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Supporting Information

Electronic structure of carbazole-based phosphine oxides as ambipolar host materials for deep blue electrophosphorescence: A Density Functional Theory study

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Table S1. DFT/B3LYP-calculated frontier molecular orbital energies of pCBZ and hosts **1-3**.[a]

	pCBZ	**1**	**2**	**3**
LUMO+2	-0.54	-0.95	-0.99/-0.99	-1.03/-1.03/-1.02
LUMO+1	-0.66	-1.07	-1.26	-1.44
LUMO	-0.86	-1.23	-1.37	-1.45
HOMO	-5.50	-5.61	-5.64/-5.67	-5.67/-5.71/-5.72
HOMO-1	-5.86	-5.96	-6.00/-6.00	-6.03/-6.04/-6.04

[a] All the values are in eV.

Table S2. Comparison of experimental and computational HOMO and LUMO energy values for hosts **1-3**.[a]

	1	**2**	**3**
		LUMO	
Koopmans' theorem[b]	-1.23	-1.37	-1.45
ΔSCF[b]	-0.16	-0.43	-0.55
Expt.	-2.6[c]	-2.19[e]	-1.67[g]
		HOMO	
Koopmans' theorem[b]	-5.61	-5.64	-5.67
ΔSCF[b]	7.10	6.88	6.86
Expt.	-6.2[d]	-5.76[f]	-5.25[g]

[a] All the values are in eV. Computation results were obtained from DFT calculations using the B3LYP functional and SV(P) basis set. [b] Koopmans' theorem corresponds to HOMO/LUMO energy values and ΔSCF to IPs/EAs. [c,e-g] Experimental data were obtained via cyclic voltammetry. [c] The value is determined from reduction potential measured in DMF; see Ref. 1. [d] Estimated from reduction potential and optical band gap. Ref. 1. [e] Data obtained on the basis of reduction potential measurement in THF from Ref. 2. [f] Oxidation potential value in CH_2Cl_2. Ref. 2. [g] Oxidation/reduction potentials estimated in CH_2Cl_2 ; see Ref. 3.

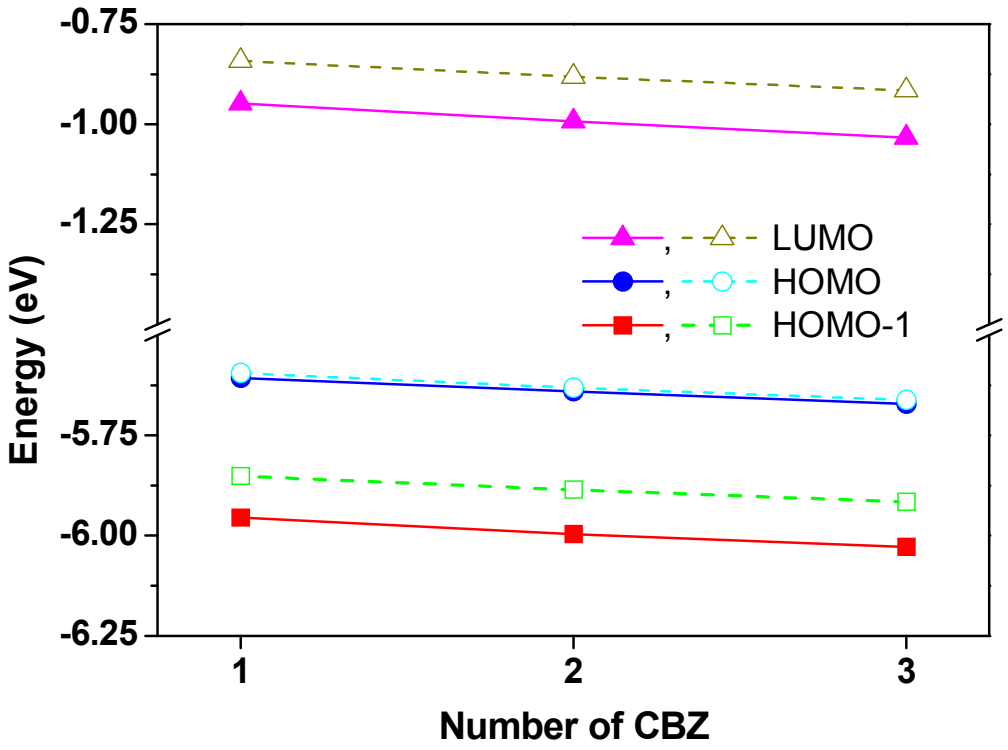

Figure S1. Evolution of the frontier molecular orbital (FMO) energis as a function of the number of carbazole (CBZ) units in the host. The closed symbols correspond to the FMOs of hosts **1-3** and the open symbols, to those of the carbazole-only systems where the triphenylphosphoryl group is removed and all carbazole units are capped with H atoms.

