

Computational Design of High Triplet Energy Host Materials for Phosphorescent Blue Emitters

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Supporting Information (5 pages including this page)

Figure S1: Triplet spin density distribution of asymmetrically substituted tph-bzi based host molecules at B3LYP/6-31G* level of theory.

Figure S2: Triplet spin density distribution of asymmetrically substituted tph-pho based host molecules at B3LYP/6-31G* level of theory.

Figure S3: Triplet spin density distribution of symmetrically substituted bzi based host molecules at B3LYP/6-31G* level of theory.

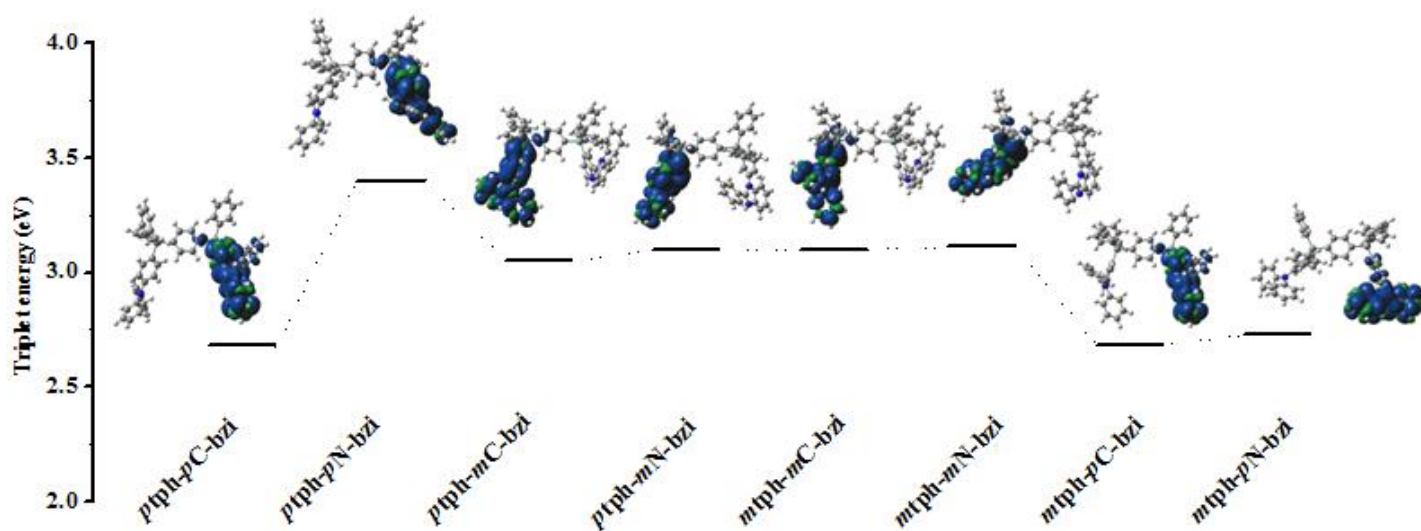
Figure S4: Triplet spin density distribution of symmetrically substituted cbz based host molecules at B3LYP/6-31G* level of theory.

Figure S5: Triplet spin density distribution of symmetrically substituted pho based host molecules at B3LYP/6-31G* level of theory.

