Supplementary Information

Unveiling the composites structures of emissive consolidated p-i-n junction nanocells for white light emission

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1. Cartesian coordinates of optimized structures.

Table S1. (a) PVK-TOP structure

atom	x	y	z
C	2.348068	-1.49185	2.369145
C	3.400676	-2.42126	2.297564
C	4.451395	-2.26063	1.396396
C	4.422043	-1.14104	0.561735
C	3.363587	-0.19758	0.615246
C	2.321708	-0.37842	1.532917
H	1.54651	-1.64813	3.08512
H	3.397848	-3.28334	2.958631
H	5.264898	-2.97691	1.34364
H	1.511068	0.343862	1.579024
N	5.341287	-0.74307	-0.41315
C	4.869352	0.428955	-1.00713
C	5.443974	1.193318	-2.02605
C	4.7684	2.343652	-2.42901
C	3.556625	2.72945	-1.82939
C	2.992174	1.969916	-0.80724
C	3.64932	0.806542	-0.38897
H	6.388272	0.907318	-2.4784
H	5.191532	2.955854	-3.22043
H	3.058574	3.63316	-2.16825
H	2.059029	2.263502	-0.33348
C	6.432733	-1.53659	-0.8971
C	7.598457	-1.57211	-0.238
C	7.949208	-0.81378	1.006045
H	8.85654	-0.2176	0.850154
H	7.143396	-0.1454	1.314236
H	8.163656	-1.49894	1.835691
C	6.144905	-2.31993	-2.1529
H	5.319026	-3.02202	-1.98755
H	5.836961	-1.65509	-2.96778
H	7.022033	-2.8842	-2.47966
H	8.3728	-2.22012	-0.64634
H	0.787913	3.633857	1.53718
H	0.241452	2.483616	2.546879

C	-1.16135	3.086336	1.176777
H	-1.13138	3.503944	0.162831
H	-1.64967	3.845734	1.813356
C	-2.01056	1.81455	1.17257
H	-1.5296	1.077246	0.518252
H	-2.00946	1.377981	2.182423
C	-3.45749	2.054039	0.72614
H	-3.92651	2.799515	1.384136
H	-3.4578	2.495825	-0.2805
C	-4.31055	0.779468	0.716838
H	-3.84152	0.035468	0.05776
H	-4.31154	0.335025	1.722137
C	-5.757	1.016653	0.2657
H	-5.75509	1.474391	-0.73376
H	-6.23149	1.749975	0.933313
C	-6.60606	-0.26176	0.233733
H	-6.611	-0.72329	1.229905
H	-6.12762	-0.98927	-0.43588
C	-8.05164	-0.01022	-0.21853
H	-8.06303	0.464346	-1.21014
H	-8.53339	0.693925	0.472823
P	-9.11846	-1.55413	-0.23749
C	-10.6958	-0.81144	-0.90502
H	-10.5366	-0.2209	-1.81452
H	-11.4081	-1.61161	-1.12781
H	-11.148	-0.16844	-0.14384
C	-8.49016	-2.36767	-1.79633
H	-9.13735	-3.21338	-2.04802
H	-8.46313	-1.6797	-2.64937
H	-7.4839	-2.76276	-1.63028
N	0.221475	2.789768	1.576008

