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Supporting Information

Azasiline-Based Thermally Activated Delayed Fluorescence Emitters for Blue Organic Light Emitting Diodes

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1. DFT Calculation

Table S1. DFT Geometry of DTPPDDA

Si	-6.73461	0.052267	-0.05573
N1	7.021699	-1.16331	-0.03585
N2	8.99982	0.144036	-0.06995
N3	6.881423	1.203462	0.050663
N4	-3.71138	-0.62441	0.392394
C1	0.544733	-0.3747	0.248398
C2	-0.08906	-1.42846	0.930666
C3	-1.47785	-1.5189	0.983724
C4	-2.27265	-0.55332	0.355547
C5	-1.65654	0.499668	-0.32508
C6	-0.26709	0.586172	-0.37795
C7	2.024252	-0.28231	0.192012
C8	2.81947	-1.43828	0.095907
C9	4.205545	-1.35521	0.044829
C10	4.848021	-0.10822	0.086012
C11	4.062249	1.050626	0.180416
C12	2.676333	0.963125	0.233557
C13	6.325782	-0.01788	0.030737
C14	8.356627	-1.03366	-0.08373
C15	8.222158	1.235691	-0.00216
C16	9.172433	-2.27013	-0.15519
C17	8.886547	2.561546	0.014996
C18	8.553338	-3.53003	-0.16463
C19	9.320832	-4.69012	-0.23058
C20	10.71425	-4.60755	-0.2883
C21	11.33736	-3.35713	-0.2795
C22	10.57301	-2.19494	-0.21329
C23	10.2864	2.654765	-0.03382
C24	10.90891	3.900353	-0.01831
C25	10.14303	5.06704	0.045843
C26	8.749399	4.982023	0.094721
C27	8.123496	3.738102	0.079504
C28	-3.60851	0.274346	2.662249
C29	-4.21007	0.823153	3.789151
C30	-5.58157	1.079871	3.816425

C31	-6.32836	0.800197	2.676782
C32	-5.74999	0.271763	1.508827
C33	-4.36429	-0.03092	1.509269
C34	-4.34882	-1.38007	-0.63172
C35	-3.58084	-2.28933	-1.39164
C36	-4.16667	-3.06989	-2.38184
C37	-5.53431	-2.98475	-2.64653
C38	-6.29344	-2.0791	-1.91293
C39	-5.73073	-1.2527	-0.92398
C40	-6.76934	1.658002	-1.06255
C41	-8.50353	-0.51398	0.28739
C42	-6.83301	2.912479	-0.42769
C43	-6.88272	4.096858	-1.16468
C44	-6.86593	4.052547	-2.56005
C45	-6.79578	2.820132	-3.21194
C46	-6.746	1.638876	-2.46944
C47	-8.73877	-1.66685	1.062518
C48	-10.0345	-2.10844	1.328518
C49	-11.1301	-1.40419	0.822553
C50	-10.9216	-0.25988	0.052446
C51	-9.62147	0.178548	-0.21056
H1	0.512265	-2.171	1.44705
H2	-1.95519	-2.33377	1.520434
H3	-2.27522	1.242197	-0.82017
H4	0.19382	1.396136	-0.93557
H5	2.342412	-2.41208	0.033048
H6	4.807675	-2.25282	-0.03728
H7	4.554247	2.015657	0.221442
H8	2.089531	1.871422	0.335985
H9	7.471596	-3.58226	-0.11936
H10	8.832005	-5.66059	-0.23706
H11	11.31205	-5.5138	-0.33982
H12	12.42089	-3.28818	-0.3242
H13	11.0457	-1.21951	-0.20551
H14	10.87036	1.742934	-0.08351
H15	11.99314	3.962026	-0.05632
H16	10.63025	6.038524	0.057763
H17	8.149913	5.886973	0.144614
H18	7.042979	3.660021	0.116556

