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

Supplementary Information:

Electronic energy levels engineering in $Zn_{1-x}Cd_xSe$ nanocrystals

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TEM Measurements

TEM measurements were carried out on Tecnai $G^2$20 microscope, operating at 200 kV. Figure S1 shows TEM image for ZnCdSe-I and ZnCdSe-Ia to ZnCdSe-Id. The Sizes of ZnCdSe-I and ZnCdSe-Id are 4.3 ± 0.3 and 4.4 ± 0.4 nm respectively. It is clear that there is no appreciable change in particle size. The exact sizes calculated from TEM are tabulated in table SI. It is evident that the sizes are within error bar and there is no appreciable change in particle size.

Sample	**Size**
ZnCdSe-I	4.3 ± 0.3
ZnCdSe-Ia	4.3 ± 0.4
ZnCdSe-Ib	4.4 ± 0.3
ZnCdSe-Ic	4.4 ± 0.4
ZnCdSe-Id	4.4 ± 0.4

Table S1 Sizes from TEM image

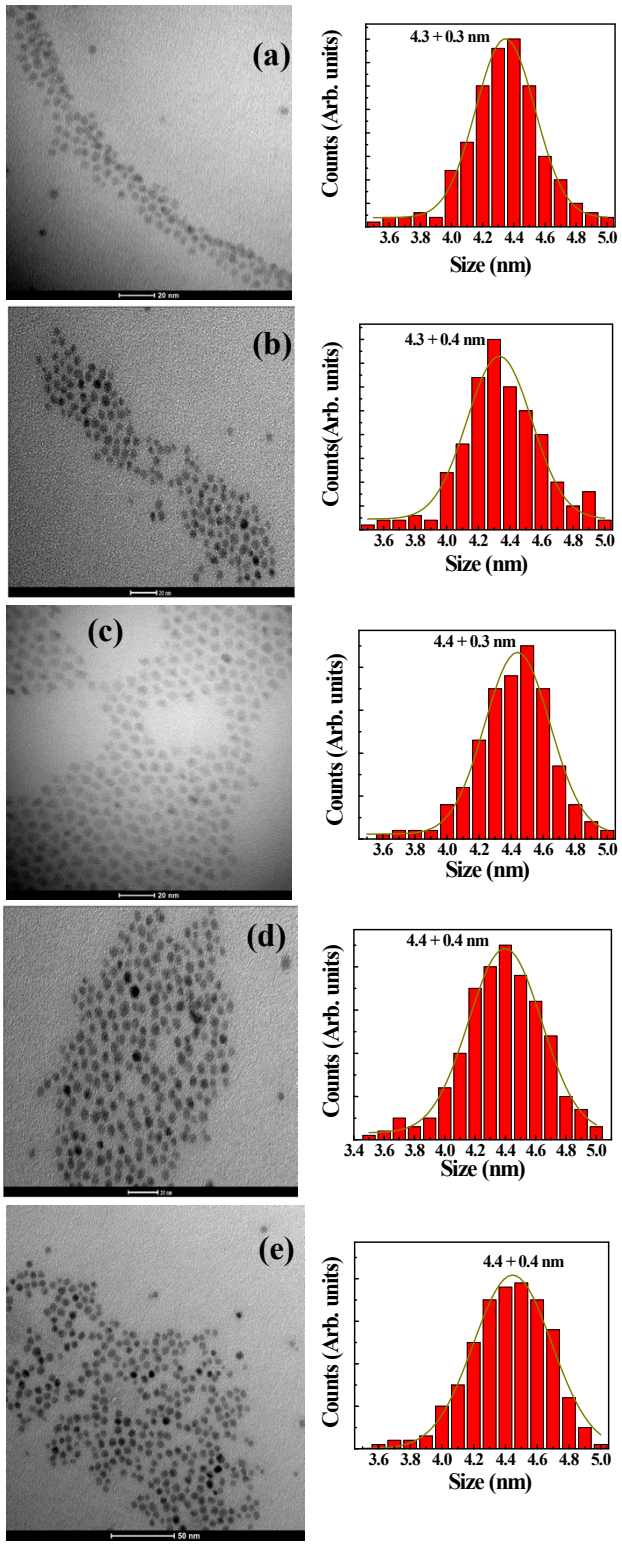

Fig. S1 TEM image of (a) ZnCdSe-I and (b) ZnCdSe-Ia (c)ZnCdSe-Ib (d)ZnCdSe-Ic (e) ZnCdSe-Id. Right panel shows respective histogram.

