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

Supporting Information for

Highly Effective Nanosegregation of Dual Dopants in a Micron-Sized Nanocluster-Based Semiconductor Molecular Single Crystal for Targeting White-Light Emission

Jian Lin,[a] Le Wang,[a] Qian Zhang,[a] Fei Bu,[c] Tao Wu*,[a] Xianhui Bu,[b] and Pingyun Feng[c]

[a] *College of Chemistry, Chemical Engineering and Materials Science, Soochow University, Jiangsu 215123, China*
[b] *Department of Chemistry and Biochemistry, California State University, Long Beach, California 90840, United States*
[c] *Department of Chemistry, University of California, Riverside, California 92521, United States*

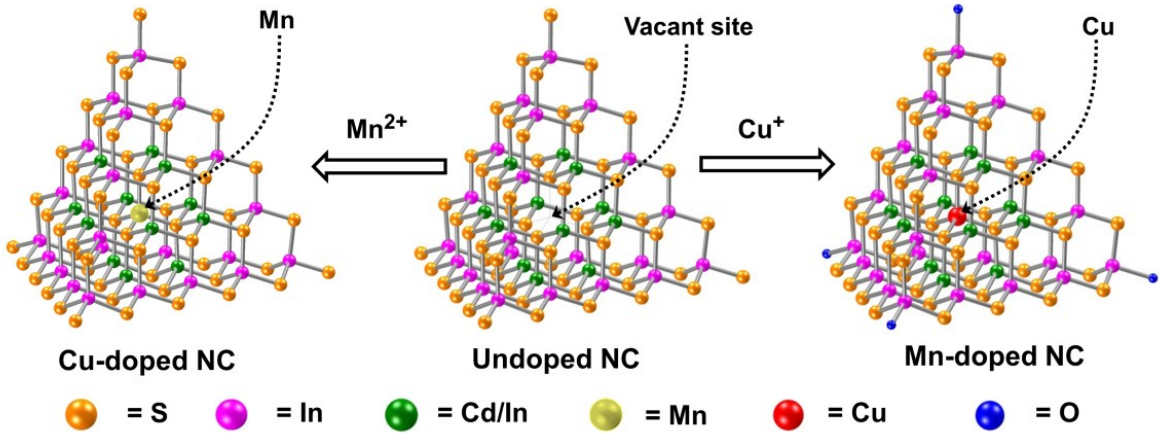

Figure S1.The doping process of transition metal ion (Cu^{+} and Mn^{2+}) into the coreless supertetrahedral nanocluster.

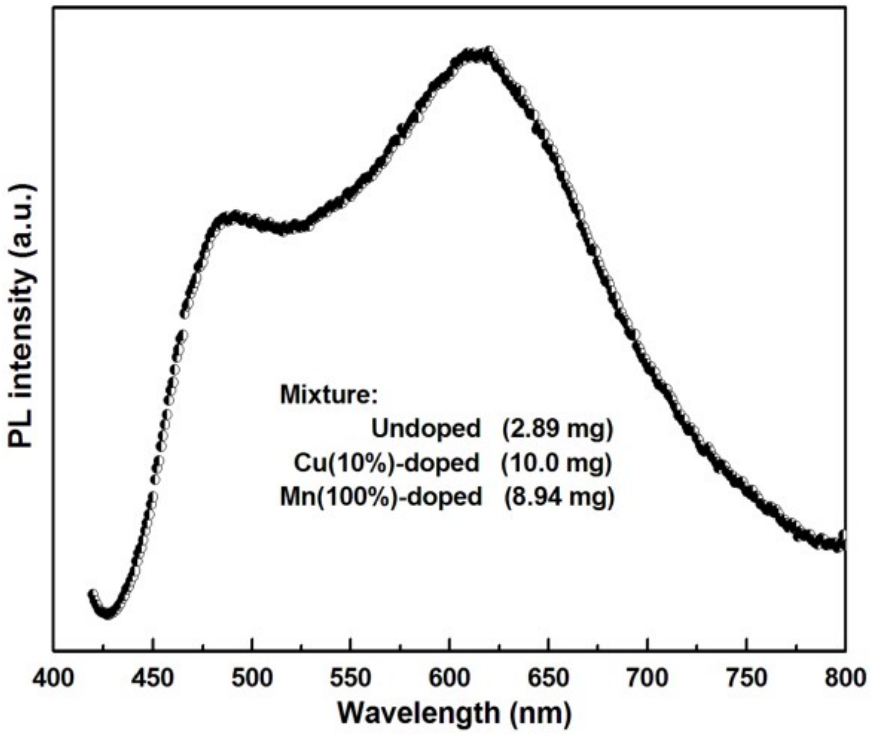

Figure S2. PL emission spectrum of mixture obtained by directly mixing separately synthesized singly Mn-doped, singly Cu-doped and undoped samples.

