Supporting Information

Aromatic imide/amide-based organic small-molecule emitters for organic light-emitting diodes

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DFT Calculations

All calculations were carried out using the Gaussian 09 program.[S1] The geometries of substances were optimized using B3LYP[S2, S3]/6-31G (d, p) method. The vibrational frequency was calculated at the same level to confirm whether the optimized geometry is a minimum on the potential energy surface. The optimized geometries of **MAI, PHI, NAI** and **PDI** are shown in Table S1, S2, S3 and S4.

Table S1. Optimized geometry of **MAI**.

Atom	X	Y	Z
C	1.151485	-0.193786	-0.000145
C	0.680894	-1.622344	0.000235
C	-0.655060	-1.633274	0.000221
C	-1.148206	-0.212035	-0.000158
N	-0.005876	0.591835	-0.000139
O	2.292794	0.220011	-0.000236
O	-2.294156	0.188618	-0.000219
C	-0.019732	2.042998	0.000325
H	1.376431	-2.451134	0.000374
H	-1.336199	-2.473899	0.000350
H	1.017696	2.378478	-0.007583
H	-0.538078	2.422441	-0.884245
H	-0.524114	2.422879	0.892849

Table S2. Optimized geometry of **PHI**.

Atom	X	Y	Z
C	-0.889875	1.168249	0.000193
C	0.527809	0.697082	0.000194
C	0.525859	-0.699431	0.000183
C	-0.894059	-1.164448	0.000193
N	-1.673234	0.001945	-0.000085
O	-1.317969	2.305144	-0.000377
O	-1.332639	-2.297332	-0.000354
C	-3.124517	-0.000641	0.000212
C	1.710565	1.420946	0.000024
C	2.909666	0.696048	0.000003
C	2.907806	-0.704281	0.000007
C	1.706832	-1.426104	0.000016
H	-3.453857	1.038565	-0.020812
H	-3.505197	-0.530166	-0.877037
H	-3.506987	-0.493157	0.89827
H	1.699381	2.505929	-0.000046
H	3.856947	1.226654	-0.000028
H	3.853706	-1.237378	-0.000009
H	1.693002	-2.511079	-0.000046

Table S3. Optimized geometry of **NAI**.

Atom	X	Y	Z
C	0.729846	2.423378	0.000926
C	2.137258	2.421471	-0.01318
C	2.831408	1.232296	-0.01762
C	2.147719	-0.01051	-0.01014
C	0.721597	-0.00285	0.00094
C	0.028533	1.231936	0.003561
C	2.817724	-1.26084	-0.01417
C	2.111031	-2.44267	-0.00722
C	0.703635	-2.42965	0.005144
C	0.016238	-1.23037	0.004629
C	-1.46424	-1.23483	0.010986
N	-2.09448	0.013371	-0.10299
C	-1.45303	1.258503	0.014519
O	-2.0844	2.299463	0.134654
O	-2.11962	-2.26141	0.125675

C	-3.5595	-0.00428	-0.12958
H	0.165872	3.355053	0.009273
H	2.682345	3.364738	-0.02087
H	3.921675	1.240028	-0.02821
H	3.907846	-1.28041	-0.02412
H	2.646305	-3.39156	-0.01187
H	0.129144	-3.35492	0.013654
H	-3.91671	1.007617	-0.32247
H	-3.91084	-0.68983	-0.90714
H	-3.9415	-0.35831	0.837354

Table S4. Optimized geometry of **PDI**.

Atom	X	Y	Z
C	-2.882571	2.418841	0.000194
C	-1.483755	2.429237	0.000186
C	-0.736499	1.249695	-0.000101
C	-1.431626	-0.001394	-0.000074
C	-2.860856	-0.002741	-0.000017
C	-3.574052	1.220238	0.000045
C	-0.734024	-1.25094	0.000253
C	-1.479545	-2.431525	0.000768
C	-2.87828	-2.423527	0.000521
C	-3.57321	-1.226568	0.000053
C	0.734024	1.25094	-0.000283
C	1.431626	0.001394	0.000075
C	0.736499	-1.249695	0.000133
C	1.479545	2.431525	-0.000882
C	2.87828	2.423527	-0.000654
C	3.57321	1.226568	-0.000119
C	2.860856	0.002741	0.000018
C	3.574052	-1.220238	0.00002
C	2.882571	-2.418841	-0.000059
C	1.483755	-2.429237	-0.000069
C	5.056878	1.251444	0.000293
N	5.704497	0.006403	0.000089
C	5.0562	-1.234817	-0.000128
C	-5.056878	-1.251443	-0.000364
N	-5.704497	-0.006403	-0.000091