H19	-2.5454	0.073889	2.687211
H20	-3.59482	1.038382	4.659304
H21	-6.05333	1.495048	4.702404
H22	-7.39795	1.000388	2.681423
H23	-2.52047	-2.39811	-1.20459
H24	-3.54227	-3.76189	-2.94154
H25	-5.99377	-3.60504	-3.41073
H26	-7.36049	-1.99843	-2.11082
H27	-6.83232	2.968046	0.658709
H28	-6.92977	5.053653	-0.65035
H29	-6.90191	4.973847	-3.13612
H30	-6.77486	2.778597	-4.29824
H31	-6.67643	0.689005	-2.99488
H32	-7.89792	-2.22731	1.465824
H33	-10.1909	-3.00065	1.929782
H34	-12.1409	-1.74697	1.028952
H35	-11.77	0.292733	-0.34375
H36	-9.47577	1.073044	-0.81074

Table S2. DFT Geometry of BDAPM

Si1	-7.7094	0.728404	-0.01854
Si2	7.769965	0.673088	0.014688
O	0.086623	-4.64758	-0.34654
N1	-5.36186	-1.3225	0.180392
N2	4.8221	-0.39333	0.294127
C1	-0.02875	-3.44379	-0.14744
C2	1.199502	-2.58885	-0.02914
C3	1.256531	-1.43409	0.767112
C4	2.445839	-0.71682	0.885738
C5	3.591191	-1.13491	0.199073
C6	3.543816	-2.29049	-0.58811
C7	2.361856	-3.01742	-0.68898
C8	-2.98762	-1.02512	-0.31885
C9	-1.68208	-1.51066	-0.38593
C10	-1.39655	-2.83693	-0.02887
C11	-2.44954	-3.6714	0.380665
C12	-3.74931	-3.18402	0.46226

C13	-4.02541	-1.85406	0.113754
C14	-5.09966	-1.14918	2.604397
C15	-5.50476	-0.67468	3.847165
C16	-6.6138	0.163776	3.96678
C17	-7.28926	0.536407	2.809035
C18	-6.89099	0.100321	1.532958
C19	-5.79173	-0.78876	1.428433
C20	-6.17039	-1.45402	-0.985
C21	-5.81923	-2.41633	-1.95564
C22	-6.59408	-2.59775	-3.09585
C23	-7.7476	-1.84071	-3.30538
C24	-8.09131	-0.8815	-2.35819
C25	-7.31593	-0.64931	-1.20814
C26	-6.91588	2.353876	-0.5838
C27	-9.56813	0.971582	0.204216
C28	-6.4713	3.308677	0.349826
C29	-5.91066	4.519078	-0.06141
C30	-5.77755	4.800342	-1.42246
C31	-6.20403	3.865068	-2.36704
C32	-6.76427	2.656266	-1.9498
C33	-10.3722	-0.10151	0.6367
C34	-11.7482	0.04765	0.806602
C35	-12.3542	1.279438	0.546388
C36	-11.578	2.356425	0.1178
C37	-10.1998	2.201817	-0.05054
C38	5.203784	-1.54135	2.416557
C39	6.00356	-1.86767	3.505843
C40	7.309768	-1.38732	3.605089
C41	7.801032	-0.59563	2.572662
C42	7.032121	-0.26793	1.441176
C43	5.691014	-0.72393	1.372684
C44	4.989574	0.692612	-0.61143
C45	3.875223	1.145715	-1.35205
C46	3.981998	2.22386	-2.22333
C47	5.192984	2.897736	-2.38444
C48	6.298537	2.444545	-1.67276
C49	6.236637	1.339186	-0.80526
C50	8.713739	-0.48339	-1.15341
C51	8.919055	2.054268	0.59741