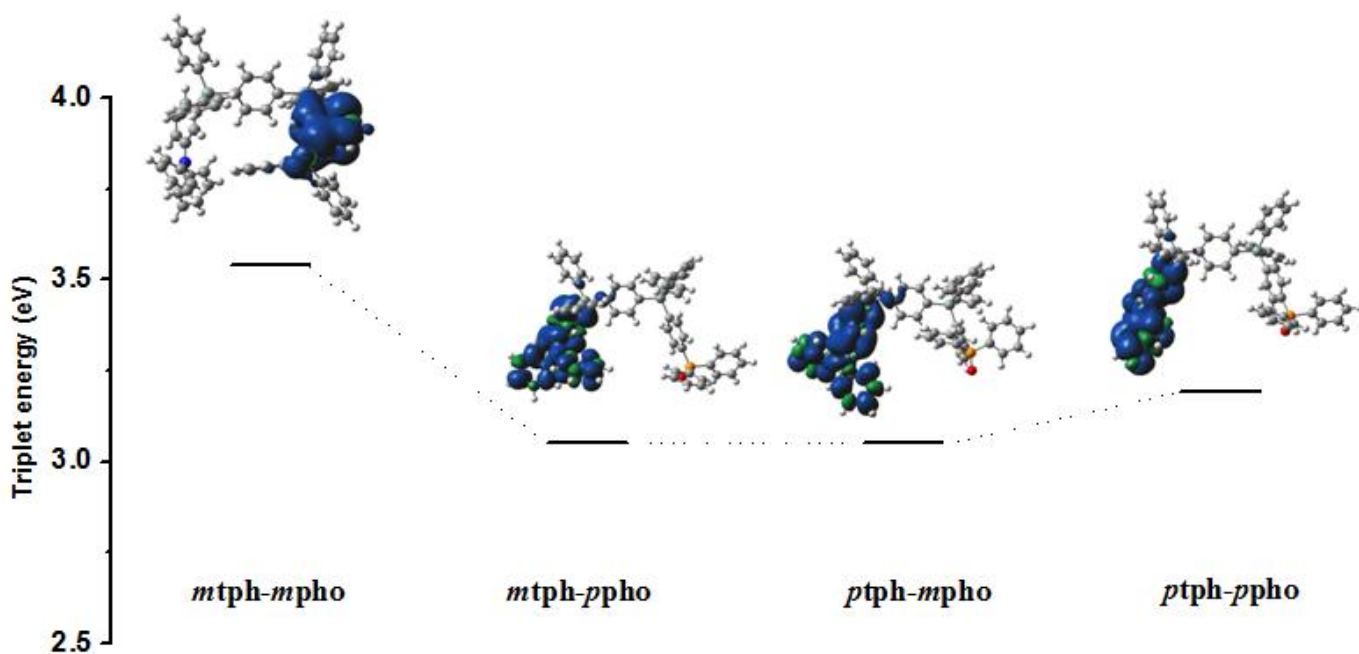
Figure S6: Triplet spin density distribution of symmetrically substituted tph based host molecules at B3LYP/6-31G* level of theory.

Figure S7: ΔE_{ST} for all the symmetrically substituted designed host molecules. ΔE_{ST} of mcp and core unit is indicated by pink dashed line and orange dot line respectively.

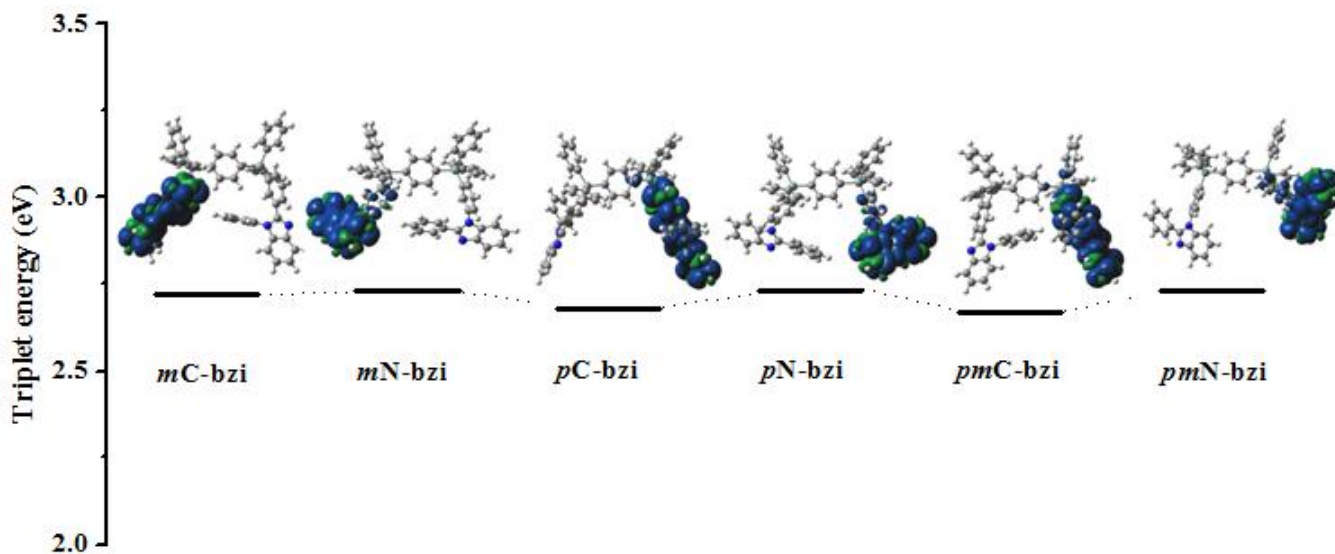
Figure S8. Total energies (in Hartree) of neutral, cation and anion hosts at their respective geometries.



