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

Supporting information

Key Host Parameter for Long Lifetime in Phosphorescent Organic Light-Emitting Diodes : Bond Dissociation Energy in Triplet Excited State

Chang Yoon Yang[1+], Sunwoo Kang[2+], Hyein Jeong[2], Ho Jin Jang[1], Yoonkyoo Lee[2], Jun Yeob Lee[1*]

[11]School of Chemical Engineering, Sungkyunkwan University
2066, Seobu-ro, Jangan-gu, Seobu-ro, Suwon, Gyeonggi, 16419, Korea
E-mail : leej17@skku.edu

[2]Display Research Center, Samsung Display Co.
1 Samsung-ro, Giheung-gu, Yongin, Gyeonggi-do, Korea

+ Chang Yoon Yang and Sunwoo Kang contributed equally.

Experimental

General information

All chemicals and reagents were purchased from commercial suppliers. 9H-3,9'-bicarbazole was purchased from Sunfine global Co. Ltd. and was further sublimed before use. 2-Fluorobenzonitile and 4-fluorobenzonitrile were purchased from TCI Co.. 3-Fluorobenzonitrile was purchased from Alfa Aesar Co.. Cesium carbonate used as a base was purchased from Samchun Chem. Toluene, tetrahydrofuran, *n*-hexane, and methylene chloride were products of Samchun pure chemical Co. Ltd. *N*,*N*-dimethylformamide (DMF) was purchased from Daejung Chemical & Metal Co.. All reactions and manipulations were performed in the oil bath. All column chromatography (methylene chloride (MC)/*n*-hexane (HEX) mixed solvent) was carried out on a stationary phase of the column on silica gel. All materials were purified by vacuum sublimation in order to get purity higher than 99.9 % before the device test.

The ^{1}H and ^{13}C nuclear magnetic resonance (NMR) spectra were recorded with a Unity Inova (Varian, 500 MHz) spectrometer. Solvent for the NMR analysis was dimethyl sulfoxide(DMSO-d_6). The HOMO and LUMO were estimated and calculated using cyclic voltammetry (Ivium Tech., Iviumstat). The UV-vis spectra were observed using UV-vis spectrophotometer (JASCO, V-730) and the PL spectra were obtained using a fluorescence spectrophotometer (PerkinElmer, LS-55). UV-vis measurements were performed using a tetrahydrofuran solution of the sample. Solution PL measurements were performed using a toluene. Tetrahydrofuran and Toluene was distilled over sodium and calcium hydride. The equipment to measure mass spectra was Advion, Expression^{L} CMS spectrometer in APCI mode. The triplet energy of the material was measured after 2 ms delay time at 77 K using a frozen tetrahydrofuran solution in liquid nitrogen. The instrument to measure mass spectra was an Advion, Expression^{L} CMS spectrometer in APCI mode. Purity of the material was

analyzed using high performance liquid chromatography (Younglin Instrument Co.) using a mobile phase of acrylonitrile: methylalcohol(9:1).

Synthesis

2-(9H-[3,9'-bicarbazol]-9-yl)benzonitrile (oCzBN).

All the reaction processes were performed in the oil bath. Reactants of 9H-3,9'-bicarbazole (1.5g, 4.51 mmol), 2-fluorobenzonitrile (0.72ml, 6.77 mmol), and cesium carbonate (2.94g, 9.03 mmol) were all added into a solution of DMF in a pressure tube. The temperature of the oil bath was adjusted to 150°C. The mixture was heated by keeping the condition and stirred overnight. The completion of the reaction was verified by a spot in the thin layer chromatography. After the reaction, the reaction vessel was cooled down, and the mixture was allowed to stand at room temperature. Then, the reaction mixture was extracted with dichloromethane and distilled water. Small amount of salt and water in organic layer were removed by anhydrous magnesium sulfate. After filtering off the magnesium sulfate, the organic phase was collected and concentrated by a rotary evaporator. A solid sample was adsorbed onto silica gel, and the crude material was purified by silica gel column chromatography using a *n*-hexane : MC (1 : 2) mixture as the eluent to obtain the desired product as a white powder with a purity of 99.7%. Subsequently, recrystallization was carried out using a mixed solvent of toluene and hexane for 24 h to obtain a high purity of 99.9%. As a final step, sublimation purification was performed for device test.

Yield 72% (1.40g), ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.59 (s, 1H), 8.38 (d, 1H, J = 8 H_Z), 8.27 (t, 3H, J = 7.5 H_Z), 8.07 (t, 1H, J= 8.5 H_Z), 7.93 (d, 1H, J = 8 H_Z), 7.86 (t, 1H, J = 8.25 H_Z), 7.64 (d, 1H, J = 9 H_Z), 7.52 (t, 1H, J = 7.75 H_Z), 7.48-7.44 (m, 3H), 7.39-7.35 (m, 3H),7.32-7.29 (m, 3H) MS (APCI) m/z 433.5 [(M + H)$^{+}$]. ^{13}C NMR (125 MHz, DMSO-d_6): δ 141, 139.4, 139, 135.6, 135, 130, 129.9, 129.8, 127.2, 126.2, 125.6, 124.2, 122.7, 122.5, 121.4, 121, 120.5, 119.8, 119.7, 116.2, 111.6, 111.1, 110, 109.6.

3-(9H-[3,9'-bicarbazol]-9-yl) benzonitrile (mCzBN)

The synthesis method of mCzBN was the same as that of oCzBN. 9H-3,9'-bicarbazole (1.5g, 4.51 mmol), 3-fluorobenzonitrile(0.72ml, 6.77 mmol), and cesium carbonate (2.94g, 9.03 mmol) were used for the synthesis.

Yield 73% (1.42 g), ^{1}H NMR (500 MHz, DMSO-d_6): δ 8.56 (s, 1H), 8.36 (d, 1H, J = 7.5 H_Z), 8.33 (s, 1H), 8.28 (d, 2H, J = 7.5 H_Z) , 8.13 (d, 1H, J = 8.5 H_Z), 8.06 (d, 1H, J = 8 H_Z), 7.93 (t, 1H, J = 8 H_Z), 7.69 (d, 1H, J = 8.5 H_Z), 7.63 (d, 1H, J = 8.5 H_Z), 7.54-7.49 (m, 2H), 7.46-7.42 (m, 2H), 7.37-7.34 (m, 3H), 7.30 (t, 2H, J = 7.8 H_Z) MS (APCI) m/z 433.5 [(M + H)$^+$]. ^{13}C NMR (125 MHz, DMSO-d_6): δ 141.1, 140.6, 139, 137.5, 132, 131.7, 131.7, 130.5, 129.7, 127.2, 126.2, 125.6, 124.2, 122.7, 122.5, 121.3, 120.9, 120.5, 119.8, 119.6, 118.1, 113.4, 111.1, 109.9,109.6.

