Supplementary Information

Electronic Structure Study of Dual Doped II-VI Semiconductor Quantum Dots Towards Single-Source White Light Emission

Payel Mondal, [a] *Sowmeya Sathiyamani,* [a] *Subham Das,* [a] *and Ranjani Viswanatha*[*,a, b]

[a]New Chemistry Unit, and [b]International Centre for Materials Science

Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064, India.

*E-mail: rv@jncasr.ac.in

Table S1 The amount of incorporated Cd (x) in $Cd_xZn_{1-x}Se$ host NCs for different samples obtained from ICP-OES analysis.

Sample	x value
S1	0.10
S2	0.175
S3	0.31
S4	0.42
S5	0.44
S6	0.51

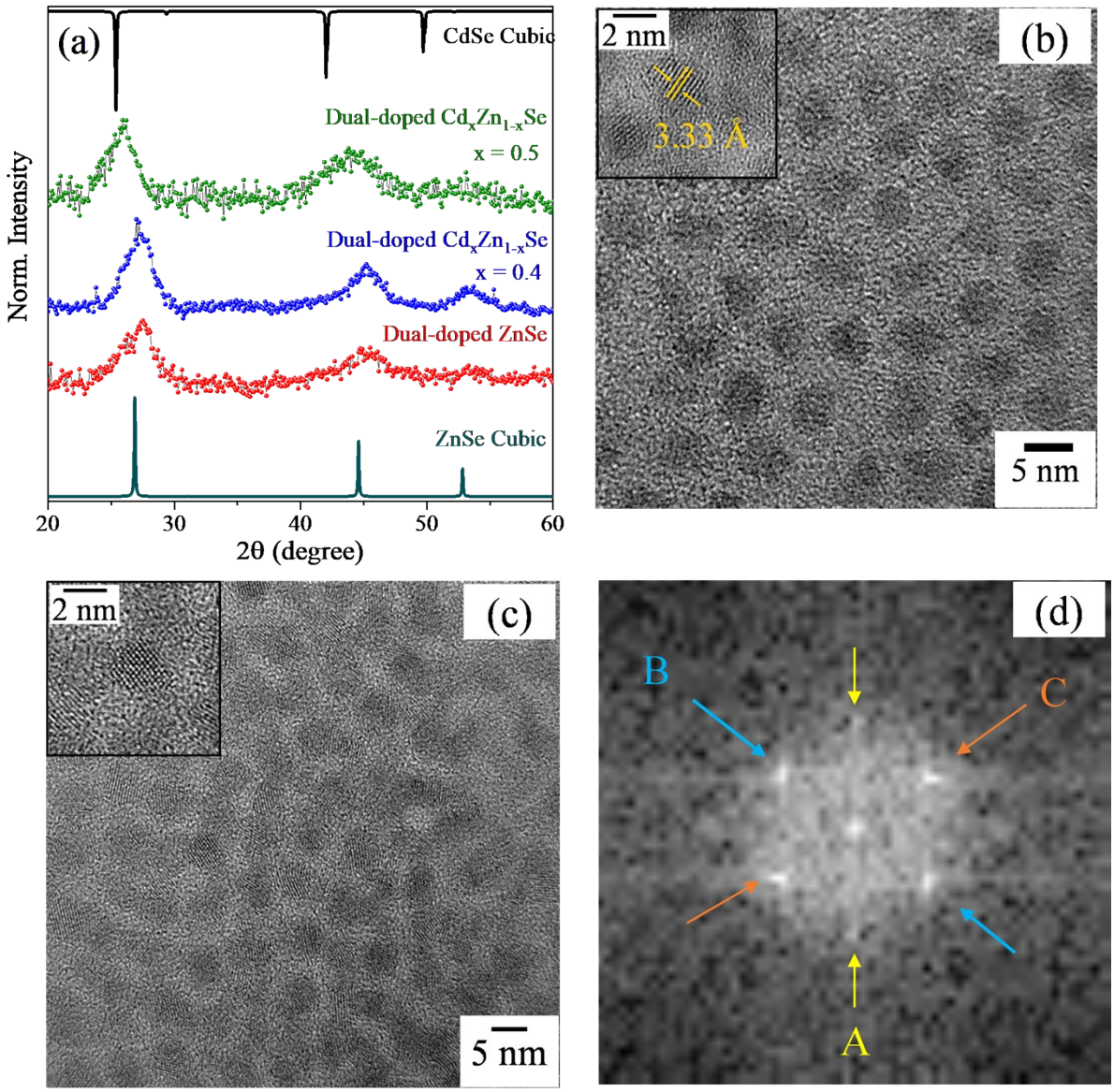

Fig. S1 (a) X-ray diffraction patterns of Cu, Mn dual-doped ZnSe and $Cd_xZn_{1-x}Se$ QDs with increasing Cd content along with the ZnSe and CdSe bulk cubic patterns. TEM images of (b) dual-doped ZnSe and (c) dual-doped $Cd_xZn_{1-x}Se$ QDs. Corresponding HRTEM images are shown in the inset to (b) and (c) respectively. (d) Fourier transform of dual-doped $Cd_xZn_{1-x}Se$ shows three distinct planes namely, $d(111)_{CdSe}$, $d(111)_{ZnSe}$ and $d(200)_{CdSe}$, marked as 'A', 'B', and 'C' respectively.

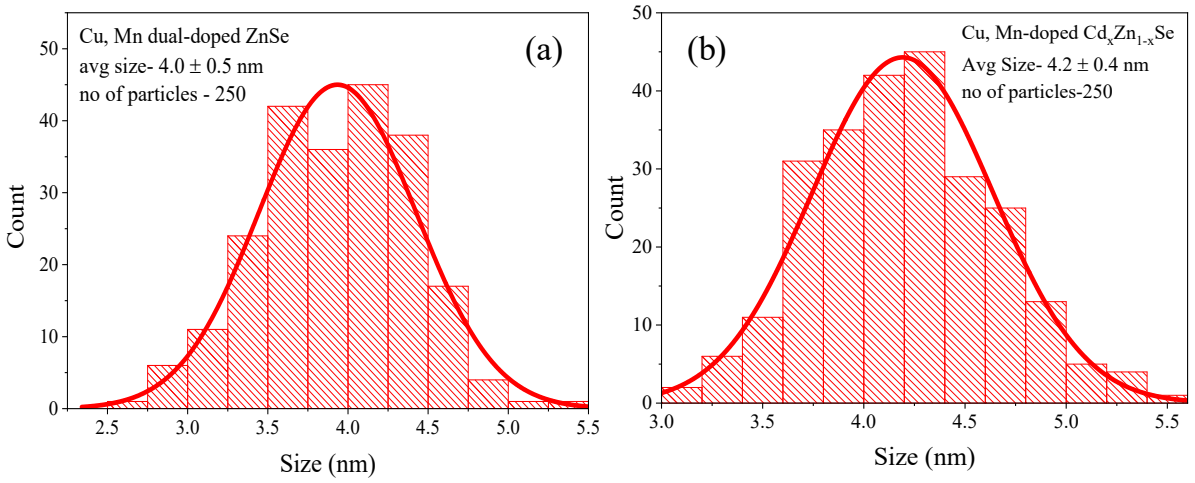