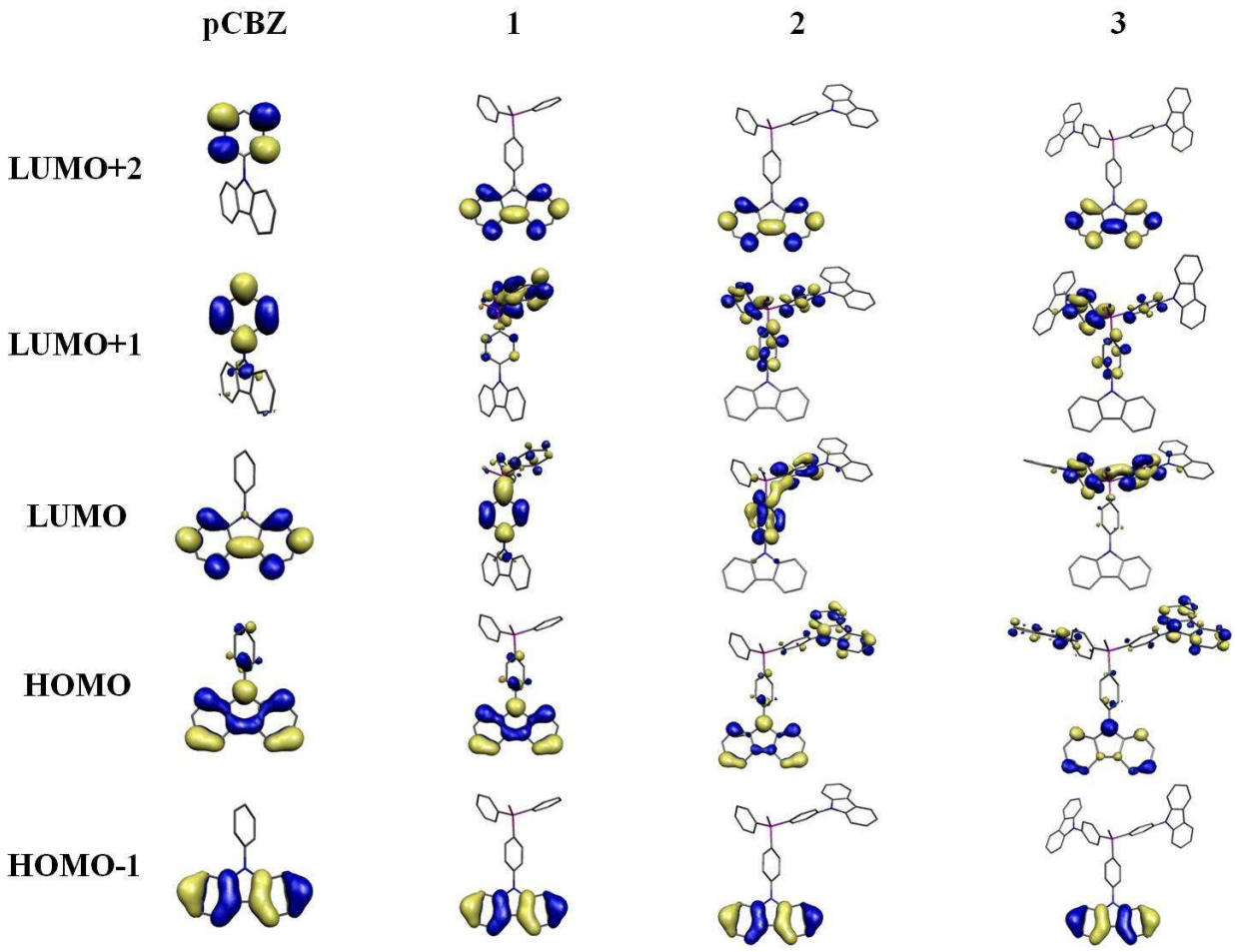

Figure S2. Illustration of frontier molecular orbitals of N-phenylcarbazole and hosts **1**-**3** in the ground state. Note that, for hosts **2** and **3**, HOMO/HOMO-1/LUMO+2 denote a set of doubly and triply (quasi-)degenerate molecular orbitals, respectively ; see Table S1.