C52	9.420132	-1.59684	-0.66156
C53	10.13742	-2.43598	-1.51578
C54	10.16202	-2.18032	-2.88802
C55	9.463131	-1.08578	-3.40012
C56	8.746576	-0.25067	-2.54102
C57	8.470277	2.987537	1.552512
C58	9.291446	4.025354	1.99183
C59	10.58634	4.154259	1.482827
C60	11.05263	3.241494	0.536538
C61	10.22608	2.202871	0.100691
H1	0.379318	-1.10641	1.315532
H2	2.495242	0.170409	1.509935
H3	4.439996	-2.60985	-1.11132
H4	2.317916	-3.92665	-1.27958
H5	-3.21314	-0.00227	-0.60454
H6	-0.89045	-0.85999	-0.74256
H7	-2.22668	-4.70429	0.627476
H8	-4.56152	-3.82661	0.789421
H9	-4.24662	-1.81365	2.555469
H10	-4.95047	-0.97963	4.73131
H11	-6.93824	0.522458	4.939345
H12	-8.15316	1.193429	2.886812
H13	-4.94316	-3.03719	-1.81843
H14	-6.29484	-3.35244	-3.81882
H15	-8.35999	-1.99263	-4.18951
H16	-8.98715	-0.28289	-2.51031
H17	-6.55289	3.101065	1.414515
H18	-5.57373	5.239916	0.67955
H19	-5.33902	5.741312	-1.7452
H20	-6.09672	4.074788	-3.42848
H21	-7.07796	1.933886	-2.70008
H22	-9.91679	-1.06764	0.843706
H23	-12.3482	-0.79486	1.141373
H24	-13.4269	1.397705	0.677975
H25	-12.044	3.317389	-0.08571
H26	-9.60874	3.050856	-0.38434
H27	4.191024	-1.92105	2.387949
H28	5.589235	-2.4964	4.289962
H29	7.929739	-1.63046	4.463128

H30	8.818958	-0.21599	2.635361
H31	2.912803	0.663304	-1.24431
H32	3.099133	2.544148	-2.77096
H33	5.272575	3.74986	-3.0532
H34	7.250837	2.957874	-1.79083
H35	9.401687	-1.82092	0.402632
H36	10.67293	-3.29136	-1.11122
H37	10.71805	-2.83405	-3.55535
H38	9.471219	-0.88539	-4.46873
H39	8.195499	0.587932	-2.96079
H40	7.465325	2.900622	1.96017
H41	8.923541	4.733357	2.730331
H42	11.22808	4.96272	1.824148
H43	12.05971	3.335876	0.137942
H44	10.60472	1.498008	-0.63512

Table S3. DFT Geometry of SPDDA

S	0.000044	4.308424	-5.3E-05
Si1	7.262044	-1.0304	0.005511
Si2	-7.26207	-1.03038	-0.00545
O1	0.200832	5.022138	1.271021
O2	-0.20079	5.022166	-1.27111
N1	4.754059	0.685915	-0.7242
N2	-4.75398	0.685908	0.724012
C1	-1.41224	3.208855	0.222862
C2	-2.16962	2.834218	-0.88775
C3	-3.26955	1.996503	-0.70798
C4	-3.60824	1.542029	0.570535
C5	-2.84347	1.934632	1.677121
C6	-1.74239	2.771889	1.50753
C7	3.269756	1.996655	0.707788
C8	2.169831	2.834372	0.887583
C9	1.412378	3.208944	-0.22301
C10	1.74246	2.771919	-1.50767
C11	2.843534	1.934657	-1.67728
C12	3.608365	1.5421	-0.57072
C13	6.015966	2.644648	-1.46573

C14	7.212928	3.288703	-1.76015
C15	8.435451	2.635431	-1.5998
C16	8.430836	1.332406	-1.11269
C17	7.242552	0.659959	-0.77654
C18	6.004921	1.317802	-0.98582
C19	4.525481	-0.71997	-0.698
C20	3.219252	-1.20753	-0.91629
C21	2.957728	-2.5734	-0.92849
C22	3.982758	-3.50016	-0.73534
C23	5.269405	-3.02464	-0.50289
C24	5.566278	-1.65119	-0.45442
C25	7.443278	-0.89878	1.887016
C26	8.634356	-2.12486	-0.68939
C27	8.195952	0.134371	2.475707
C28	8.354187	0.21804	3.860272
C29	7.75655	-0.73201	4.690326
C30	6.99878	-1.76184	4.129416
C31	6.84417	-1.84052	2.744361
C32	8.692668	-2.39286	-2.07141
C33	9.697487	-3.1951	-2.61104
C34	10.67143	-3.7497	-1.77663
C35	10.63381	-3.49784	-0.40503
C36	9.624859	-2.6937	0.130633
C37	-3.21926	-1.20756	0.916266
C38	-2.95778	-2.57344	0.928594
C39	-3.98285	-3.50019	0.735568
C40	-5.26949	-3.02464	0.503092
C41	-5.56631	-1.65119	0.454487
C42	-4.52548	-0.71998	0.697962
C43	-6.00481	1.317892	0.985537
C44	-6.0158	2.644828	1.465213
C45	-7.21273	3.288978	1.759547
C46	-8.43528	2.635721	1.599349
C47	-8.43072	1.332611	1.112469
C48	-7.24247	0.66006	0.776411
C49	-8.63446	-2.12461	0.689666
C50	-7.44335	-0.89905	-1.88697
C51	-8.69336	-2.39154	2.071873
C52	-9.69817	-3.19368	2.611645