4-(9H-[3,9'-bicarbazol]-9-yl)benzonitrile (pCzBN).

The synthesis method of pCzBN was the same as that of oCzBN. 9H-3,9'-bicarbazole (2g, 6.02 mmol), 4-fluorobenzonitrile (0.99ml, 9.03 mmol), and cesium carbonate (3.95g, 12.03 mmol) were used for the synthesis.

Yield 76% (1.98 g),^{1}H NMR (500 MHz, DMSO-d_6): δ 8.57 (s, 1H), 8.37 (d, 1H, J = 8 H_Z), 8.28 (d, 2H, J = 7.5 H_Z), 8.19 (d, 2H, J = 8.5 H_Z), 8.01 (d, 2H, J = 8.5 H_Z), 7.74 (d, 1H, J = 9 H_Z), 7.64 (d, 1H, J = 9 H_Z), 7.57–7.51 (m, 2H), 7.44 (t, 2H, J = 7.5 H_Z), 7.37-7.35 (m, 3H), 7.30 (t, 2H, J = 7.5 H_Z).' MS(APCI) m/z 433.5 [(M + H)$^+$]. ^{13}C NMR (125 MHz, DMSO-d_6): δ 141.6, 141.5, 140.7, 139, 130.5, 127.9, 127.8, 126.7, 126.2, 125.1, 123. 5, 123, 121.9, 121.7, 121, 120.3, 120.2, 119, 111.8, 110.6, 110.5, 110.2

Computational Details

The ground state geometries of three different host materials were carried out the by employing a non-local density functional of Becke's three parameterized Lee-Yang-Parr exchange functional (B3LYP)

with 6-31G* level of theory as implemented in the suite of Gaussian 09 package[1]. To obtain the molecular structures and excitation energies in singlet and triplet excited state, two different approaches were taken. The time-dependent density functional theory (TDDFT) simulations for singlet excited state were preferentially carried out by employing CAM-B3LYP functional with same basis set. It is already known that the B3LYP functional generally gives underestimated the excitation energy of charge transfer molecule due to inappropriate description of Coulomb coupling.[2,3] Therefore, range separated (RS) functionals including short- and long-range Coulomb operator should be applied to exactly obtain the transition characteristics. Nevertheless, the CAM-B3LYP functional (ω =33) should be carefully modified to predict accurate values of singlet adiabatic excitation energies of three host materials due to overestimation of excitation energies. Accordingly, the ω value was set to be 25, which gives a quantitative prediction of singlet adiabatic excitation energies as compared experimental results. For triplet excited state, it is well known that spin unrestricted simulation has been known to be provided qualitative prediction of the lowest triplet excited state energy.[4] In addition, the spin unrestricted simulation is very efficient method to reduce the time cost for geometrical optimization of triplet excited state. Therefore, the molecular structures in triplet excited states were performed by spin unrestricted B3LYP functional with same basis set. The corresponding lowest triplet transition energies of three host materials were calculated by means of the ΔSCF method. To obtain the degradation reaction profiles of three host materials in singlet and triplet excited states, the fully relaxed potential energy surface simulations were carried out based on the bond elongation of targeted bond. The initial bond distances of singlet and triplet excited states were set from each of singlet and triplet excited states optimized structures. The interval distances set to be 0.1 angstrom. In degradation reaction pathway, the activation energy should be considered and compared in these materials. However, it should be noticed that the triplet-triplet annihilation (TTA) process can provide a sufficient energy to overcome activation energy in these complexes. Furthermore, TTA rate behaves to impact on the degradation rate. Therefore, the chemical stability of three host materials was investigated by energy differences between initial and final state. In the same perspectives, the chemical stability in singlet excited state was determined.

1. M. Frisch, G. Trucks, H. B. Schlegel, G. Scuseria, M. Robb, J. Cheeseman, G. Scalmani, V. Barone, B. Mennucci and G. Petersson, *Inc., Wallingford, CT*, 2009, **200**, 28.
2. M. A. Rohrdanz, K. M. Martins and J. M. Herbert, *The Journal of chemical physics*, 2009, **130**, 054112.
3. Y. Tawada, T. Tsuneda, S. Yanagisawa, T. Yanai and K. Hirao, *The Journal of chemical physics*, 2004, **120**, 8425-8433.
4. A. Berces and M. Z. Zgierski, *Chemical Physic Letters*, 1996, **257**, 61-67.

Table S1. Bond dissociation energy calculation results. The units are in eV

Materials	C-N bond (at carbazolycarbazole)			C-N bond (at benzonitrile)		
	Neutral	Cation	Anion	Neutral	Cation	Anion
oCzBN	3.672	4.620	2.042	3.534	3.662	1.54
mCzBN	3.663	4.493	2.057	3.569	3.58	1.60
pCzBN	3.659	4.465	2.085	3.585	3.573	1.648

Materials	C-N bond (at carbazolycarbazole)		C-N bond (at benzonitrile)	
	Singlet	Triplet	Singlet	Triplet
oCzBN	1.177	0.648	0.982	0.396
mCzBN	0.999	0.526	0.886	0.432
pCzBN	1.087	0.396	0.901	0.648

Table S2. Blue PhOLEDs device results

		oCzBN	**mCzBN**	**pCzBN**
EQE[a)] (%)	1000 cd/m^2	5.4	5.2	9.4
	Max	5.5	5.9	9.7
PE[b)] (lm/W)	1000 cd/m^2	4.7	5.1	11.1
	Max	6.3	9.1	14.5
CIE[c)]		(0.15,0.23)	(0.15,0.23)	(0.15,0.24)
Device lifetime[d)] (h)		48.8	48.9	103.6

[a)] External quantum efficiency, [b)] power efficiency, [c)] color coordinates, [d)] device lifetime of 50% luminance decay at initial luminance of 100 cd/m^2

