

To dope Mn²⁺ in a semiconducting nanocrystal

Angshuman Nag,¹ S. Chakraborty² and D. D. Sarma^{1,2,*}

Supporting Information

¹ *Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560 012, India*
² *Centre for Advanced Materials, Indian Association for the Cultivation of Science, Kolkata-700032, India*

Table S1: Ionic radius values for the relevant ions, taken from ref. 1 and ref. 2

Ion	Ionic radius ^{ref. 1} (Å)	Ionic radius ^{ref. 2} (Å)
Zn ²⁺	0.83	0.83
Mn ²⁺	0.91	0.91
Cd ²⁺	1.03	0.99
S ²⁻	1.74	-

Fig. S1: Powder X-ray diffraction pattern of ZnS nanocrystals along with the reference patterns for bulk ZnS in both wurtzite (WZ) and zinc-blende (ZB) phase.

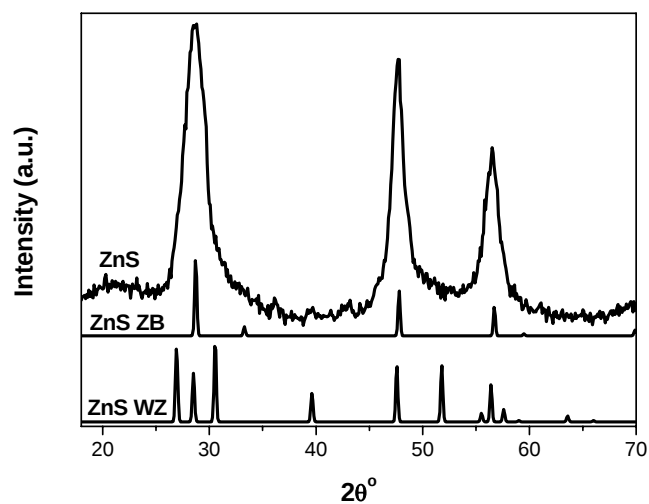


Fig. S2: UV-visible absorption spectra of $\text{Zn}_x\text{Cd}_{1-x}\text{S}$ NCs for different values of “x”.

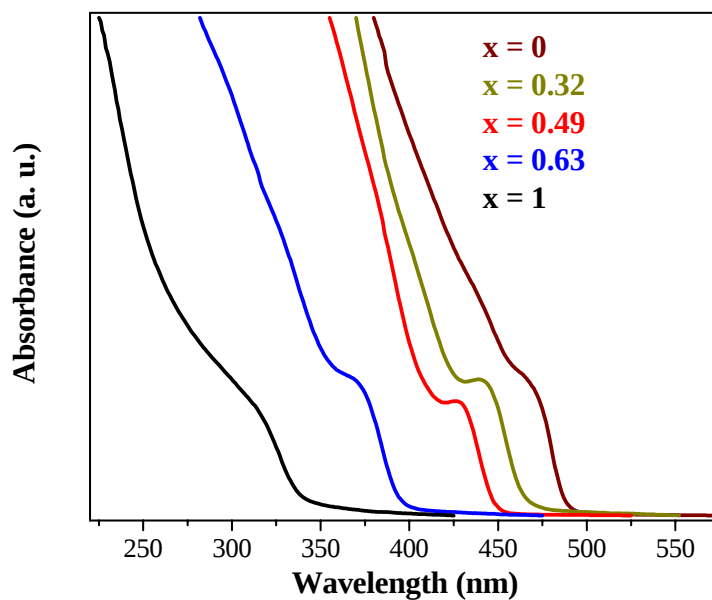


Fig. S3: Powder X-ray diffraction patterns for $\text{Zn}_{0.49}\text{Cd}_{0.51}\text{S}$ NCs doped with different concentration of manganese. Reference XRD pattern for bulk WZ of CdS, MnS and ZnS are taken from ICSD.