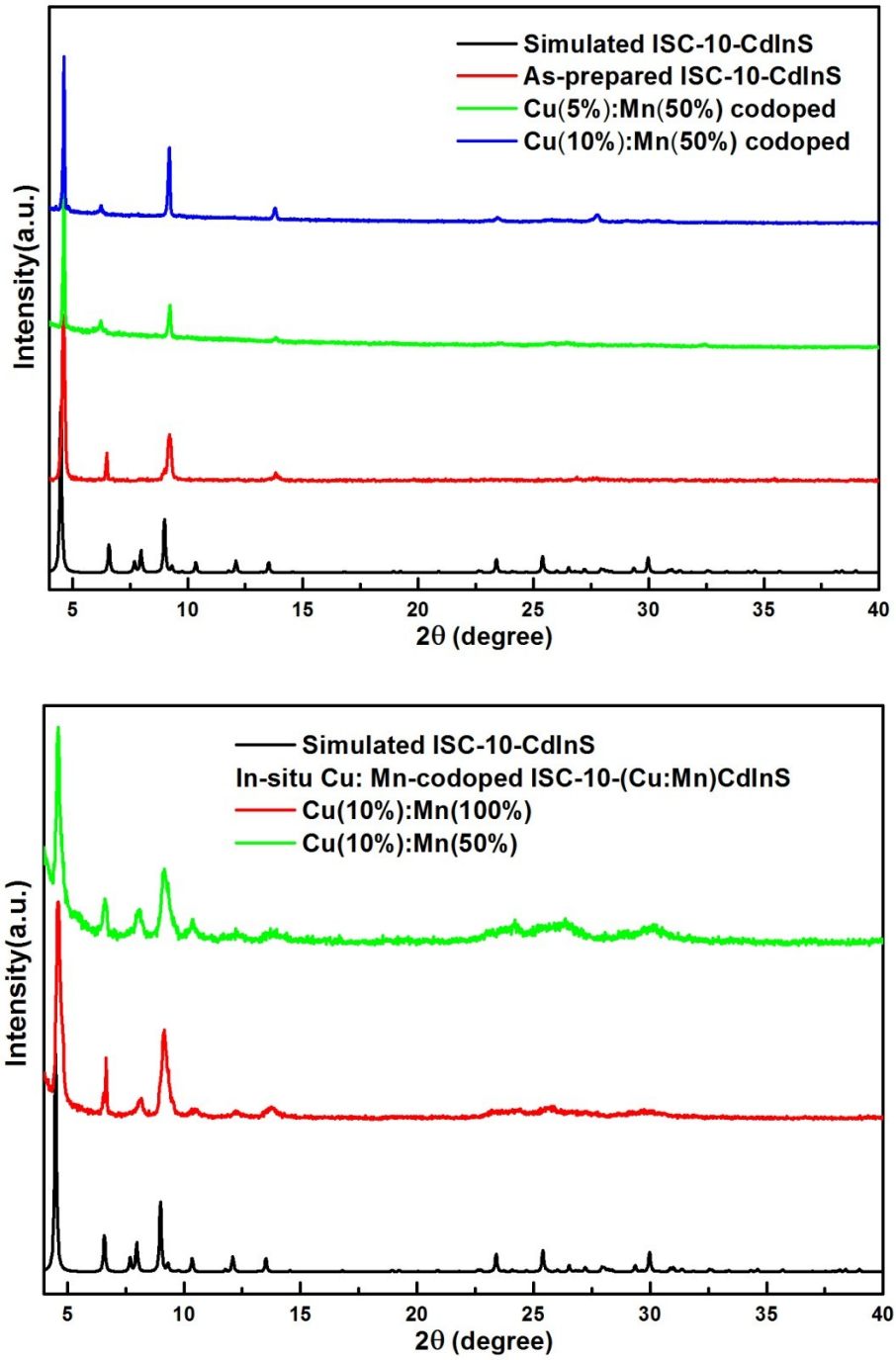

Figure S3. Top: powder X-ray diffraction patterns of as-synthesized and codoped sample; bottom: powder X-ray diffraction patterns of in-situ synthesized Cu:Mn-codoped samples.