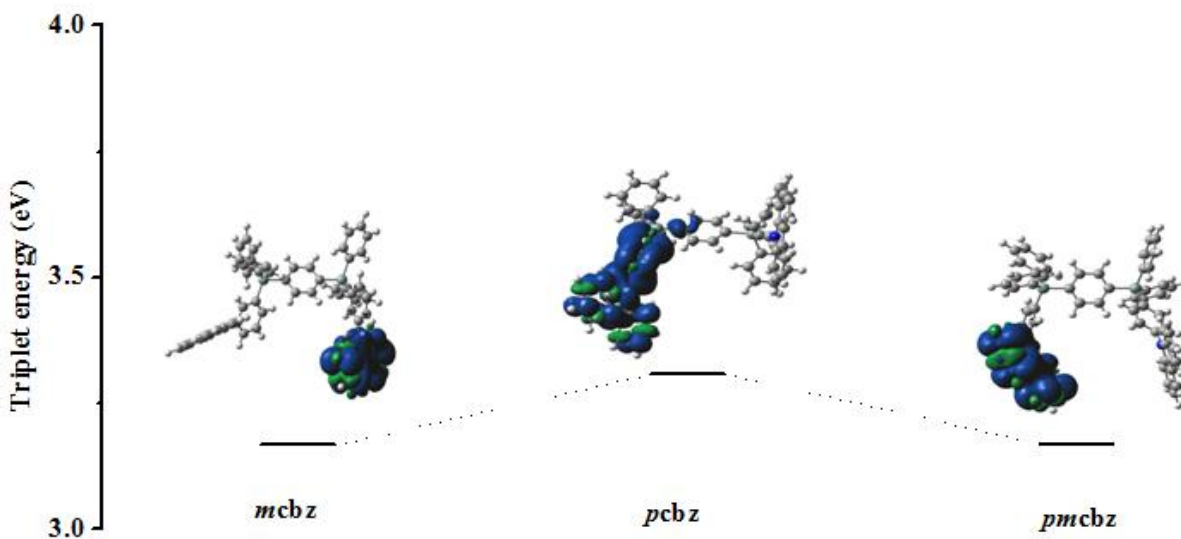
SI 1. Triplet spin density distribution of asymmetrically substituted tph-bzi based host molecules at B3LYP/6-31G* level of theory.



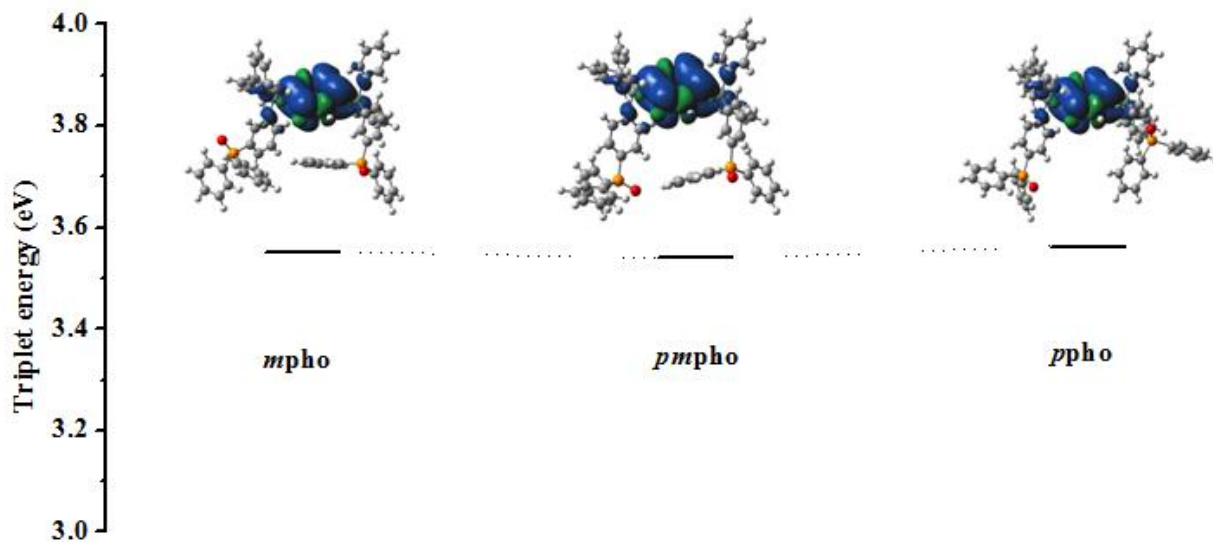
SI 2. Triplet spin density distribution of asymmetrically substituted tph-pho based host molecules at B3LYP/6-31G* level of theory.