Fig. S2 Particle size distribution histogram of (a) Cu, Mn dual-doped ZnSe, and (b) Cu, Mn dual-doped $Cd_xZn_{1-x}Se$ QDs showing the average size of the QDs are 4.0 ± 0.5 nm, and 4.2 ± 0.4 nm respectively.

Table S2 Fitting summary of decay dynamics of Mn emission. Cu, Mn ZnSe_1, 2, 3, 4 represents the Cu annealing time of 20, 30, 45, and 60 minutes respectively.

Sample name	A_1	t_1 (µs)	A_2	t_2 (µs)	A_3	t_3 (µs)
Mn-ZnSe	---	---	---	---	0.88	244
Cu, Mn ZnSe_1	0.29	5	0.22	111	0.49	476
Cu, Mn ZnSe_2	0.33	5	0.20	159	0.46	630
Cu, Mn ZnSe_3	0.62	12	0.14	291	0.25	872
Cu, Mn ZnSe_4	0.77	10	0.08	275	0.16	923

Table S3 Fitting summary of decay dynamics of Cu emission. Cu, Mn ZnSe_1, 2, 3, 4 represents the Cu annealing time of 20, 30, 45, and 60 minutes respectively.

Sample name	A_1	t_1 (ns)	A_2	t_2 (ns)	A_3	t_3 (ns)
Cu-ZnSe	---	---	0.82	4.6	0.18	21
Cu, Mn ZnSe_1	0.68	3.7	0.38	13.2	0.07	95
Cu, Mn ZnSe_2	0.66	3.5	0.40	12.9	0.08	96

Cu, Mn ZnSe_3	0.65	3.9	0.37	13.7	0.08	96
Cu, Mn ZnSe_4	0.68	4.1	0.30	16.6	0.14	111

Table S4 The stoichiometric percentages of Cu precursor, percentages of Cu ions incorporated into ZnSe host lattice for different samples and their quantum yield.