C53	-10.6715	-3.74927	1.777208
C54	-10.6333	-3.49848	0.405427
C55	-9.62438	-2.69443	-0.13039
C56	-6.84357	-1.84037	-2.74428
C57	-6.99825	-1.76185	-4.12934
C58	-7.75677	-0.73259	-4.69028
C59	-8.35509	0.217053	-3.86025
C60	-8.19679	0.133541	-2.47569
H1	-1.91317	3.214399	-1.87083
H2	-3.87964	1.69501	-1.55378
H3	-3.12435	1.587256	2.666736
H4	-1.15893	3.104064	2.359678
H5	3.8799	1.695196	1.55357
H6	1.913428	3.21461	1.870654
H7	1.158959	3.104047	-2.35981
H8	3.124343	1.587221	-2.6669
H9	5.088517	3.180494	-1.62153
H10	7.181235	4.309661	-2.13192
H11	9.369039	3.134334	-1.84314
H12	9.377194	0.81228	-0.97943
H13	2.399896	-0.52168	-1.0895
H14	1.939769	-2.91098	-1.1065
H15	3.780571	-4.56707	-0.75935
H16	6.077554	-3.73618	-0.34604
H17	8.65765	0.891755	1.846073
H18	8.939482	1.026843	4.290765
H19	7.876195	-0.66727	5.768891
H20	6.524599	-2.50093	4.770521
H21	6.238494	-2.64211	2.327112
H22	7.94232	-1.96928	-2.73573
H23	9.722178	-3.38828	-3.68059
H24	11.4557	-4.37534	-2.19539
H25	11.389	-3.92685	0.248865
H26	9.608198	-2.5068	1.201247
H27	-2.39987	-0.52173	1.089384
H28	-1.93983	-2.91104	1.106622
H29	-3.7807	-4.5671	0.759687
H30	-6.07767	-3.73617	0.346335
H31	-5.08833	3.180674	1.620892

H32	-7.18099	4.310005	2.131122
H33	-9.36884	3.134697	1.842633
H34	-9.37711	0.812492	0.979345
H35	-7.94349	-1.96715	2.736218
H36	-9.72332	-3.38602	3.681344
H37	-11.4558	-4.37484	2.196082
H38	-11.3881	-3.92825	-0.2485
H39	-9.6073	-2.50833	-1.20113
H40	-6.23731	-2.6415	-2.327
H41	-6.52354	-2.50062	-4.77042
H42	-7.87646	-0.66797	-5.76885
H43	-8.94097	1.025419	-4.29077
H44	-8.65903	0.890618	-1.84608

2. Materials and methods

All starting materials were purchased from Aldrich, TCI and Alfa Aesar. Pd catalyst was purchased from Umicore. Solvents were purified by distillation using Na or CaH_2. n-BuLi was used without further purification. ^{1}H and ^{13}C-NMR spectra were recorded using a Bruker Avance 300 MHz and Bruker 500 FT-NMR spectrometer; chemical shifts (ppm) were reported with tetramethylsilane as an internal standard. Thermal analysis was performed using a TA TGA 2100 thermogravimetric analyzer under a nitrogen atmosphere at a heating rate of 10 °C/min. Differential scanning calorimeter (DSC) was conducted under nitrogen using a TA instrument 2100 DSC. The sample was heated at 10 °C /min from 50 °C to 400 °C. UV–vis absorption spectra were measured using a Perkin-Elmer LAMBDA-900 UV spectrophotometer.