Table S1. (b) TPBi-TOP structure

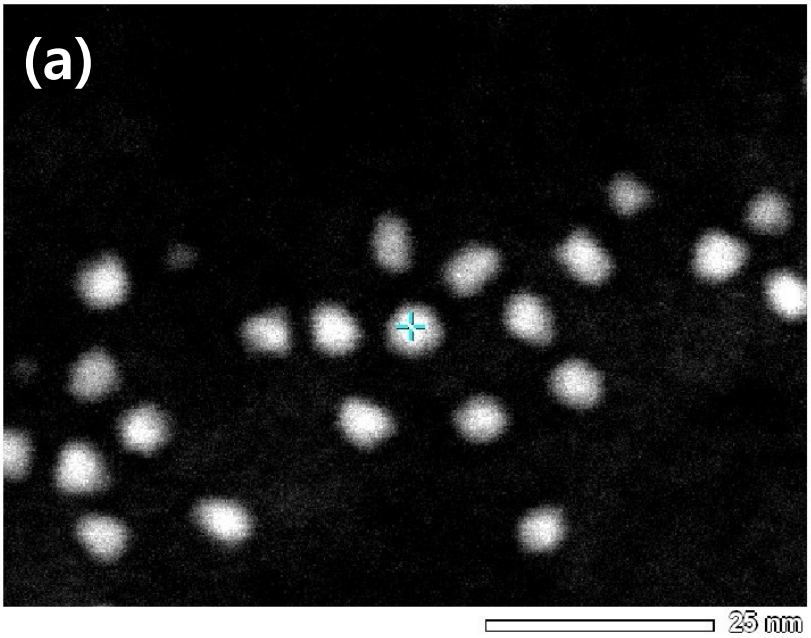
Atom	x	y	z
C	2.737093	-3.23903	-0.9013
C	2.230078	-2.08303	-1.4986
C	0.874829	-1.98867	-1.81075
C	0.017611	-3.05018	-1.50202
C	0.519403	-4.20879	-0.89973
C	1.880975	-4.30178	-0.60841
N	-1.37247	-2.97012	-1.8235
C	-2.01399	-3.78673	-2.75438
C	-1.58716	-4.90079	-3.47996
C	-2.51084	-5.47157	-4.35186
C	-3.8109	-4.94676	-4.49839
C	-4.22327	-3.82955	-3.78142
C	-3.30795	-3.23771	-2.90081
N	-3.45251	-2.12744	-2.09108
C	-2.30244	-1.9877	-1.46752
C	-2.05721	-0.92015	-0.48135
C	-2.69258	0.314239	-0.68222
C	-2.501	1.367164	0.220969
C	-1.67481	1.170245	1.336184
C	-1.05069	-0.06241	1.558927
C	-1.24602	-1.10783	0.645078
C	-0.15105	-0.17967	2.720815
N	0.58144	0.825103	3.154273
C	1.317214	0.32963	4.214251
C	2.250682	0.974744	5.036174
C	2.842834	0.234307	6.05254
C	2.516211	-1.1217	6.257551
C	1.593643	-1.78116	5.449474
C	1.012344	-1.03354	4.423313
N	0.063033	-1.35079	3.451156
C	-0.65105	-2.58664	3.392352
C	-2.03298	-2.61214	3.606363
C	-2.71577	-3.82656	3.559457
C	-2.02342	-5.01553	3.32104
C	-0.64242	-4.98688	3.12067
C	0.046951	-3.7741	3.14864

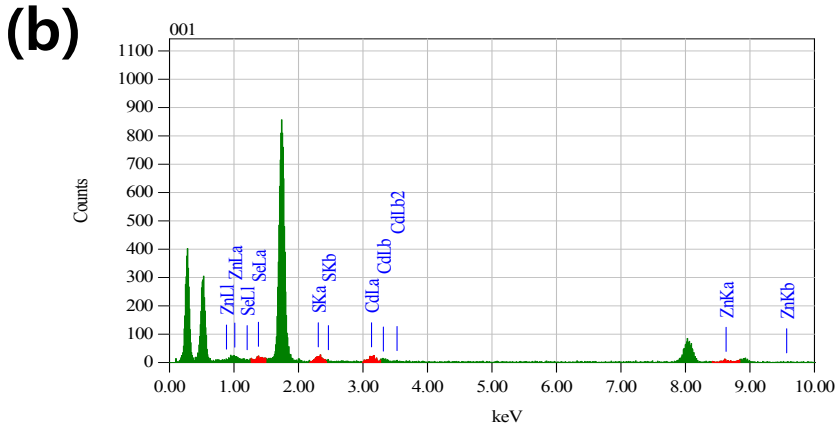
C	-3.06218	2.715355	0.017901
N	-2.42631	3.806436	0.394622
C	-3.22742	4.86416	0.010256
C	-3.0309	6.242455	0.170058
C	-4.01787	7.098572	-0.30353
C	-5.18352	6.602853	-0.92307
C	-5.39546	5.237523	-1.09429
C	-4.39384	4.384513	-0.62586
N	-4.27384	2.995152	-0.61547
C	-5.30285	2.092005	-1.02645
C	-5.72018	2.086613	-2.36117
C	-6.74215	1.225565	-2.76104
C	-7.33726	0.365448	-1.83743
C	-6.91527	0.373903	-0.50687
C	-5.90632	1.242439	-0.09444
H	3.794504	-3.31058	-0.66629
H	2.891403	-1.25398	-1.73067
H	0.476075	-1.09929	-2.28655
H	-0.15899	-5.01953	-0.65535
H	2.27	-5.2039	-0.14577
H	-0.58508	-5.30227	-3.37435
H	-2.22096	-6.34145	-4.93358
H	-4.49888	-5.42538	-5.18879
H	-5.21867	-3.4125	-3.89348
H	-3.31324	0.431765	-1.56108
H	-1.51102	1.985193	2.028636
H	-0.76125	-2.06133	0.80571
H	2.489416	2.020663	4.874272
H	3.569797	0.706982	6.705903
H	2.994906	-1.66635	7.065802
H	1.340184	-2.82309	5.612993
H	-2.55946	-1.68522	3.806854
H	-3.78934	-3.84399	3.719619
H	-2.55827	-5.95982	3.292751
H	-0.09896	-5.90851	2.935494
H	1.116738	-3.73689	2.971877
H	-2.13356	6.613377	0.654219