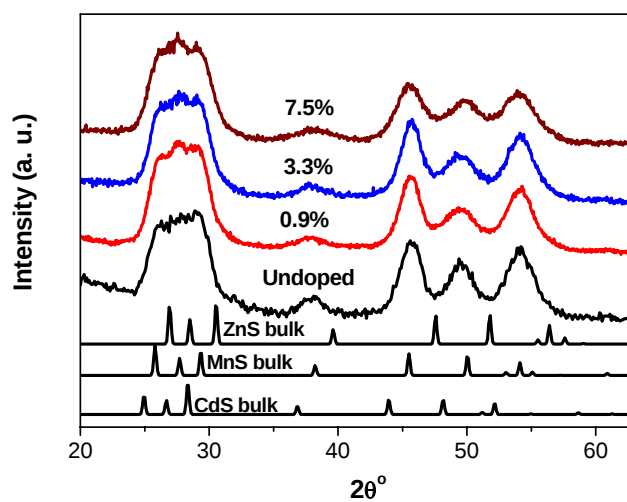
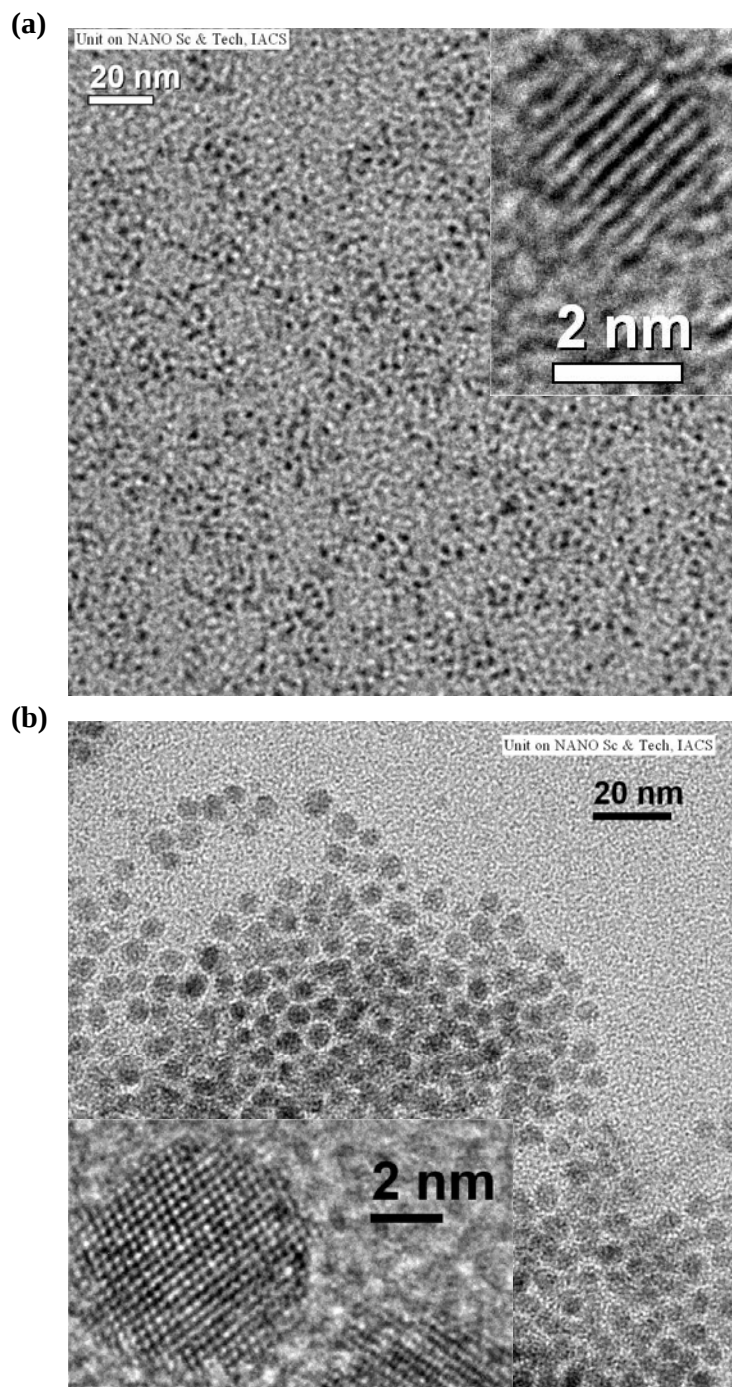