Table S3. Green PhOLEDs device results

		oCzBN	**mCzBN**	**pCzBN**
EQE[a)] (%)	1000 cd/m^2	15.6	17.7	17.3
	Max	16.2	18.4	18.1
PE[b)] (lm/W)	1000 cd/m^2	23.2	29.0	33.6
	Max	27.7	41.1	46.6
CIE[c)]		(0.28, 0.63)	(0.28, 0.64)	(0.28, 0.64)
Device lifetime[d)] (h)		350.5	472.4	743.6

[a)] External quantum efficiency, [b)] power efficiency, [c)] color coordinates, [d)] device lifetime of 70% luminance decay at initial luminance of 200 cd/m^2

Table S4. Bond dissociation energy calculation results at weakest bond

Materials	BDE				
	Neutral	Cation	Anion	Triplet	Singlet
oCzBN	3.534	3.662	1.54	0.396	0.982
mCzBN	3.569	3.58	1.60	0.432	0.886
pCzBN	3.585	3.573	1.648	0.648	0.901

Table S5. Cartesian coordinates of oCzBN, mCzBN, and pCzBN in singlet and triplet excited states.

The geometry of oCzBN in singlet excited state				
1	C	5.71869	2.530504	1.011819
2	C	4.415013	2.986142	1.234529
3	C	3.312366	2.175137	0.986548
4	C	3.549079	0.89595	0.487257
5	C	4.857446	0.412839	0.290716
6	C	5.947235	1.239056	0.549788
7	H	6.558987	3.186891	1.216292
8	H	4.255783	3.989443	1.618244
9	H	2.310082	2.529879	1.197743
10	H	6.960419	0.875885	0.402437
11	C	3.370402	-1.27457	-0.19962
12	C	2.913201	-2.50327	-0.67252
13	C	3.868517	-3.44401	-1.04226
14	C	5.237355	-3.16521	-0.96233
15	C	5.682345	-1.92082	-0.52782
16	C	4.74318	-0.96616	-0.15023
17	H	1.856582	-2.72141	-0.77756
18	H	3.538301	-4.4104	-1.41068
19	H	5.957058	-3.92188	-1.25937
20	H	6.744135	-1.69431	-0.49493
21	N	2.63514	-0.1357	0.192634
22	C	1.251333	-0.05023	0.272195
23	C	0.515459	-1.12813	0.824789
24	C	0.593341	1.106176	-0.21448
25	C	-0.85607	-1.09045	0.893148
26	H	1.056446	-1.97433	1.231035
27	C	-0.7776	1.151832	-0.16974
28	H	1.172725	1.89731	-0.67723
29	C	-1.50606	0.049476	0.380363
30	H	-1.4339	-1.89984	1.320729
31	C	-1.7815	2.10568	-0.62559
32	N	-2.83214	0.279206	0.288689
33	C	-3.03079	1.521851	-0.33597
34	C	-1.72987	3.348396	-1.23779
35	C	-4.2318	2.139011	-0.64475
36	C	-2.93377	3.986737	-1.554
37	H	-0.77941	3.81779	-1.47633
38	C	-4.16074	3.389284	-1.26372
39	H	-5.17636	1.66003	-0.41438
40	H	-2.91167	4.958854	-2.03684
41	H	-5.08053	3.903262	-1.52563
42	C	-3.85501	-0.66875	0.627066
43	C	-3.99598	-1.83163	-0.23098
44	C	-4.67574	-0.44314	1.717715
45	C	-5.08588	-2.70588	0.112026
46	C	-5.70053	-1.32939	2.034835
47	H	-4.50656	0.443472	2.325306
48	C	-5.89047	-2.46579	1.191816

49	H	-5.25739	-3.57425	-0.51719
50	H	-6.34378	-1.15093	2.887928
51	H	-6.69937	-3.15862	1.409627
52	C	-3.13671	-2.06668	-1.30201
53	N	-2.3716	-2.23702	-2.18189

The geometry of oCzBN in triplet excited state				
1	6	-5.73095	-2.52999	1.066146
2	6	-4.42559	-2.96907	1.333907
3	6	-3.3208	-2.15312	1.090494
4	6	-3.55558	-0.88961	0.540871
5	6	-4.86906	-0.42147	0.295548
6	6	-5.96018	-1.25165	0.55684
7	1	-6.57143	-3.18615	1.272887
8	1	-4.26807	-3.95928	1.751767
9	1	-2.31715	-2.48566	1.328413
10	1	-6.97348	-0.90356	0.37603
11	6	-3.37046	1.256997	-0.20982
12	6	-2.90791	2.481068	-0.69963
13	6	-3.85894	3.410371	-1.12012
14	6	-5.23225	3.126671	-1.06821
15	6	-5.68475	1.889581	-0.61054
16	6	-4.7509	0.943596	-0.18405
17	1	-1.8487	2.699231	-0.76908
18	1	-3.52332	4.370098	-1.50212
19	1	-5.9479	3.872946	-1.40078
20	1	-6.74691	1.660863	-0.59658
21	7	-2.63786	0.134205	0.231566
22	6	-1.24712	0.044784	0.333607
23	6	-0.51384	1.106085	0.866524
24	6	-0.59835	-1.1682	-0.16137
25	6	0.88854	1.058253	0.937545
26	1	-1.04368	1.949279	1.294591
27	6	0.805298	-1.17568	-0.18639
28	1	-1.18595	-1.93117	-0.65433
29	6	1.521238	-0.07919	0.347474
30	1	1.459076	1.826607	1.44164
31	6	1.790672	-2.11681	-0.66513
32	7	2.866333	-0.29967	0.212965
33	6	3.068604	-1.5579	-0.39518
34	6	1.724057	-3.36678	-1.29555
35	6	4.257329	-2.18939	-0.73219
36	6	2.915727	-4.01679	-1.62941
37	1	0.764883	-3.81817	-1.53245
38	6	4.165007	-3.44374	-1.35401
39	1	5.219016	-1.72993	-0.52966
40	1	2.872399	-4.98601	-2.11916
41	1	5.07375	-3.97148	-1.62677
42	6	3.886467	0.634654	0.538454
43	6	3.89738	1.928297	-0.06197
44	6	4.867908	0.283901	1.467307
45	6	4.901089	2.840551	0.340031
46	6	5.858549	1.192576	1.833007

