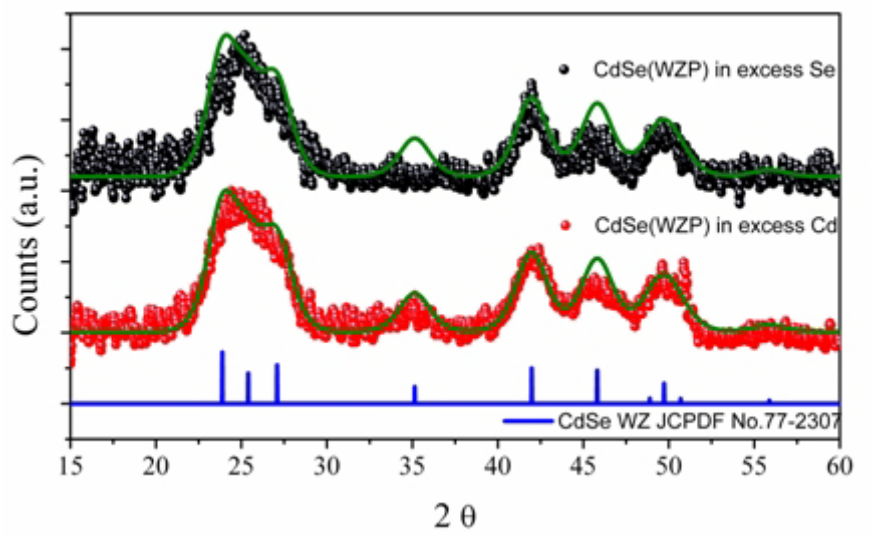


**Fig. S2.** PXRD data of CdSe synthesized by using WZ process (WZP) in both cases we obtain WZ only (size obtained 4.0 nm by Scherrer formula).

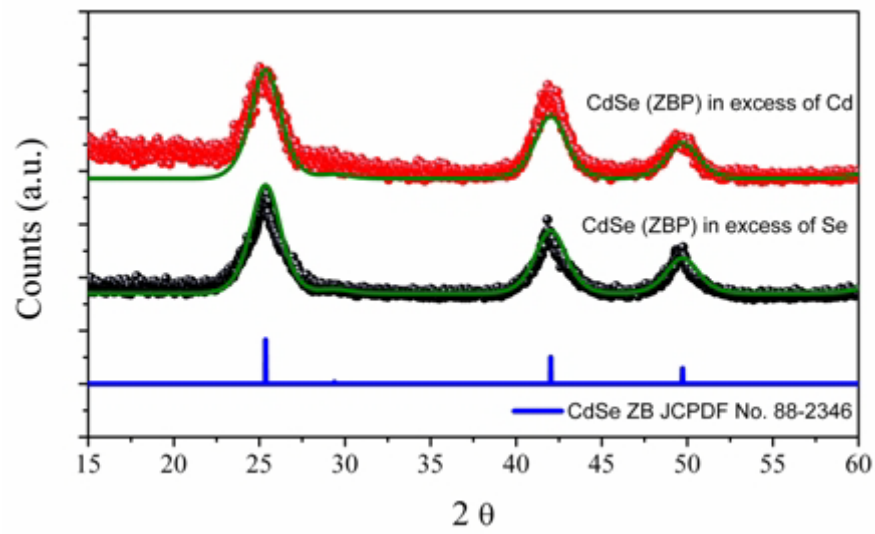


**Fig. S3.** PXRD data of CdSe synthesized by using ZB process (ZBP) in both cases we obtain ZB only (size obtained 4.2 nm by Scherrer formula).

**Table 1.** Optimized reaction conditions for phase transformations

| Nanocrystals | Phase before annealing | Coated Ion | Annealing Temperature (ºC) | Phase after annealing |
|---|---|---|---|---|
| CdSe | WZ | Se | 240 | ZB |
| CdSe | WZ | Cd | 240 | WZ |
| CdSe | ZB | Se | 240 | ZB |
| CdSe | ZB | Cd | 240 | WZ |
| CdS | WZ | S | 250 | ZB |
| CdS | WZ | Cd | 250 | WZ |
| CdTe | ZB | Te | 150 | ZB |
| CdTe | ZB | Cd | 150 | WZ |

WZ-Wurtzite, ZB-Zinc blende