Synthesis of 10,10-dipheny-5,10-dihydrodibenzo[b,e][1,4]azasiline : The synthesis was prepared following reported literature. (*Chem. Mater. 2015, 27, 6675−6681.*)Yield: 27% (7. 5g). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 9.43 (s, 1H), 7.48-7.32 (m, 14H), 7.10-7.07 (m, 2H), 6.90-6.85 (m, 2H)

Synthesis of 2,4-diphenyl-6-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)-1,3,5-triazine *:* 10 g (25.8 mmol) of 2-(4-Bromophenyl)-4,6-diphenyl-1,3,5-triazine, 13.1 g (51.5 mmol) of bispinacolatodiboron, 7.58 g (77.3 mmol) of potassium acetate are suspended in 150 mL of N,N-dimethylformamide. 0.84 g (1.0 mmol) of 1,1-Bis(diphenylphosphino)- ferrocene-dichloro-palladium(II) is added to this suspension, and the reaction mixture is heated under reflux for 16 h. After cooling, 300 mL of ethyl acetate and 200 mL of water are added, and the organic phase is separated, washed three times with 200 mL of water, dried with $MgSO_4$ and subsequently evaporated to dryness. The crude product was purified by silica gel chromatography (hexane–methylenechloride, gradient from 1:1). Yield: 53 % (6 g).
^{1}H-NMR (300MHz, $CDCl_3$, ppm): 8.83-8.77 (m, 6H), 8.04-8.02 (d, 2H), 7.65-7.58 (m, 6H),1.42 (s, 12H).

Synthesis of 5-(4'-(4,6-diphenyl-1,3,5-triazin-2-yl)-[1,1'-biphenyl]-4-yl)-10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline *:* A mixture of 2-(4'-bromo-[1,1'-biphenyl]-4-yl)-4,6-diphenyl-1,3,5-triazine (0.5 g, 1.07 mmol), 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4] azasiline (0.38 g, 1.07 mmol), sodium-*t*-butoxide (0.31 g, 3.23 mmol), tris(*t*-butyl)phosphine (0.02 g, 0.11 mmol), $Pd_2(dba)_3$ (0.05 g, 0.05 mmol), and anhydrous toluene(10 mL) was stirred at 110 °C for 18 h under nitrogen atmosphere. After cooling to room temperature, the mixture was poured into water and then extracted with chloroform. The combined organic phase was washed with brine and dried over MgSO4. The crude product was purified by column chromatography (hexane–methylenechloride, gradient from 1:1). Yield: 43 % (0.34 g). Tm=352 °C. ^{1}H NMR (300 MHz, $CDCl_3$, δ): 8.95-8.92 (d, 2H), 8.86-8.83 (d, 4H), 8.00-7.93 (m, 4H), 7.69-7.63 (m, 12H), 7.46-7.41 (m, 8H), 7.24-7.20 (d, 2H), 7.00-6.96 (t, 2H), 6.58-6.55 (d, 2H) ; ^{13}C NMR (500 MHz, $CDCl_3$, δ):177.03, 171.74, 164.55, 149.95, 140.06, 136.27, 136.11, 135.99, 135.42, 132.59, 131.89, 130.38, 129.77, 129.64, 129.59, 129.02, 128.70, 127.93, 127.41, 120.03, 117.26, 115. 65. HR-Mass: $C_{51}H_{36}N_4Si$ calcd. 732.2709, found. 732.2710

Synthesis of 4,4'-dibromobenzophenone*:* The synthesis was prepared following reported literature. *[Trans. Mat. Res. Soc. Japan 37[3] 459-462 (2012)]* Yield: 62% (9 g). ^{1}H-NMR (300 MHz, $CDCl_3$)[ppm] δ = 7.47-7.42 (d, 4H), 7.22-7.18 (d, 4H).