47	1	4.829572	-0.70397	1.916433
48	6	5.862379	2.481613	1.271571
49	1	4.91279	3.827753	-0.11092
50	1	6.612293	0.906679	2.559892
51	1	6.624098	3.199683	1.560599
52	6	2.995477	2.30485	-1.0991
53	7	2.31215	2.656234	-1.97889

The geometry of mCzBN in singlet excited state				
1	C	6.032372	2.194958	1.028844
2	C	4.747512	2.693955	1.267093
3	C	3.613429	1.942669	0.976585
4	C	3.799602	0.679285	0.418427
5	C	5.087854	0.1512	0.207385
6	C	6.209779	0.917441	0.509088
7	H	6.897945	2.805059	1.26788
8	H	4.627917	3.683477	1.697861
9	H	2.626228	2.328935	1.202536
10	H	7.207755	0.518519	0.351259
11	C	3.535508	-1.45149	-0.36022
12	C	3.035627	-2.64544	-0.87682
13	C	3.954602	-3.60986	-1.27672
14	C	5.332521	-3.38765	-1.18277
15	C	5.822526	-2.17922	-0.70043
16	C	4.919639	-1.20294	-0.29197
17	H	1.972136	-2.8228	-0.9852
18	H	3.589076	-4.55071	-1.67666
19	H	6.023851	-4.16101	-1.50291
20	H	6.892117	-1.99558	-0.65252
21	N	2.844741	-0.29883	0.071238
22	C	1.464833	-0.14784	0.131934
23	C	0.661221	-1.20992	0.61592
24	C	0.876936	1.066098	-0.30124
25	C	-0.70876	-1.0957	0.681105
26	H	1.146997	-2.10458	0.986682
27	C	-0.4898	1.194396	-0.25054
28	H	1.504022	1.846542	-0.71754
29	C	-1.28564	0.112409	0.241745
30	H	-1.33649	-1.87951	1.085579
31	C	-1.43092	2.241461	-0.63022
32	N	-2.59381	0.442282	0.185671
33	C	-2.71496	1.734621	-0.3379
34	C	-1.30086	3.515054	-1.16127
35	C	-3.87355	2.46439	-0.56041
36	C	-2.46052	4.263728	-1.39239
37	H	-0.32392	3.928569	-1.39601
38	C	-3.72148	3.745336	-1.09548
39	H	-4.84587	2.045217	-0.3304
40	H	-2.37638	5.261461	-1.81178
41	H	-4.60503	4.346544	-1.28588
42	C	-3.67551	-0.40614	0.629272
43	C	-4.53455	-0.90576	-0.31316
44	C	-3.74525	-0.6992	2.015257

45	C	-5.606	-1.76351	0.090313
46	C	-4.84064	-1.52386	2.411017
47	H	-3.12921	-0.17387	2.733613
48	C	-5.72207	-2.04258	1.503866
49	H	-4.97322	-1.74707	3.466674
50	H	-6.53585	-2.67941	1.837191
51	H	-4.39238	-0.67925	-1.36516
52	C	-6.49672	-2.29068	-0.85353
53	N	-7.23522	-2.73027	-1.65147

The geometry of mCzBN in triplet excited state				
1	6	6.067858	2.056583	1.564331
2	6	4.770044	2.500506	1.81872
3	6	3.603677	1.762282	1.329067
4	6	3.833756	0.626618	0.613333
5	6	5.167103	0.132716	0.342743
6	6	6.30783	0.891787	0.837784
7	1	6.908884	2.633318	1.940456
8	1	4.60576	3.409761	2.388057
9	1	2.602732	2.116804	1.546638
10	1	7.316954	0.54555	0.641376
11	6	3.623342	-1.31474	-0.56852
12	6	3.1773	-2.40807	-1.27575
13	6	4.150342	-3.29549	-1.80317
14	6	5.542867	-3.06754	-1.60997
15	6	6.011517	-1.97942	-0.91453
16	6	5.053224	-1.04413	-0.36692
17	1	2.119524	-2.58654	-1.43541
18	1	3.826029	-4.16394	-2.36758
19	1	6.248982	-3.77937	-2.0302
20	1	7.07449	-1.81126	-0.77497
21	7	2.917046	-0.28395	0.038193
22	6	1.500912	-0.16832	0.094207
23	6	0.739351	-1.21181	0.657776
24	6	0.873416	0.973038	-0.40798
25	6	-0.64821	-1.1376	0.727875
26	1	1.25386	-2.08524	1.04482
27	6	-0.51801	1.073706	-0.32833
28	1	1.468028	1.759781	-0.86159
29	6	-1.26939	0.01734	0.245491
30	1	-1.22079	-1.95608	1.151067
31	6	-1.46554	2.08106	-0.75865
32	7	-2.63021	0.341551	0.181213
33	6	-2.75683	1.598275	-0.43144
34	6	-1.32986	3.332581	-1.37075
35	6	-3.90587	2.351769	-0.68407
36	6	-2.47147	4.081407	-1.63895
37	1	-0.34572	3.714537	-1.62867
38	6	-3.74358	3.594236	-1.29357
39	1	-4.89233	1.991029	-0.4125
40	1	-2.38048	5.053047	-2.11544
41	1	-4.62248	4.197485	-1.50298
42	6	-3.69586	-0.46481	0.650975

43	6	-4.75184	-0.79524	-0.20353
44	6	-3.69732	-0.93553	1.971946
45	6	-5.81065	-1.58419	0.270423
46	6	-4.74178	-1.73864	2.429254
47	1	-2.88523	-0.65782	2.636002
48	6	-5.80475	-2.06389	1.59045
49	1	-4.7331	-2.09906	3.453465
50	1	-6.62552	-2.67897	1.943505
51	1	-4.74741	-0.45157	-1.23185
52	6	-6.89742	-1.91366	-0.60709
53	7	-7.78073	-2.17995	-1.31528