PLE measurements:

The absorption of ZnCdSe-I correspond to CdSe of size ~ 3.2 nm. PLE spectra are recorded at 10K. The recorded PLE spectra for ZnCdSe-I is compared with that of CdSe of size 3.2 nm.[1] Peak position of ZnCdSe-I and CdSe of size 3.2 nm matches. This clearly indicates that the emission is caused by CdSe like core. Even with increasing the annealing time the PLE spectra does not show crossing of any energy levels [See Fig. S2(a)]. However a continuous blue shift in energy of all the peaks is observed. The PLE spectra is fitted with Gaussian fit as discussed in ref. 1. The peak positions are assigned as in case of CdSe.

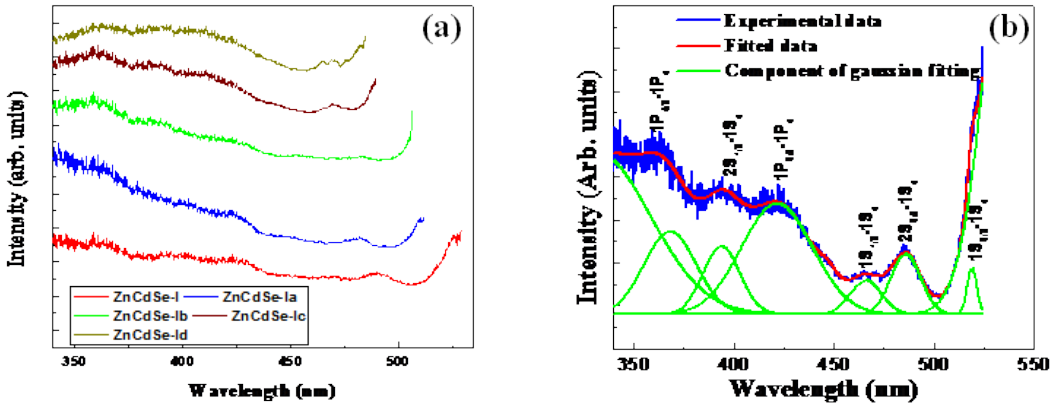

FIG. S2 (a) PLE spectra recorded on ZnCdSe-I, ZnCdSe-Ia, ZnCdSe-Ib, ZnCdSe-Ic, and ZnCdSe-Id. (b) Fitting of PLE spectra and assignment of the peak.

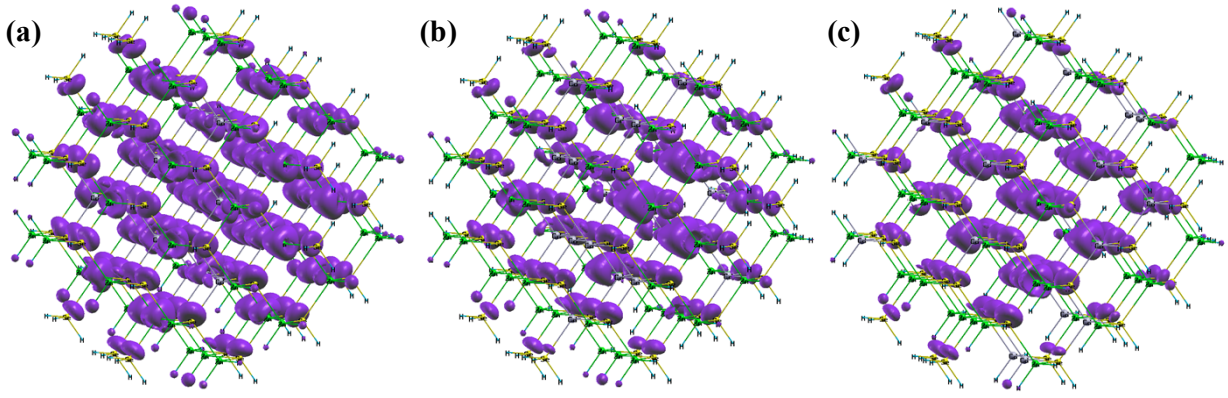

FIG. S3 (Color online)Partial charge density of LUMO level for (a) core/shell, (b) graded, and (c) alloyed structure. The spatial extent of LUMO partial charge density is seen to shrink toward center of NC (core region) with uniform Zn distribution on alloying.