Synthesis of bis(4-(10,10-diphenyldibenzo[b,e][1,4]azasilin-5(10H)-yl)phenyl)methanone : A mixture of bis(4-bromophenyl)methanone (0.7 g, 2.06 mmol), 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (1.58 g, 4.53 mmol), sodium-*t*-butoxide (0.4 g, 4.12 mmol), tris(*t*-butyl)phosphine (0.04 g, 0.21 mmol), $Pd_2(dba)_3$ (0.09 g, 0.10 mmol), and anhydrous toluene(10 mL) was stirred at 110 °C for 18 h under nitrogen atmosphere. After cooling to room temperature, the mixture was poured into water and then extracted with chloroform. The combined organic phase was washed with brine and dried over $MgSO_4$. The crude product was purified by column chromatography

(ethyl acetate/n-hexane = 7/1). Yield: 38 % (1.5 g). Tm=299 °C. ^{1}H NMR (300 MHz, $CDCl_3$, δ): 8.07-8.04 (d, 4H), 7.63-7.60 (m, 12H), 7.43-7.36 (m, 16H), 7.29 (d, 1H), 7.27-7.26 (d, 2H), 7.24(d, 1H), 7.06-7.01 (t, 4H), 6.65-6.62 (d, 4H) *;* ^{13}C NMR (500 MHz, $CDCl_3$, δ):194.78, 149.55, 148.19, 136.10, 136.06, 135.59, 134.51, 132.58, 130.41, 129.73, 128.80, 127.94, 121.22, 118.89, 118.80. HR-Mass: $C_{61}H_{44}N_2OSi_2$ calcd. 877.2060, found. 877.3060

Synthesis of 4,4'-sulfonylbis(bromobenzene) : The synthesis was prepared following reported literature. *Chem. Mater. 2015, 27, 6675−6681* Yield: 51% (5 g). ^{1}H NMR (300 MHz, $CDCl_3$, δ): 7.81-7.79 (d, 4H), 7.68-7.65 (d, 4H).

Synthesis of 5,5'-(sulfonylbis(4,1-phenylene))bis(10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline) : A mixture of 4,4'-sulfonylbis(bromobenzene) (0.7 g, 1.29 mmol), 10,10-diphenyl-5,10-dihydrodibenzo[b,e][1,4]azasiline (1.43 g, 4.10 mmol), sodium-*t*-butoxide (0.36 g, 3.72 mmol), tris(*t*-butyl)phosphine (0.04 g, 0.19 mmol), $Pd_2(dba)_3$ (0.09 g, 0.09 mmol), and anhydrous toluene(10 mL) was stirred at 110 °C for 18 h under nitrogen atmosphere. After cooling to room temperature, the mixture was poured into water and then extracted with chloroform. The combined organic phase was washed with brine and dried over $MgSO_4$. The crude product was purified by column chromatography (ethyl acetate/n-hexane = 7/1). Yield: 45 % (1.7 g). Tm=314 °C. ^{1}H NMR (300 MHz, $CDCl_3$, δ): 7.93-7.90 (d, 4H), 7.60-7.58 (d, 4H), 7.55-7.52 (d, 8H), 7.37-7.29 (m, 16H), 7.22-7.19 (d, 4H), 7.13-7.08(t, 4H), 6.81-6.78 (d, 4H) ; ^{13}C NMR (500 MHz, $CDCl_3$, 149.36, 149.29, 137.07, 136.08, 133.32, 130.41, 129.88, 129.79, 127.91, 125.45, 123.31, 122.71, 121.05. HR-Mass: $C_{60}H_{44}N_2O_2SSi_2$ calcd. 913.2540, found. 913.2747

Purification

The obtained materials were purified by sublimation for device fabrication.

Elemental Analysis data

No	Sample name	Type	Weight[mg]	N	C	H	S
	bypass	By-Pass		0	0	0	0
	blank	Blank		0	0	0	0
	s1	STD	1.296	6.539999962	72.58999634	6.059999943	7.429999828
	s2	STD	1.036	6.539999962	72.58999634	6.059999943	7.429999828
	s3	STD	1.662	6.539999962	72.58999634	6.059999943	7.429999828
	test	UNK	1.302	6.52816391	72.10095215	6.029181957	7.282568932
1	DTPPDDA	Calcd	-	7.64	83.57	4.91	0
1	DTPPDDA	UNK	0.73	7.545599937	83.14569092	4.816615582	0