The geometry of pCzBN in singlet excited state				
1	C	6.013034	1.759418	1.608452
2	C	4.744361	2.313916	1.808174
3	C	3.59735	1.689313	1.32947
4	C	3.755716	0.497868	0.624072
5	C	5.023471	-0.08885	0.446901
6	C	6.15852	0.550547	0.937281
7	H	6.889118	2.270315	1.995816
8	H	4.646814	3.245696	2.357121
9	H	2.619055	2.11308	1.5251
10	H	7.140727	0.105168	0.80709
11	C	3.433792	-1.49126	-0.45099
12	C	2.910287	-2.57156	-1.15778
13	C	3.801264	-3.53914	-1.61082
14	C	5.176768	-3.42837	-1.38096
15	C	5.694075	-2.32962	-0.70449
16	C	4.819047	-1.35107	-0.24116
17	H	1.85124	-2.65918	-1.37092
18	H	3.416209	-4.39363	-2.1589
19	H	5.845829	-4.20141	-1.74605
20	H	6.764443	-2.22994	-0.54808
21	N	2.778054	-0.35723	0.074353
22	C	1.409405	-0.11798	0.045107
23	C	0.504611	-1.17247	0.319513
24	C	0.935501	1.180788	-0.26731
25	C	-0.85669	-0.96793	0.290699
26	H	0.900911	-2.13911	0.606563
27	C	-0.41973	1.397703	-0.30828
28	H	1.643772	1.962257	-0.51943
29	C	-1.31902	0.32124	-0.03098
30	H	-1.56382	-1.75372	0.526798
31	C	-1.26222	2.551978	-0.60864
32	N	-2.60243	0.743012	-0.13536
33	C	-2.59238	2.100587	-0.48466
34	C	-1.01629	3.871496	-0.9513
35	C	-3.68511	2.927143	-0.69328
36	C	-2.10992	4.720042	-1.16599
37	H	-0.00196	4.246815	-1.05578
38	C	-3.41885	4.254265	-1.0387
39	H	-4.69199	2.539986	-0.5874
40	H	-1.93415	5.756398	-1.43751

41	H	-4.24726	4.934336	-1.21146
42	C	-3.76958	-0.06459	0.065287
43	C	-4.21488	-0.91799	-0.99405
44	C	-4.22198	-0.31224	1.400654
45	C	-5.13135	-1.89939	-0.74219
46	C	-5.13826	-1.29698	1.6403
47	H	-3.85217	0.303321	2.216445
48	C	-5.63768	-2.12823	0.581661
49	H	-5.50701	-1.45787	2.648936
50	H	-3.83966	-0.76341	-2.00229
51	H	-5.49513	-2.52062	-1.55517
52	C	-6.57371	-3.14433	0.83572
53	N	-7.35309	-3.99213	1.047442

The geometry of pCzBN in triplet excited state				
1	6	5.990975	1.706815	1.969016
2	6	4.683371	2.169893	2.191161
3	6	3.58338	1.551319	1.599738
4	6	3.823502	0.454545	0.767369
5	6	5.13495	-0.03636	0.547039
6	6	6.221937	0.602203	1.153372
7	1	6.827075	2.211844	2.443995
8	1	4.521704	3.025408	2.841152
9	1	2.576229	1.906534	1.79026
10	1	7.232771	0.236307	0.993888
11	6	3.631756	-1.36168	-0.58827
12	6	3.171443	-2.37287	-1.43601
13	6	4.116282	-3.23361	-1.99164
14	6	5.487044	-3.09072	-1.71929
15	6	5.941018	-2.07005	-0.88837
16	6	5.012872	-1.19226	-0.31789
17	1	2.116796	-2.48344	-1.6642
18	1	3.781777	-4.02888	-2.65203
19	1	6.197713	-3.77959	-2.16664
20	1	7.002925	-1.95189	-0.68959
21	7	2.911803	-0.35652	0.075579
22	6	1.508106	-0.17962	0.041077
23	6	0.656134	-1.26383	0.33666
24	6	0.969414	1.0689	-0.30606
25	6	-0.72741	-1.12768	0.29833
26	1	1.094848	-2.21924	0.603457
27	6	-0.41213	1.226588	-0.32422
28	1	1.631754	1.882492	-0.58366
29	6	-1.25622	0.132252	-0.00312
30	1	-1.36882	-1.97746	0.5
31	6	-1.27983	2.337636	-0.67453
32	7	-2.59581	0.526497	-0.12406
33	6	-2.61126	1.876416	-0.53165
34	6	-1.04214	3.658433	-1.05378
35	6	-3.7057	2.725347	-0.71499
36	6	-2.13161	4.502317	-1.27813
37	1	-0.02659	4.028759	-1.16356
38	6	-3.44481	4.039628	-1.10281

39	1	-4.7207	2.384179	-0.54778
40	1	-1.9612	5.532311	-1.57694
41	1	-4.27738	4.719182	-1.25953
42	6	-3.71336	-0.26762	0.125332
43	6	-4.83764	-0.27254	-0.79465
44	6	-3.77139	-1.11308	1.304127
45	6	-5.91571	-1.06272	-0.57033
46	6	-4.85698	-1.8851	1.55404
47	1	-2.96067	-1.06291	2.024231
48	6	-5.99	-1.91092	0.622989
49	1	-4.91815	-2.47979	2.459257
50	1	-4.7709	0.313781	-1.70552
51	1	-6.73417	-1.09828	-1.28148
52	6	-7.09846	-2.71183	0.865172
53	7	-8.0403	-3.39259	1.070862