Fig. S4: TEM images of Mn^{2+} -doped $\text{Zn}_{0.49}\text{Cd}_{0.51}\text{S}$ NCs with 15% Mn^{2+} precursor in the reaction mixture; (a) after 5 seconds of the reaction time, (b) the final product obtained after 1800 seconds of reaction time and (c) NCs obtained after etching the final product in Fig. S3b.



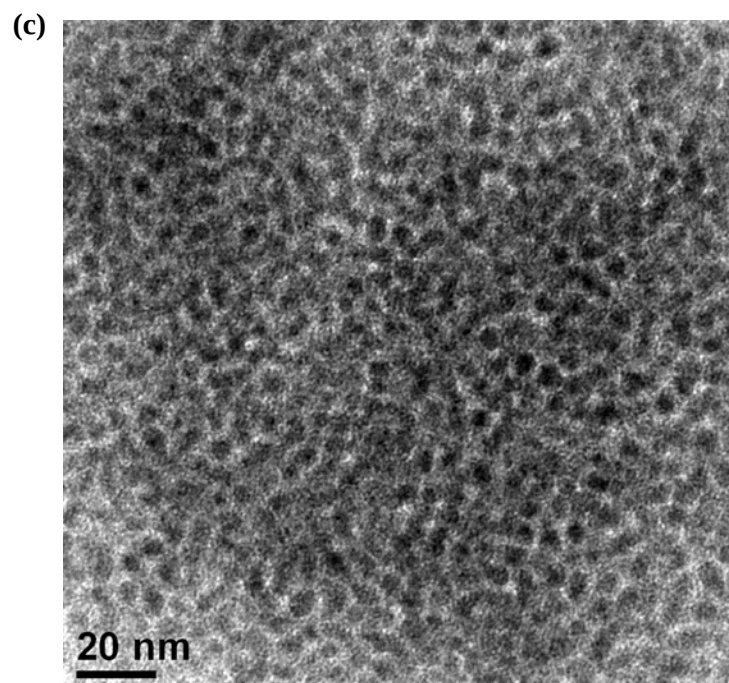


Table S2: Emission intensities for bandgap emission, Mn^{2+} d-emission, total PL emission and Mn^{2+} d-emission per Mn^{2+} ion from Mn^{2+} -doped $\text{Zn}_{0.49}\text{Cd}_{0.51}\text{S}$ NCs with different dopant concentrations. All the intensities mentioned here are normalized by their corresponding absorbance at the excitation wavelength.

% of manganese	Bandgap emission intensity	Mn^{2+} d-emission intensity	Total emission intensity	Average number of manganese per NC	Mn^{2+} d emission intensity per Mn^{2+} ion
0	998237	0	998237	0	-
0.5	308025	634067	942092	18.0	35177.1
0.9	161077	801944	963021	32.4	24717.0
1.7	103764	681867	785631	61.3	11126.2
3.3	74691	339208	413899	119.0	2851.3
7.5	37612	48122	85734	270.4	178.0

Reference:

1. Chen, D. M.; Yang, C. S.; Chuang, F. B.; Tzeng, Y. W.; Wei, C. C.; Ro, C. S.; Lan, K. Y.; Chou, W. C.; Lan, W. H.; Uen, W. Y. *Chinese J.l of Phys.* **2000**, 38, 74.
2. Zhikharevich, V.V.; Ostapov, S.E.; Deibuk, V.G. *Semiconductor Physics, Quantum Electronics and Optoelectronics* **2006**, 9, 17.