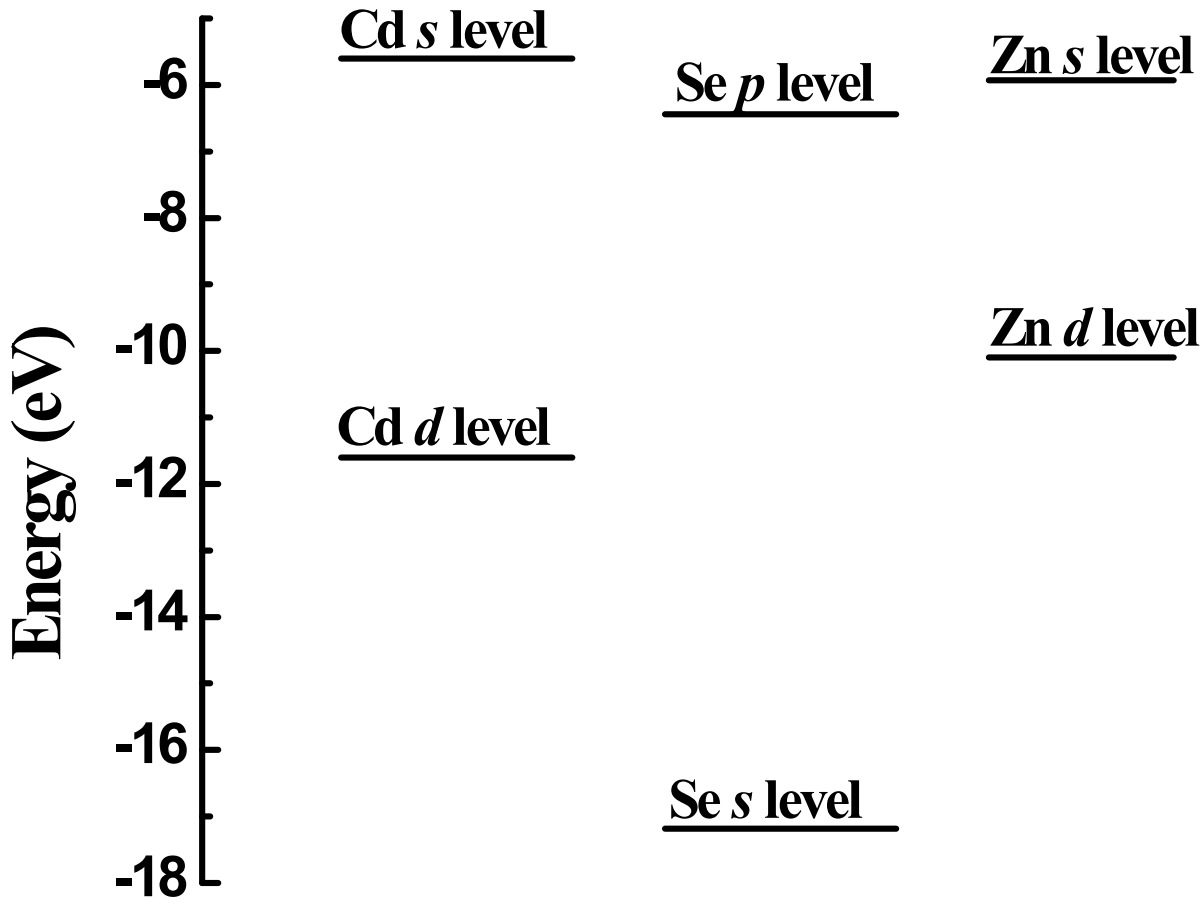

FIG. S4 Relative positions of the relevant energy Zn, Cd and Se atoms.