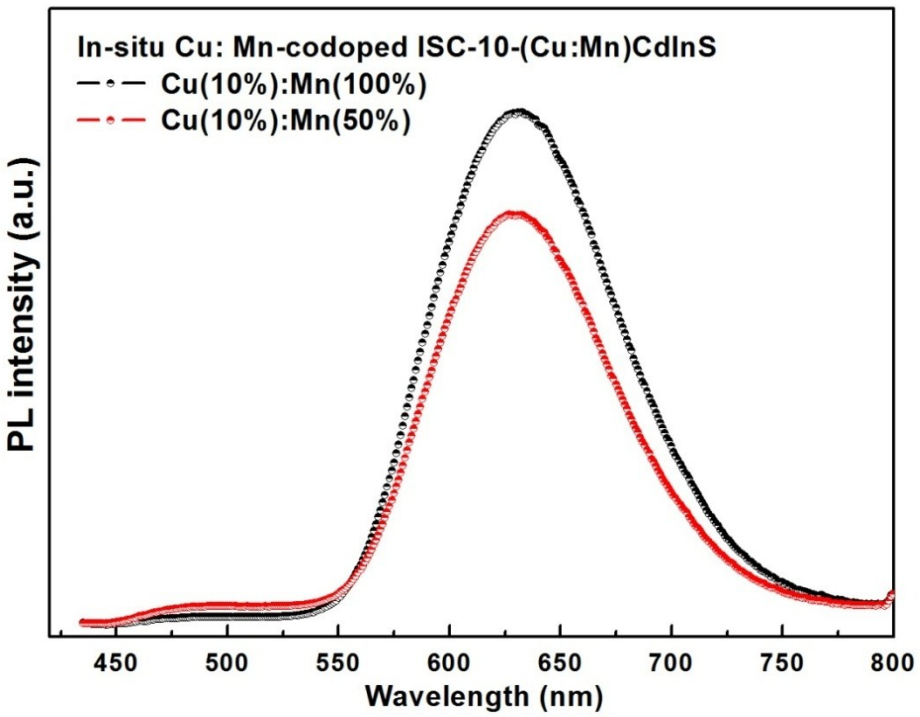

Figure S4. PL emission spectra of in-situ synthesized Cu:Mn-codoped samples (excited at 420 nm).

Table S1. Measured molar ratios of Cd:In:Mn:Cu in doped samples determined by EDS. The doping level of Cu^{+} or Mn^{2+} ions for doped sample is given as N%, with N being the moles of Cu^{+} or Mn^{2+} ions per 100 moles of T5 nanolcuster. The value of *N* for the nominal doping level and actual doping level represents the added number of moles of Cu^{+} or Mn^{2+} per 100 moles of T5 nanocluster and measured one, respectively.

Crystal Surface	**The molar ratio of Cd : In : Mn : Cu by EDS**				**Nominal Doping Level (N%)**		**Actual Doping Level (N%)**	
	Cd	In	Mn	Cu	Mn	Cu	Mn	Cu
Crystal 1	8.8	35.2	0.2	-	100%	-	15.8%	-
Crystal 2	8.4	34.4	0.1	-	100%	-	8.2%	-
Crystal 3	7.9	31.7	0.1	-	100%	-	8.8%	-
Crystal 4	8.1	32.6	0.1	-	100%	-	8.6%	-
Average	**8.3**	**33.5**	**0.125**	**-**	100%	**-**	**10.4%**	-
Inner Surface								
Crystal 1	8.7	34.5	0.1	-	100%	-	8.1%	-
Crystal 2	8.4	33.0	0.1	-	100%	-	8.4%	-
Crystal 3	8.9	33.0	0.2	-	100%	-	16.6%	-
Average	**8.7**	**33.5**	**0.13**	**-**	100%	**-**	**11.0%**	-
Crystal Surface								
Crystal 1	7.9	31.8	-	0.8	-	10%	-	69.1%
Crystal 2	7.9	32.4	-	0.3	-	10%	-	25.9%
Crystal 3	7.8	33.5	-	0.8	-	10%	-	66.5%
Average	**7.9**	**32.6**	**-**	**0.63**	**-**	10%	**-**	**54.0%**
Inner Surface								
Crystal 1	8.7	32.1	-	0.1	-	10%	-	8.6%
Crystal 2	8.9	31.8	-	0.0	-	10%	-	0.0%
Crystal 3	8.7	31.4	-	0.4	-	10%	-	34.6%
Average	**8.8**	**31.8**	**-**	**0.17**	**-**	10%	**-**	**14.3%**
Crystal Surface								