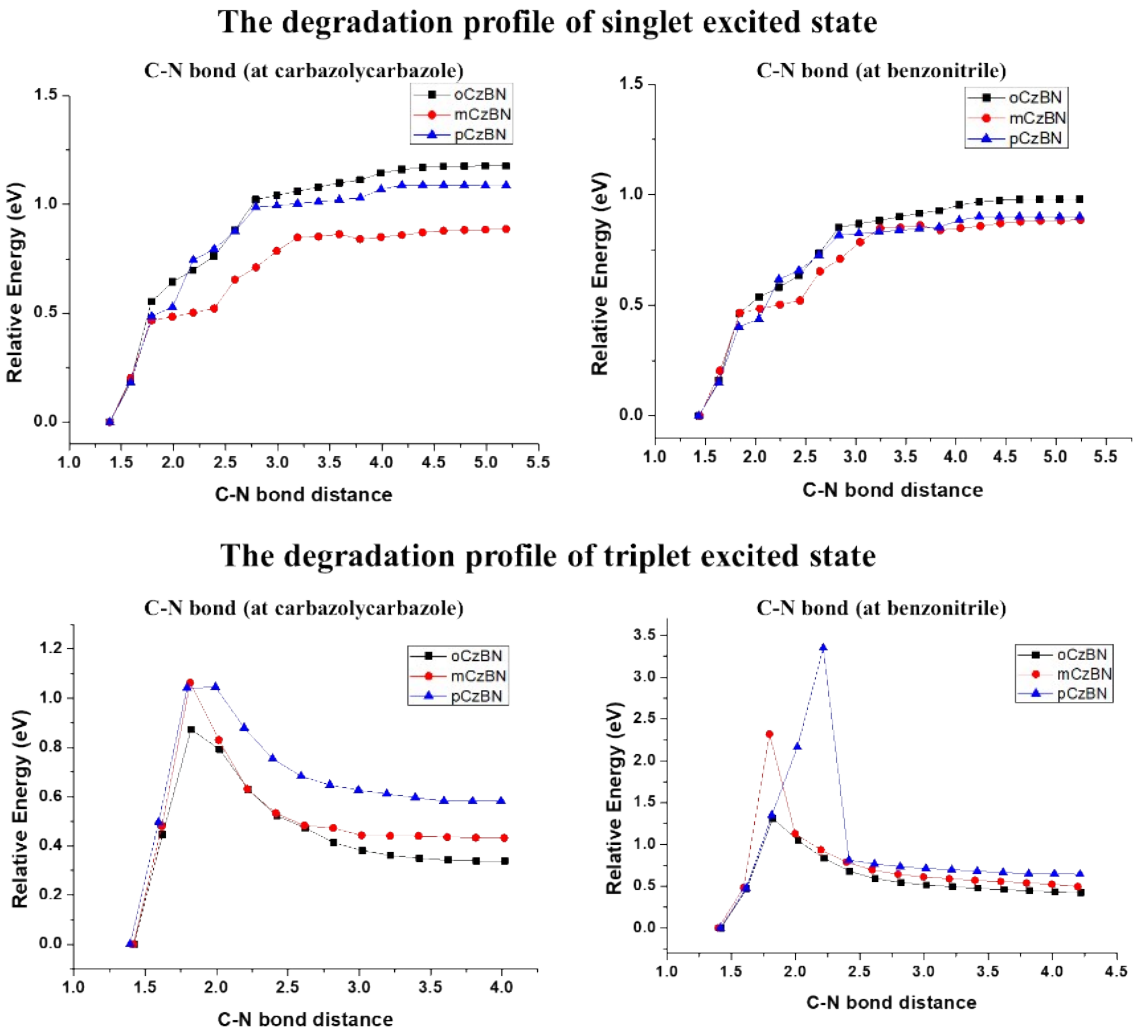


Figure S1. The degradation profiles of singlet and triplet excited states.

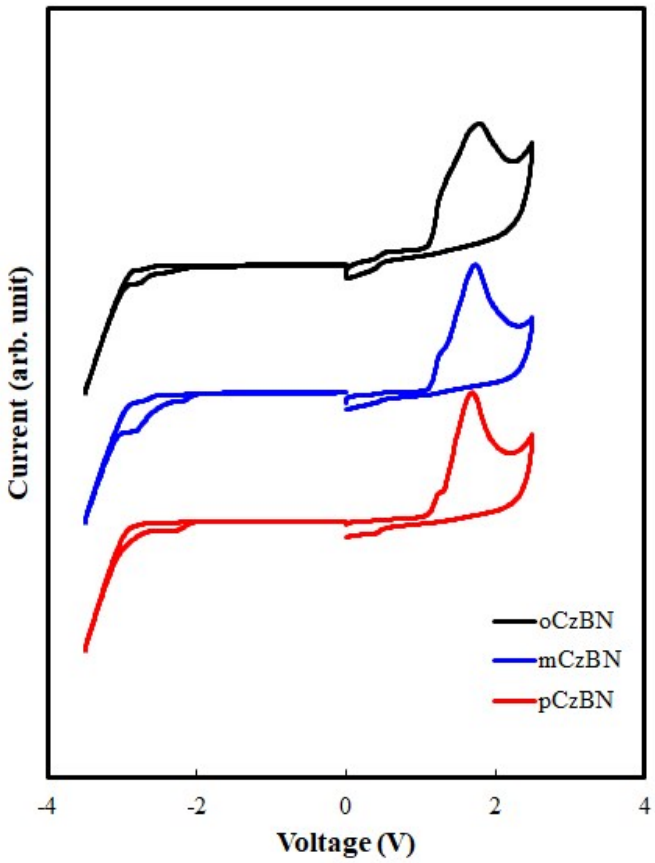


Figure S2. Cyclic voltammetry (CV) data of the hosts.