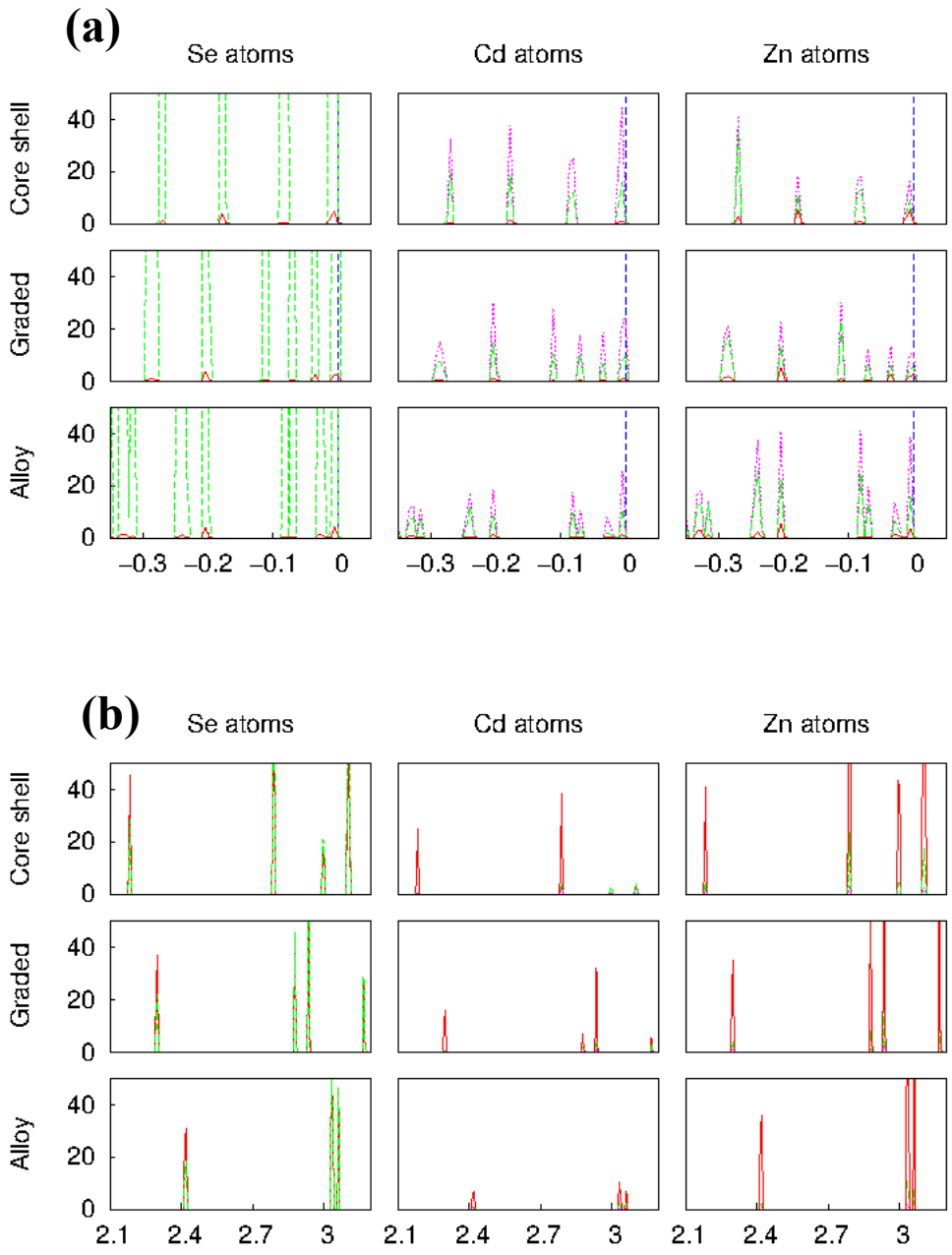

Fig. S5 Site projected DOS in the region near the (a) HOMO, (b) LUMO, for core/shell, graded and alloyed NCs. Red color indicates *s* orbitals, green color *p* orbitals, magenta colour *d* orbitals, while the Fermi level is shown in blue color. Maximum for Se-*p* state is ~340.

References

1 Norris, D. J.; Bawendi, M. G. *Phys. Rev. B* **1996**, *53*, 16338.