Sample name	Stoichiometric Cu percentages	Cu percentages from ICP	Quantum yield (%)
Cu_1	1.5 %	1 %	20 %
Cu_2	3.0 %	1 %	22 %
Cu_3	4.5 %	1 %	9.5 %

Table S5 Quantum yield of the dual-doped NCs with varying the TOP concentration

Sample name	TOP amount (mL)	Quantum yield (%)
TOP_1	1.00 mL	18 %
TOP_2	0.50 mL	35 %
TOP_3	0.25 mL	32 %

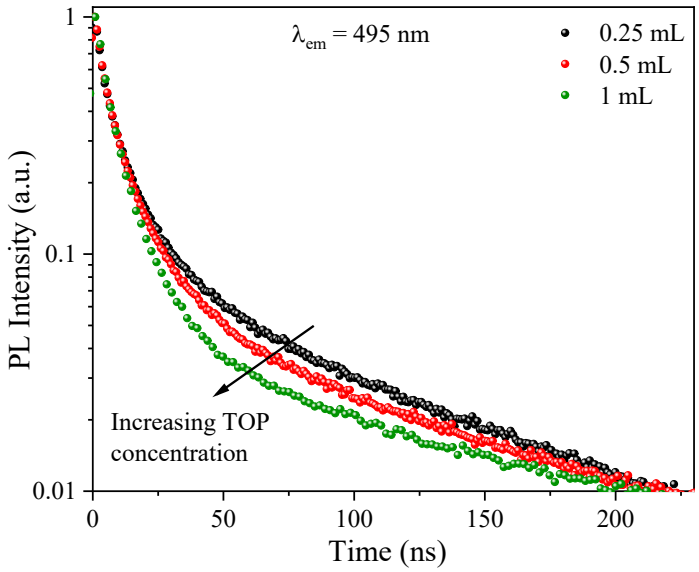

Fig. S3 TrPL dynamics of Cu emission (495 nm) in Cu, Mn dual-doped ZnSe nanocrystals with varying TOP concentration.

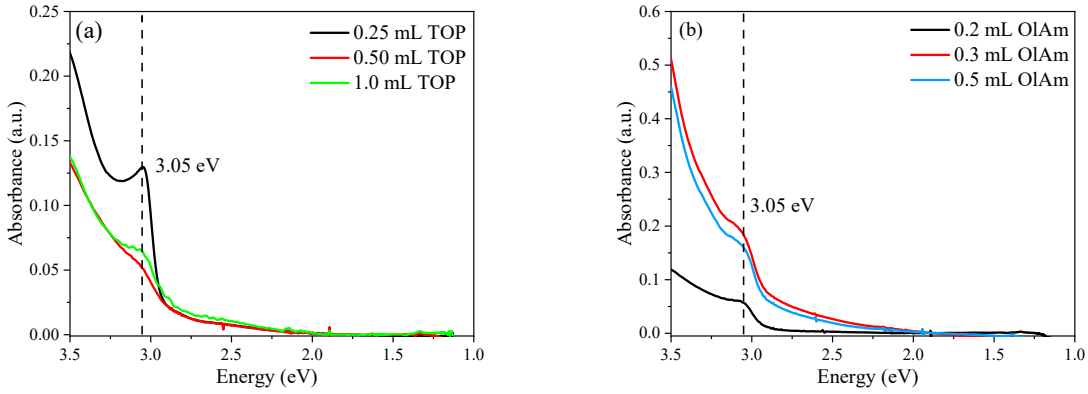

Fig. S4 Absorbance of the Mn, Cu dual doped QDs with varying concentrations of (a) TOP and (b) OlAm.