C	-5.0562	1.234817	0.000197
O	-5.707598	2.271095	0.000462
O	-5.690148	-2.298795	-0.000858
O	5.690147	2.298796	0.000727
O	5.707598	-2.271095	-0.000334
C	-7.171416	0.024293	-0.000019
C	7.171416	-0.024294	0.000018
H	-3.447667	3.344435	0.0004
H	-0.984853	3.390455	0.000528
H	-0.979294	-3.392035	0.001433
H	-3.441022	-3.350435	0.000675
H	0.979294	3.392035	-0.001609
H	3.441022	3.350435	-0.00087
H	3.447667	-3.344435	-0.000203
H	0.984854	-3.390455	-0.000349
H	-7.52343	-1.003927	0.000499
H	-7.529569	0.555055	0.884379
H	-7.529796	0.554014	-0.884973
H	7.523431	1.003926	-0.000564
H	7.529796	-0.553961	0.885004
H	7.529567	-0.555111	-0.884347

The abbreviations of material names mentioned in the review

ITO: indium-tin oxide

NPB: (*N*,*N*′-di(1-naphthyl)-*N*,*N*′-diphenyl-(1,1′-biphenyl)-4,4′-diamine)

BCP: 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline

α-NPD(NPD): 4,4'-bis[*N*-(1-naphthyl)-*N*-phenyl]biphenyl diamine

TPBi: 1,3,5-tris(*N*-phenylbenzimid-azole-2-yl)benzene

TPBI (1,3,5-tris(1-phenyl-1*H*-benzo[*d*]imidazol-2-yl)benzene)

mCBP: 3,3’-di(9*H*-carbazol-9-yl)biphenyl

CBP: 4,4'-bis(9-carbazolyl)-1,1'-biphenyl

HAT-CN: dipyrazino(2,3-f:2',3'-*h*)-quinoxaline-2,3,6,7,10,11-hexacarbonitrile

TAPC: 1,1-bis-[4-[*N*,*N*-di(*p*-tolyl)amino]phenyl]cyclohexane

TmPyPB: 1,3,5-tri(*m*-pyrid-3-yl-phenyl)benzene

TCTA: 4,4',4''-tris(carbazol-9-yl)triphenylamine

TcTa: (4,4',4''-tri(*N*-carbazolyl)triphenylamine)

PVK : poly(9-vynylcarbazole)

mCP: 3-bis(9-carbazolyl)benzene

TSPO1: diphenyl-4-triphenylsilylphenyl-phosphineoxide

CuPc：phthalocyanine copper

TAPC: 1,1-bis-[4-[*N*,*N*-di(*p*-tolyl)amino]phenyl]cyclohexane

3TPYMB: tris-[3-(3-pyridyl)mesityl]borane

mCPCN: 9-(3-(9*H*carbazol-9-yl)phenyl)-9*H*-carbazole-3-carbonitrile

PFO: poly(9,9-dioctylfluorene

Bphen: 4,7-diphenyl-1,10-phenanthroline

4CzTNA: 2-(4-tert-butylphenyl)-6-(9-(4-tertbutylphenyl)-9H-carbazol-3-yl)-1H-benzo[*de*]isoquinoline-1,3-(2H)-dione

CzPhONI: 6-{3,5-Bis-[9-(4-*t*-butylphenyl)-9H-carbazol-3-yl]-phenoxy}-2-(4-*t*-butylphenyl)benzo[*de*]isoquinoline-1,3-dione

References

S1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, R. E. Stratmann, J. C. Burant, S. J. Dapprich, M. A. Millam, D. K. Daniels, N. M. Kudin, C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, A. D. Malick, K. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. Pople, *Gaussian 09*, G. I. Revision A. 1-SMP, Wallingford, CT, 2009.

S2 A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange, *Journal of Chemical Physics*, 1993, **98**, 5648–5652.

S3 C. Lee, W. Yang, R. G. Parr, Development of the Colle-Salvetti correlation- formula into a functional of the electron density, *Physical Review B*, 1988, **37**, 785–789.