H	-3.89403	8.171651	-0.19373
H	-5.93534	7.302625	-1.27547
H	-6.29472	4.857716	-1.56707
H	-5.23703	2.746586	-3.07428
H	-7.0637	1.220567	-3.79796
H	-8.12583	-0.3105	-2.15316
H	-7.37714	-0.29216	0.215281
H	-5.58191	1.267378	0.940375
C	1.592061	3.202551	0.143584
H	1.534607	3.969976	-0.64076
H	1.154728	2.284105	-0.29492
C	3.063065	2.932721	0.47137
H	3.497021	3.84915	0.891086
H	3.114052	2.175428	1.266894
C	3.886282	2.462743	-0.73273
H	3.843763	3.22516	-1.52404
H	3.426107	1.559513	-1.16133
C	5.352987	2.167811	-0.39499
H	5.39657	1.392978	0.383651
H	5.808436	3.064811	0.047901
C	6.187276	1.722396	-1.60223
H	6.155239	2.503931	-2.3746
H	5.728293	0.831779	-2.05617
C	7.650111	1.412303	-1.25523
H	7.683927	0.619032	-0.49659
H	8.099685	2.298519	-0.78744
C	8.484284	0.990102	-2.47339
H	8.483015	1.787061	-3.2305
H	8.026129	0.109438	-2.94335
N	0.880177	3.69906	1.321362
H	-0.08669	3.904384	1.069962
H	0.838414	2.952615	2.016097
P	10.24769	0.507552	-2.05343
C	10.88746	0.209002	-3.78212
H	10.67861	1.043708	-4.46111
H	11.96923	0.048054	-3.74775
H	10.4301	-0.69769	-4.18969

C	10.99078	2.194202	-1.75183
H	12.07727	2.099381	-1.66197
H	10.76534	2.903367	-2.55676
H	10.6178	2.602568	-0.80832

2. STEM EDS data of QD in consolidated p-i-n junction NCs structures.





Thin Film Standardless Standardless Quantitative Analysis
Fitting Coefficient : 0.9781

Element	(keV)	Mass%	Counts	Error%	Atom%	Compound	Mass%	Cation	K
S K	2.307	13.32	172.13	0.97	31.24			0.3050	
Zn K	8.630	11.01	73.56	3.57	12.66			0.5898	
Se L	1.379	19.25	66.68	2.68	18.34			1.1381	
Cd L (Ref.)	3.133	56.42	222.39	0.89	37.76			1.0000	
Total		100.00			100.00				

Fig S2. (a) STEM image of CdSe/ZnS QD. (b) EDS spectra of the CdSe/ZnS QD.

3. PL lifetimes of the consolidated p-i-n junction NCs.

Table S3. PL lifetimes of the consolidated p-i-n NCs. (Unit: ns)

	τ_1	τ_2	τ_{ave}	A_1	A_2
TPBi 388 nm	4.756	15.668	10.068	0.257	0.074
PVK 403 nm	4.704	15.799	12.626	0.148	0.110
Blue QDs 440 nm	10.258	30.021	18.523	0.171	0.042
Green QDs 554 nm	11.616	32.915	17.4	0.152	0.020
Red QDs 620 nm	16.389	40.398	20.096	0.189	0.014

Table S3. PL lifetimes of the consolidated p-i-n NCs. (Unit: ns) Excitation: 350nm, 2nd harmonic of fs Ti:Sapphire laser. The PL decay curves were fitted by a bi-exponential function to calculate the lifetimes of the samples. τ_1 and τ_2 are lifetimes.