Table S6 Quantum yield of the dual-doped NCs with varying the oleylamine (OlAm) concentration

Sample name	OlAm amount (mL)	Quantum yield (%)
OlAm_1	0.2 mL	26.0 %
OlAm_2	0.3 mL	26.5 %
OlAm_3	0.5 mL	28.0 %

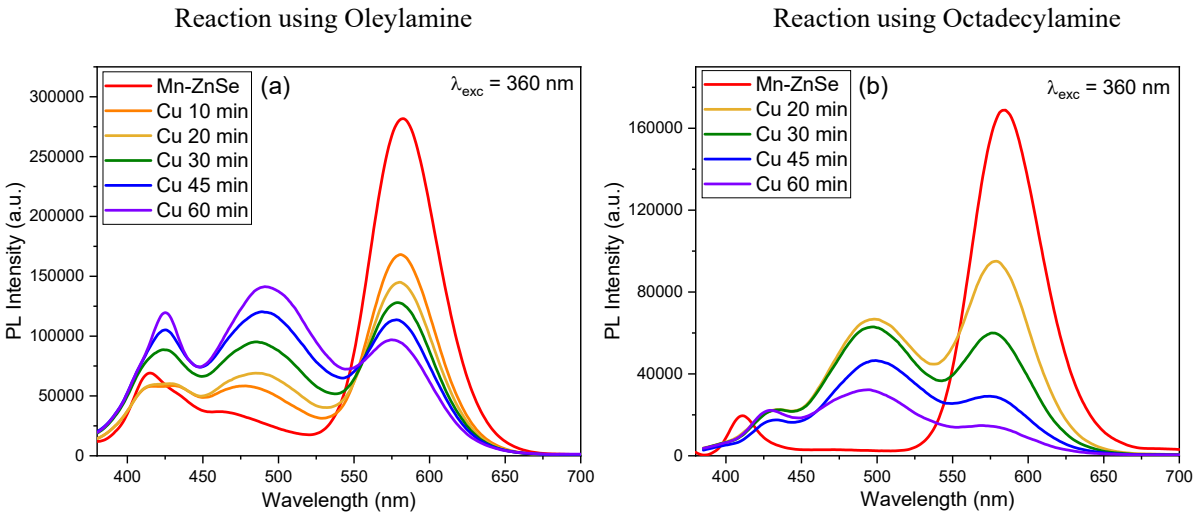

Fig. S5 Evolution of PL bands in Cu, Mn dual-doped ZnSe QDs when reacted with (a) oleylamine and (b) octadecylamine.

Table S7 Quantum yield of the dual-doped ZnSe QDs as a function of annealing time.

Sample name with annealing time	Quantum yield (%)
1_5 min	19.5 %
2_10 min	19 %
3_15 min	18 %
4_20 min	22 %
5_30 min	23 %
6_45 min	24 %
7_60 min	26 %

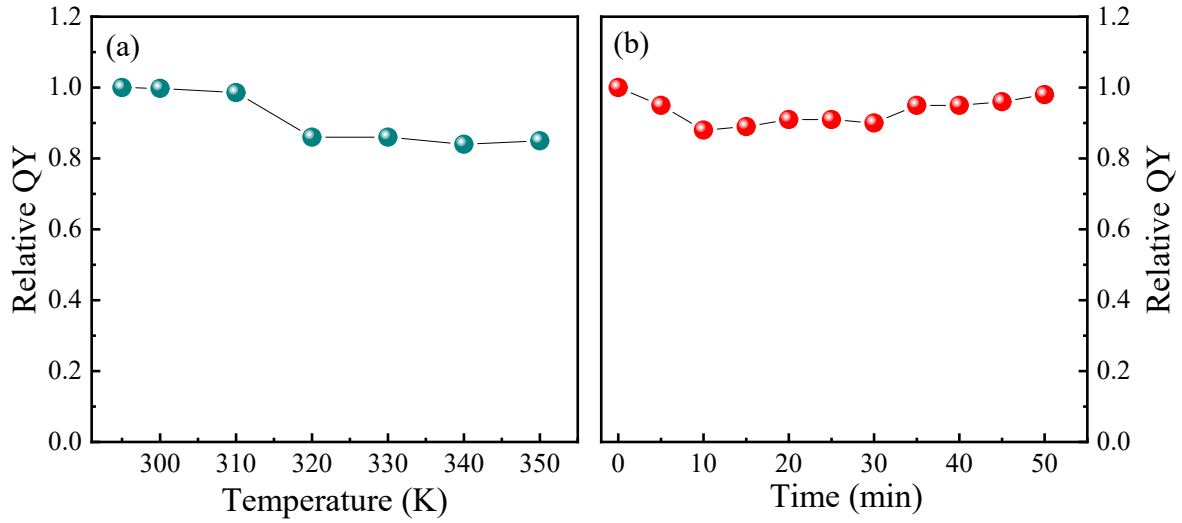

Fig. S6 The relative quantum yield of Cu, Mn dual-doped ZnSe QDs as a function of (a) temperature, and (b) continuous excitation.