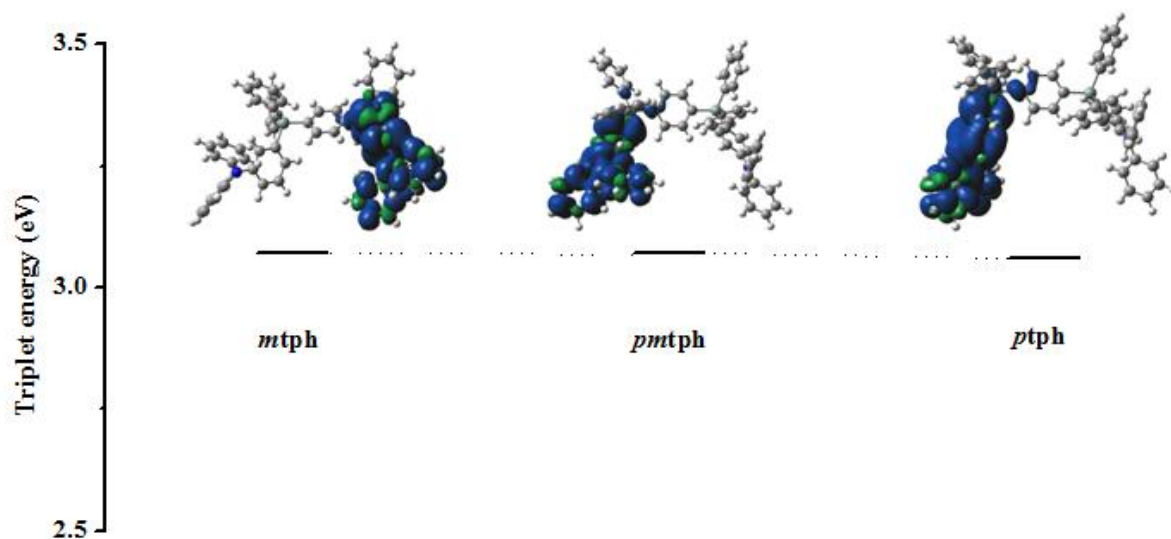
SI 3. Triplet spin density distribution of symmetrically substituted bzi based host molecules at B3LYP/6-31G* level of theory.