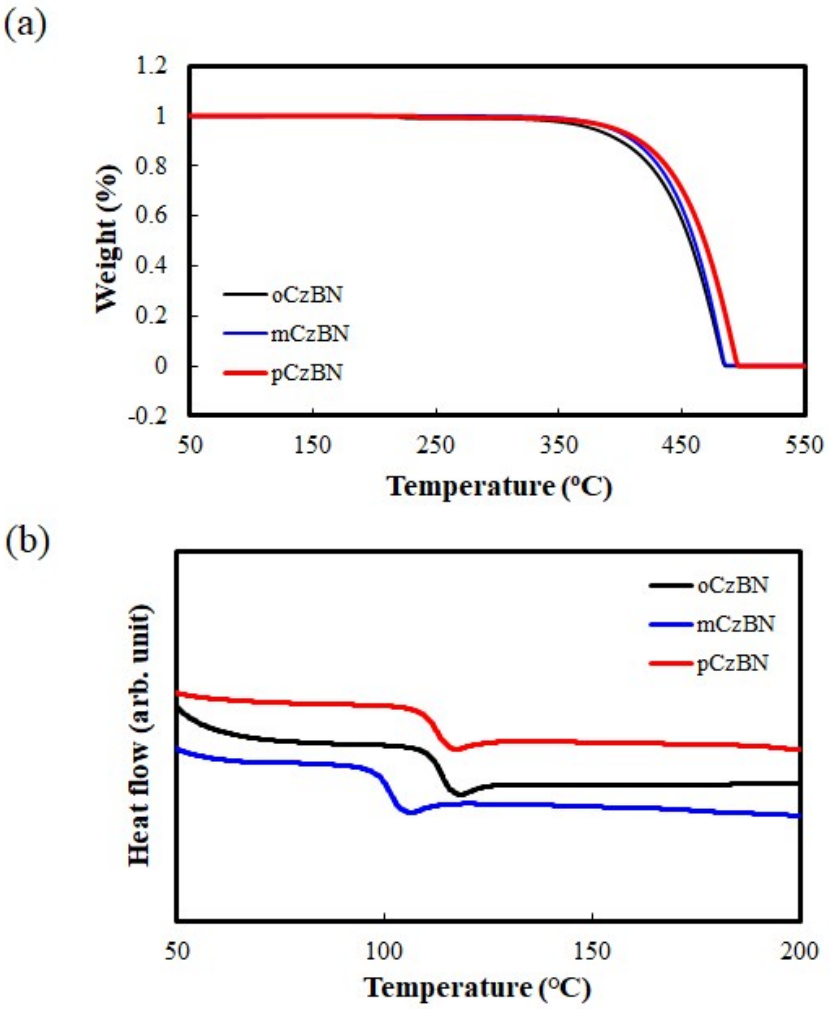


Figure S3. (a) Thermogravimetric analysis data of oCzBN, mCzBN, pCzBN at a heating rate of 10 ℃/min in nitrogen atmosphere. and (b) DSC thermograms of oCzBN, mCzBN, pCzBN at a heating rate of 10 ℃/min in nitrogen atmosphere.

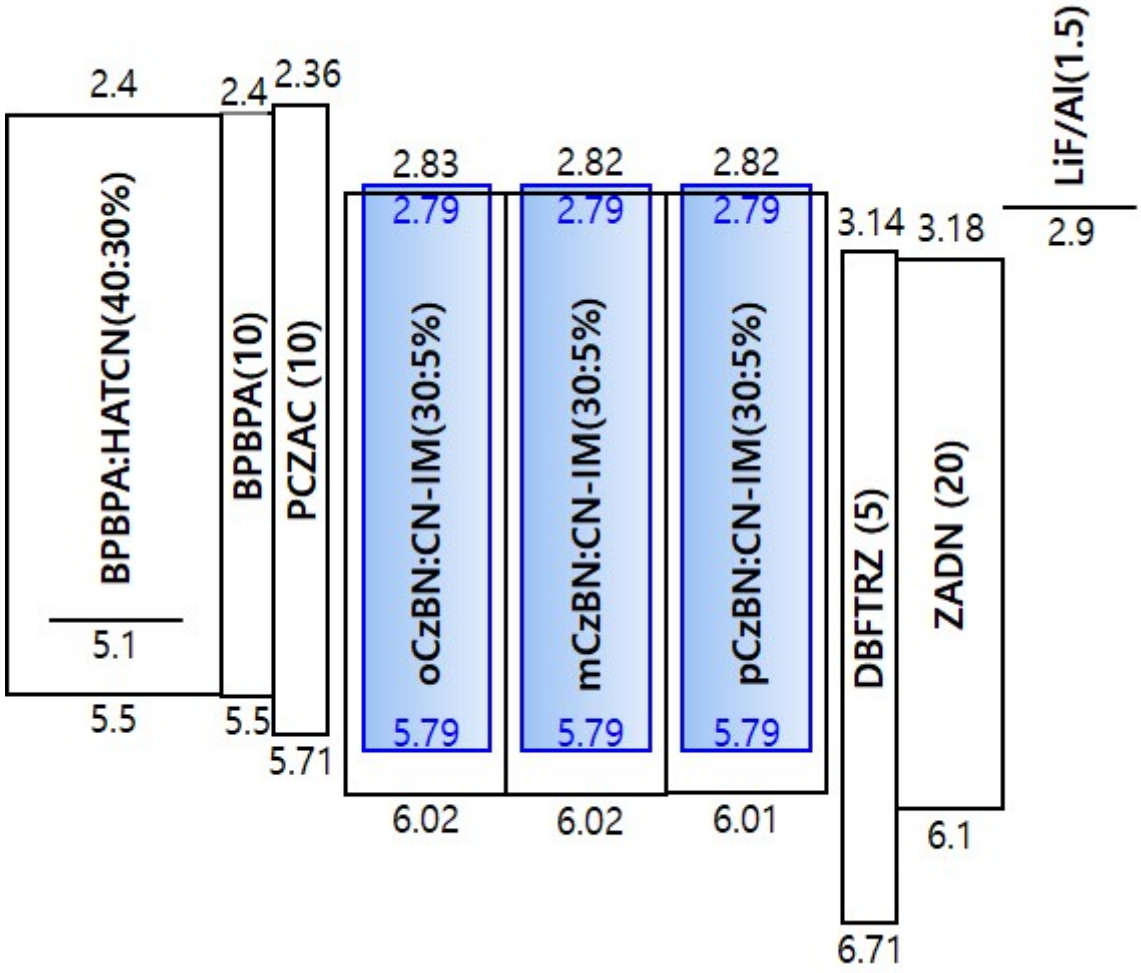


Figure S4. Blue PhOLEDs device structure.