No	Sample name	Type	Weight[mg]	N	C	H	S
	bypass	By-Pass		0	0	0	0
	blank	Blank		0	0	0	0
	s1	STD	1.296	6.539999962	72.58999634	6.059999943	7.429999828
	s2	STD	1.036	6.539999962	72.58999634	6.059999943	7.429999828
	s3	STD	1.662	6.539999962	72.58999634	6.059999943	7.429999828
	test	UNK	1.302	6.52816391	72.10095215	6.029181957	7.282568932
1	BDAPM	Calcd	-	3.20	83.52	5.01	0
1	BDAPM	UNK	0.75	3.208084106	83.00067139	4.843986511	0

No	Sample name	Type	Weight[mg]	N	C	H	S
	bypass	By-Pass		0	0	0	0
	blank	Blank		0	0	0	0
	s1	STD	1.296	6.539999962	72.58999634	6.059999943	7.429999828
	s2	STD	1.036	6.539999962	72.58999634	6.059999943	7.429999828
	s3	STD	1.662	6.539999962	72.58999634	6.059999943	7.429999828
	test	UNK	1.302	6.52816391	72.10095215	6.029181957	7.282568932
1	SPDDA	calcd	-	3.06	78.83	4.81	3.50
1	SPDDA	UNK	0.959	3.044113874	78.21221924	4.683484554	3.399706125

3. TGA and DSC thermograms

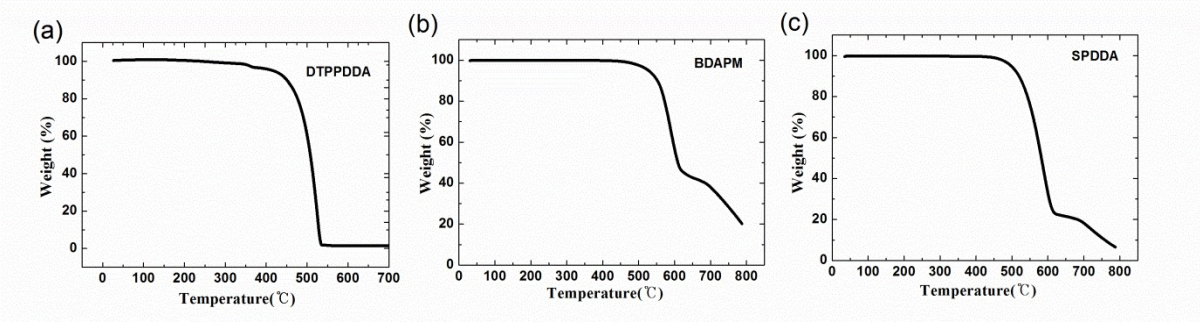

Figure S1. TGA data of (a) DTPPDDA, (b) BDAPM, and (c) SPDDA.

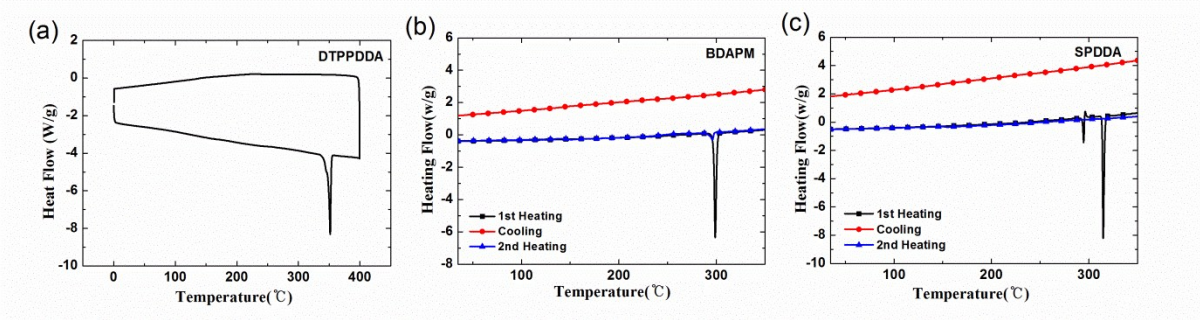

Figure S2. DSC data of (a) DTPPDDA, (b) BDAPM, and (c) SPDDA.