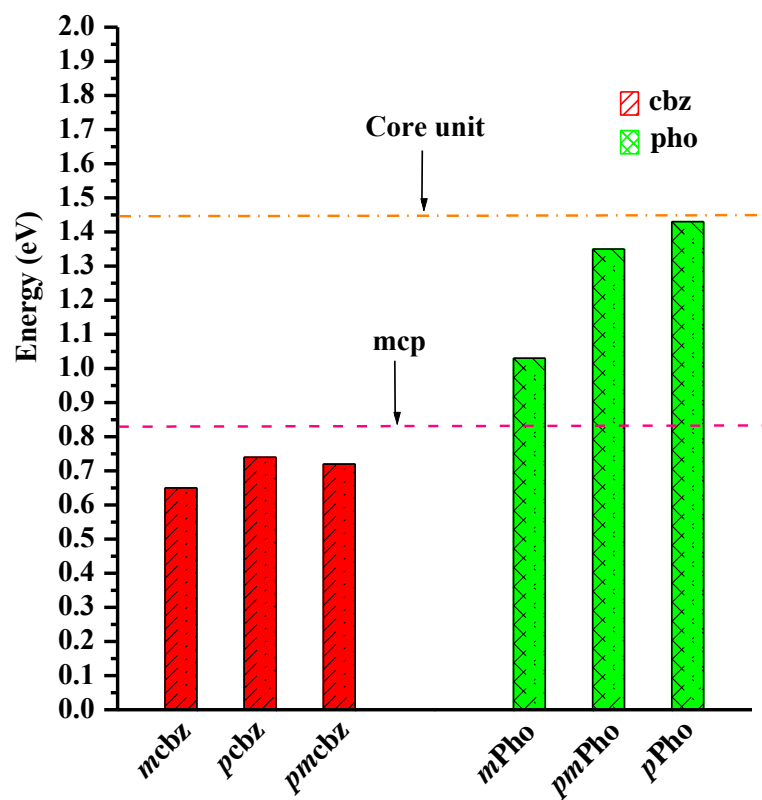
SI 4. Triplet spin density distribution of symmetrically substituted cbz based host molecules at B3LYP/6-31G* level of theory.



SI 5. Triplet spin density distribution of symmetrically substituted pho based host molecules at B3LYP/6-31G* level of theory.



SI 6. Triplet spin density distribution of symmetrically substituted tph based host molecules at B3LYP/6-31G* level of theory.



SI 7. ΔE_{ST} for all the symmetrically substituted designed host molecules. ΔE_{ST} of mcp and core unit is indicated by pink dashed line and orange dot line respectively.

SI 8. Total energies (in Hartree) of neutral, cation and anion hosts at their respective geometries.

Asymmetric systems	Neutral	Cation	Anion
cbz-bzi:			
<i>mcbz-mN-bzi</i>	-3326.003025	-3325.769035	-3326.009716
<i>mcbz-pN-bzi</i>	-3326.002468	-3325.769388	-3326.012182
<i>pcbz-mN-bzi</i>	-3326.003475	-3325.768519	-3326.009426
<i>pcbz-pN-bzi</i>	-3326.002846	-3325.768943	-3326.012303
cbz-pho:			
<i>mcbz-mpho</i>	-3595.576313	-3595.333143	-3595.581067
<i>mcbz-ppho</i>	-3595.576365	-3595.33795	-3595.582945
<i>pcbz-mpho</i>	-3595.577223	-3595.332973	-3595.58178
<i>pcbz-ppho</i>	-3595.576803	-3595.333491	-3595.583265
tph-bzi:			
<i>mtph-mC-bzi</i>	-3327.176866	-3326.95461	-3327.182362
<i>mtph-mN-bzi</i>	-3327.177788	-3326.954924	-3327.182558
<i>ptph-mN-bzi</i>	-3327.17928	-3326.955099	-3327.183208
<i>ptph-pN-bzi</i>	-3327.179764	-3326.954534	-3327.186954
tph-pho:			
<i>mtph-mpho</i>	-3596.752186	-3596.535993	-3596.754633
<i>Ptph-ppho</i>	-3596.752792	-3596.525879	-3596.758551
Symmetric systems			
cbz:			
<i>mcbz</i>	-3232.546334	-3232.319287	-3232.54794
<i>pcbz</i>	-3232.5473	-3232.318857	-3232.550055
<i>pmcbz</i>	-3232.546674	-3232.318763	-3232.548238
pho:			
<i>mpho</i>	-3958.606725	-3958.332456	-3958.611559
<i>pmpho</i>	-3958.610062	-3958.33824	-3958.61631
<i>ppho</i>	-3958.605508	-3958.332658	-3958.614472
Core unit	-2200.001659	-2199.726521	-2199.993425
<i>mcp</i>	-1264.792091	-1264.551301	-1264.780477
<i>NPD</i>	-1805.486405	-1805.280691	-1805.492849
<i>TAZ</i>	-1323.72191	-1323.480044	-1323.730992
<i>Flrpic</i>	-1895.47567	-1895.234495	-1895.5004