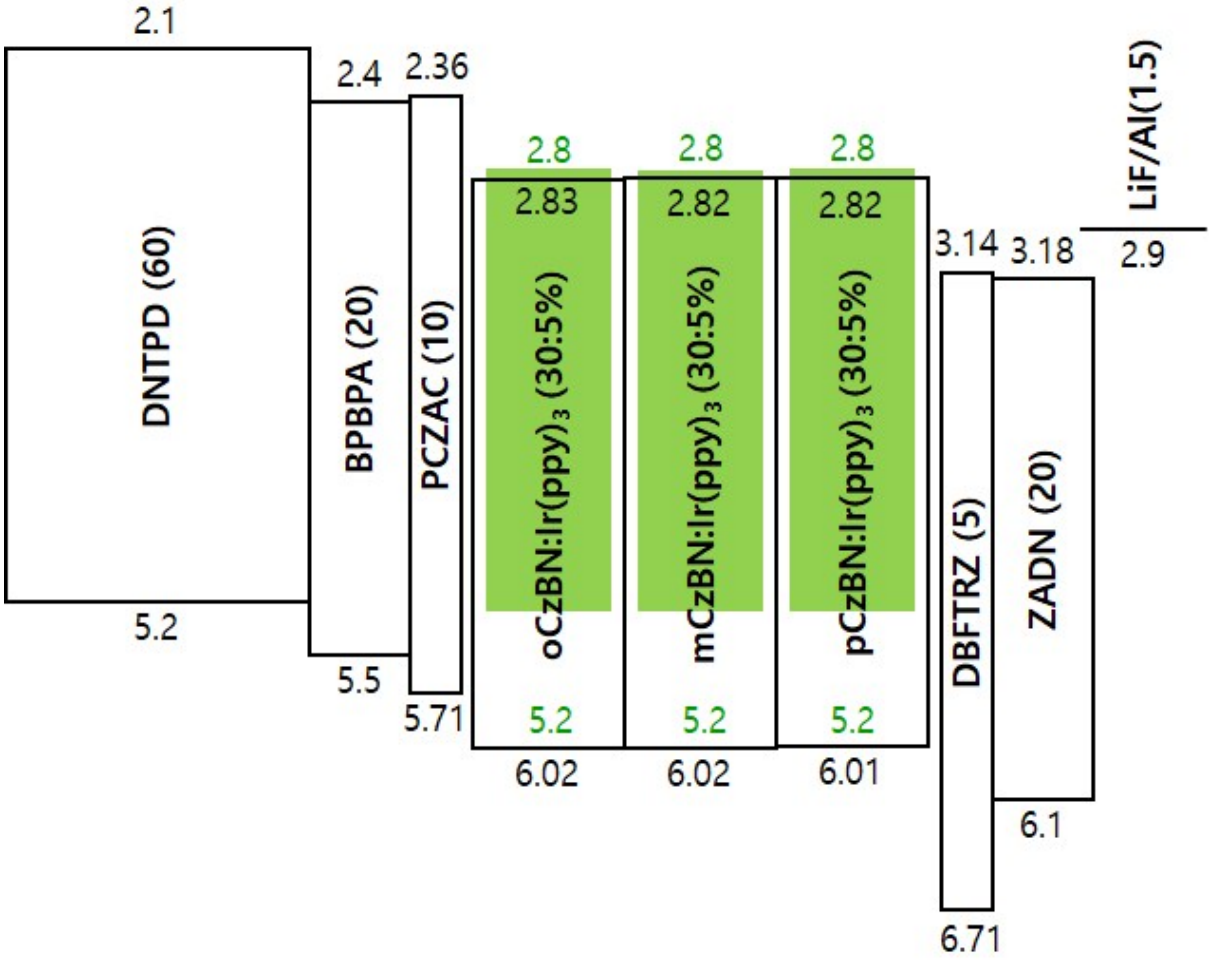
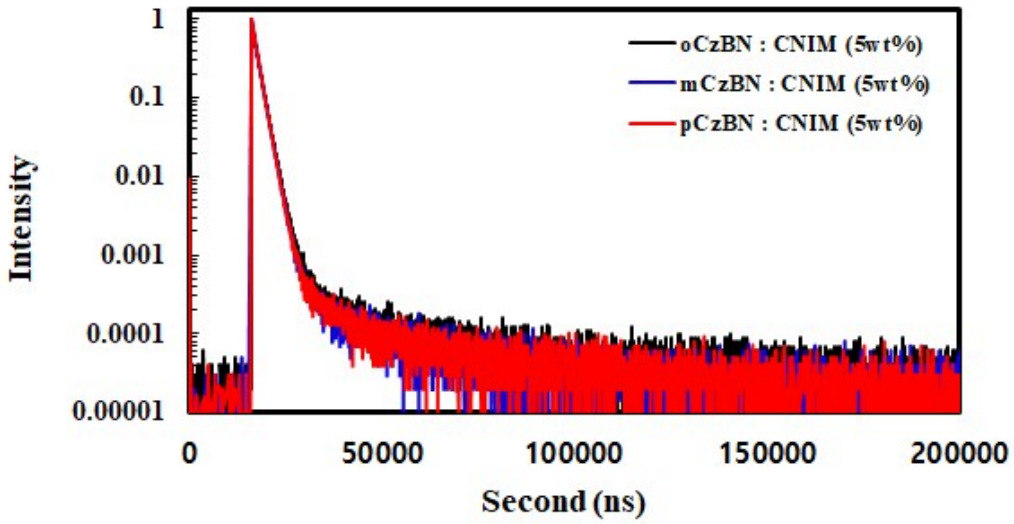


Figure S5. Green PhOLEDs device structure



Name	Excited state lifetime (μs)
oCzBN	1.52
mCzBN	1.52
pCzBN	1.52

Figure S6. Transient PL spectra of the CNIM 5 doped oCzBN, mCzBN and pCzBN film at 5% doping concentration. The data were collected at room temperature.

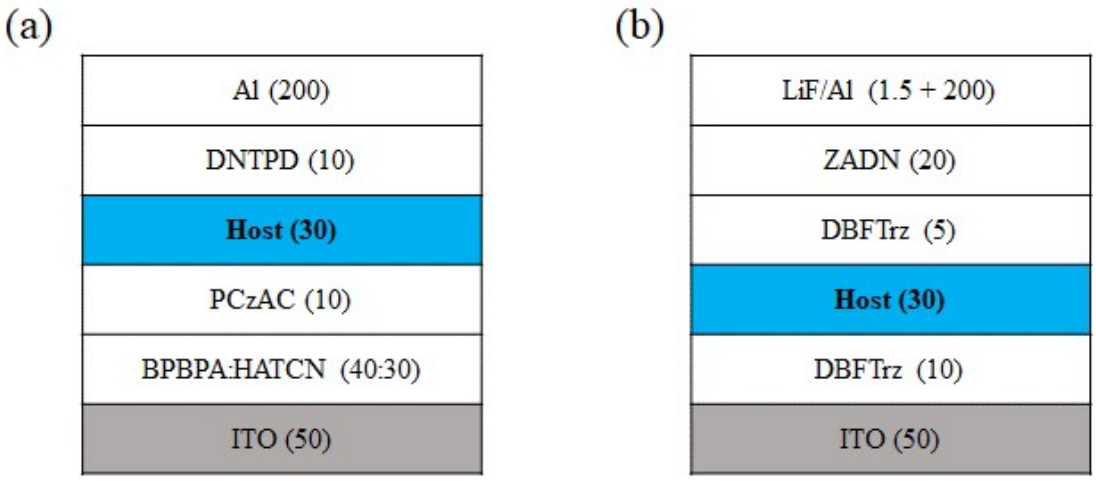


Figure S7. (a) HOD device structure and (b) EOD device structure