4. Cyclic voltammetry

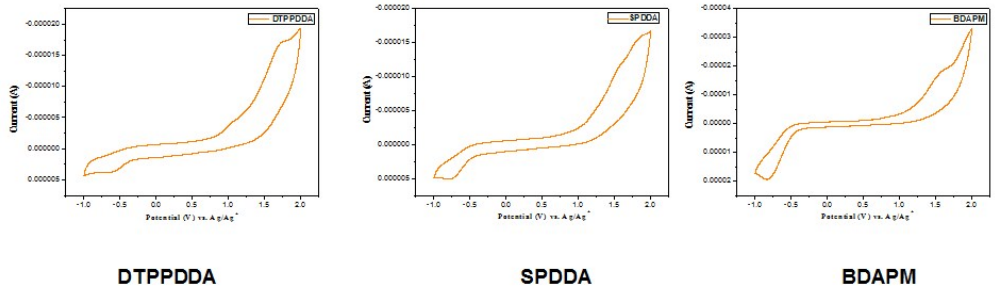

Figure S3. CV data of (a) DTPPDDA, (b) BDAPM, and (c) SPDDA

5. Max. EQEs of OLED devices in various doping ratio of the TADF emitters.

Table S4. Max. EQEs of OLED devices in various doping ratio of the TADF emitters.

Doping Ratio	Max. EQEs of the OLED devices of		
	DTPPDDA	BDAPM	SPDDA
2 wt%	3.4%	3.8%	2.3%
8 wt%	4.7%	10.2%	1.7%
16 wt%	3.2%	11.4%	1.1%

6. Calculation of theoretical EQE.

The EQE of an OLED can be expressed by the following equation,

$EQE = \gamma \times \eta_{S/T} \times q_{PL} \times \eta_{out}$

,where γ is the charge balance factor, $\eta_{S/T}$ is the singlet-triplet factor, q_{PL} is the PL quantum yield, and η_{out} is the out-coupling efficiency of the emitted light. Derivation of q_{PL} and η_{out} are explained before.(assume γ=1)[1]

$\eta_{S/T}$ can be acquired from knowing prompt, delayed and total PLQYs, efficiency of RISC and internal quantum efficiency(IQE). Prompt, delayed and total PLQYs can be achievable from experiment and calculation method of IQE was previously reported.[2]

Table S5. PLQYs and RISC efficiencies of film samples of DTPPDDA, BDAPM and SPDDA doped into mCP:TSPO1, and IQE and $\eta_{S/T}$ of the OLEDs.

Values	DTPPDDA	BDAPM	SPDDA
PLQY (prompt)	35.6%	62%	18%
PLQY (delayed)	2.4%	8%	2%
PLQY (total)	38%	70%	20%
Efficiency of RISC	3.8%	21%	2.4%
IQE	12.3%	33.3%	6.8%
$\eta_{S/T}$	0.32	0.48	0.34

7. Singlet & triplet energy levels, Experimental and calculated singlet-triplet splittings and decay rates

Table S6. Singlet(S_1) & triplet(T_1) energy levels, Experimental and calculated singlet-triplet splittings(ΔE_{ST}) and prompt(τ_p) and delayed(τ_d) decay rates.

Name	S_1 (eV)	T_1 (eV)	ΔE_{ST} (eV) (Experimental)	ΔE_{ST} (eV) (Calculated)	Decay time	
					Prompt(τ_p)	Delayed(τ_d)
DTPPDDA	2.79	2.75	0.04	0.01	6 ns	20 ns
BDAPM	2.7	2.64	0.06	0.01	134 ns	5,2 μs, 42.96 μs
SPDDA	3.0	2.93	0.07	0.02	4 ns	16 ns

8. Oscillator strength

Table S7. Oscillator strength for the materials

	DTPPDDA	**BDAPM**	**SPDDA**
Oscillator strength (f)	0.0012	0.0004	0.0011

Reference for Supporting Information

1 S. -Y. Kim, W. -I. Jeong, C. Mayr, Y. -S. Park, K. -H. Kim, J. -H. Lee, C. -K. Moon, W. Brütting, J. -J. Kim, *Adv. Funct. Mater*. 2013, **23**, 3896.

2 K. Masui, H. Nakanotani, C. Adachi, *Org. Elec*., 2013, **14**, 2721.