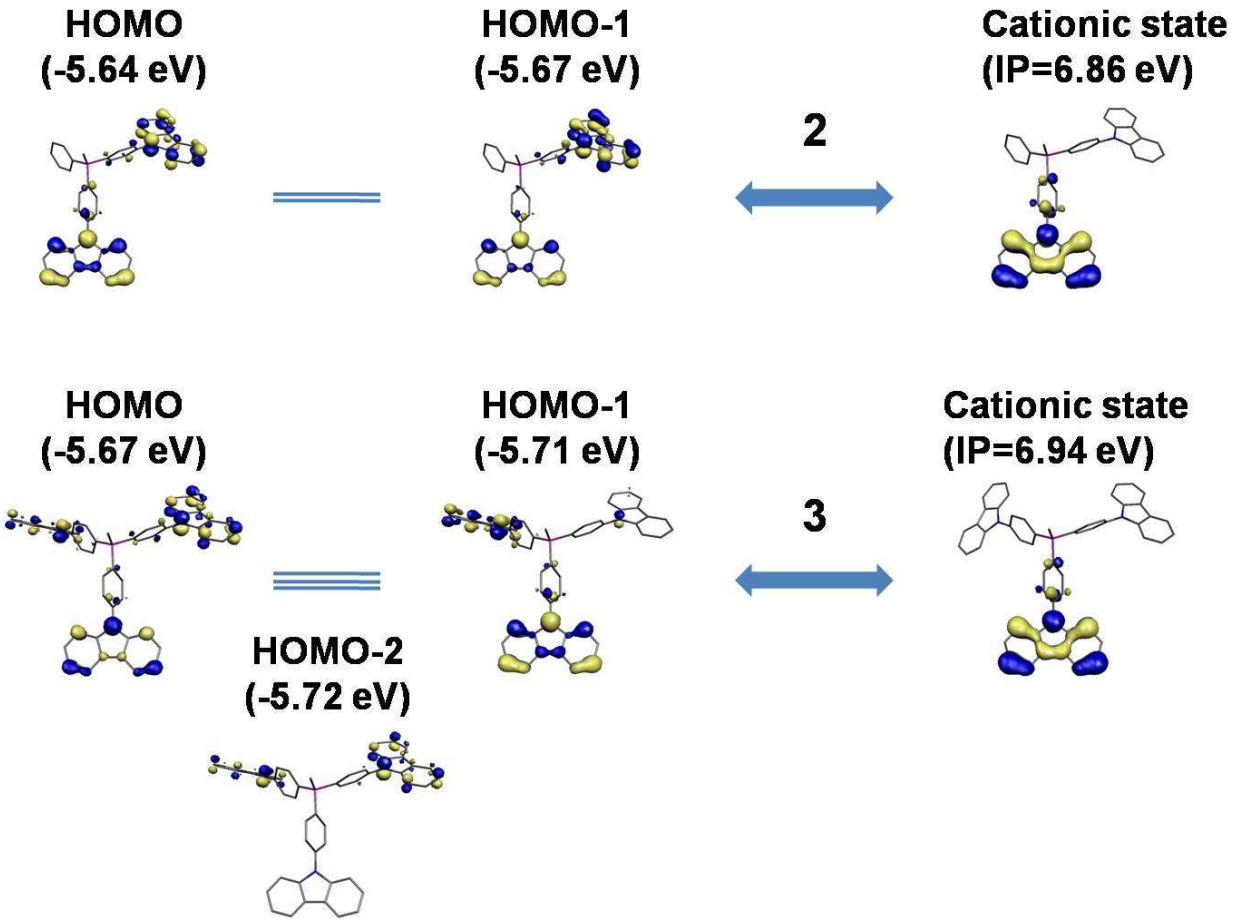

Figure S3. Illustration of the HOMOs in the ground-state (left) and cation-state (right) geometries of hosts **2** and **3**. Note that the HOMOs in the cation state of hosts **2** and **3** are localized within a single carbazole unit, while those in the neutral ground state are delocalized, which illustrates the broken-symmetry effect in the cation.

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