Crystal 1	7.9	35.1	0.1	0.9	50%	10%	8.0%	71.6%
Crystal 2	7.4	31.0	0.1	0.3	50%	10%	9.0%	27.1%
Average	**7.7**	**33.1**	**0.1**	**0.6**	50%	10%	**8.5%**	**50.7%**
Inner Surface								
Crystal 1	9.0	31.3	0.3	0.1	50%	10%	25.8%	8.6%
Crystal 2	9.0	29.4	0.1	0.2	50%	10%	9.0%	18.1%
Crystal 3	8.5	30.9	0.2	0.8	50%	10%	17.3%	69.3%
Average	**8.8**	**30.5**	**0.2**	**0.37**	50%	10%	**17.5%**	**32.1%**
Crystal Surface								
Crystal 1	8.1	31.6	0.0	0.5	100%	10%	0.0%	43.5%
Crystal 2	8.3	36.0	0.2	0.7	100%	10%	15.5%	54.2%
Average	**8.2**	**33.8**	**0.1**	**0.6**	100%	10%	**8.2%**	**49.2%**
Inner Surface								
Crystal 1	8.6	32.3	0.3	0.2	100%	10%	25.4%	16.9%
Crystal 2	8.7	32.1	0.3	0.3	100%	10%	25.4%	25.4%
Crystal 3	9.2	33.5	0.3	0.2	100%	10%	24.3%	16.2%
Average	**8.8**	**32.6**	**0.3**	**0.23**	100%	10%	**25.0%**	**19.4%**

Table S2. Time constants τ_1, τ_2, and τ_3, the corresponding amplitudes of the components A1, A2 and A3 at different emission sites of Mn^{2+}(100%)-doped ISC-10-CdInS under interband excitation at 400nm. Fit parameter deriving from $I(t) = A\ I(t)=\Sigma A_i \exp(-t/\tau_i)$, and weighted average lifetime $\tau_{ave} = \Sigma A_i\tau_{i2} / \Sigma A_i\tau_i$.

100% Mn Doped	τ_1(ms)	A_1(%)	τ_2(ms)	A_2(%)	τ_3(ms)	A_3(%)	τ_{ave}(ms)
550	0.27	23%	1.33	77%			1.267
580	0.29	15%	1.36	85%			1.324
600	0.21	11%	1.17	89%			1.147
630	0.15	3%	0.51	21%	1.46	76%	1.377
650	0.07	1%	0.37	16%	1.34	83%	1.288
700	0.11	1%	0.38	17%	1.31	82%	1.260

Table S3. Time constants τ_1, τ_2, and τ_3, the corresponding amplitudes of the components A1, A2 and A3 at different emission sites of Cu^{+},Mn^{2+}(10%,50%)-codoped ISC-10-CdInS under interband excitation at 400nm. Fit parameter deriving from $I(t) = A\ I(t)=\Sigma A_i \exp(-t/\tau_i)$, and weighted average lifetime $\tau_{ave} = \Sigma A_i\tau_{i2} / \Sigma A_i\tau_i$.

Codoped 10-50%	τ_1(ms)	A_1(%)	τ_2(ms)	A_2(%)	τ_3(ms)	A_3(%)	τ_{ave}(ms)
550	0.06	2%	0.28	30%	0.96	68%	0.885
580	0.24	26%	1.00	74%			0.937
600	0.04	1%	0.30	28%	1.05	71%	0.971
630	0.07	2%	0.35	30%	1.11	68%	1.011
650	0.04	2%	0.32	28%	1.07	70%	0.987
700	0.23	20%	0.96	80%			0.916

Table S4. Time constants τ_1, τ_2, and τ_3, the corresponding amplitudes of the components A1, A2 and A3 at different emission sites of Cu^{+},Mn^{2+}(10%, 100%)-codoped ISC-10-CdInS under interband excitation at 400nm. Fit parameter deriving from $I(t) = A\ I(t)=\Sigma A_i \exp(-t/\tau_i)$, and weighted average lifetime $\tau_{ave} = \Sigma A_i\tau_{i2} / \Sigma A_i\tau_i$.

Codoped 10-100%	τ_1(ms)	A_1(%)	τ_2(ms)	A_2(%)	τ_3(ms)	A_3(%)	τ_{ave}(ms)
550	0.11	6%	0.38	39%	1.37	55%	1.196
600	0.19	21%	0.77	79%			0.734
630	0.03	2%	0.29	31%	1.10	67%	1.006
650	0.02	2%	0.28	29%	1.08	69%	0.999
700	0.14	7%	0.51	39%	1.52	54%	1.312