

## Supplementary Information

# Explore the Role of Varied-Length Spacers in the Charge Transfer: a Theoretical Investigation on the Pyrimidine-Bridged Porphyrin Dyes

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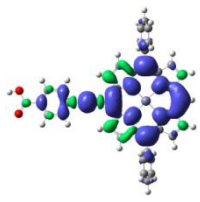
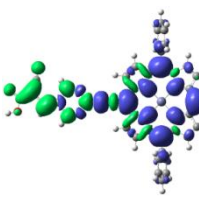
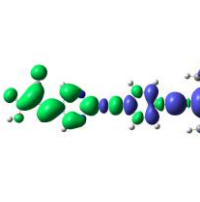
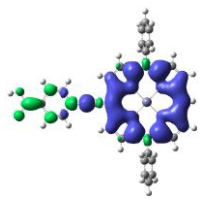
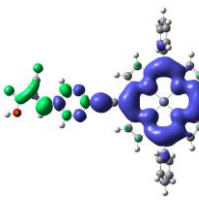
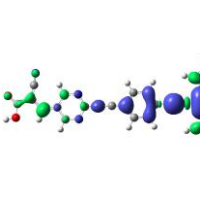
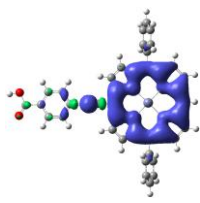
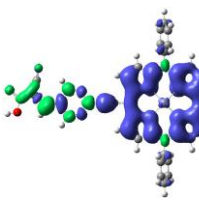
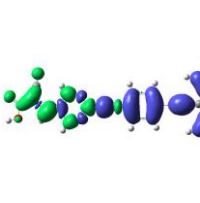
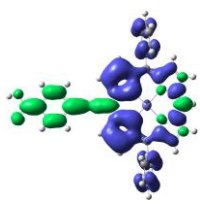
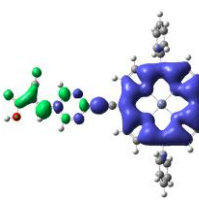
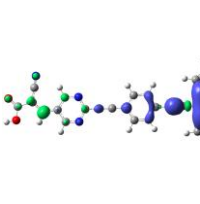
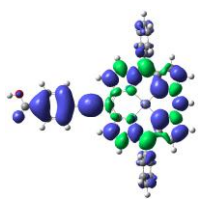
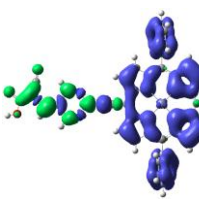
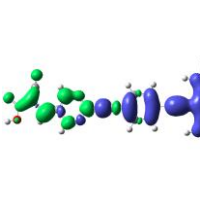
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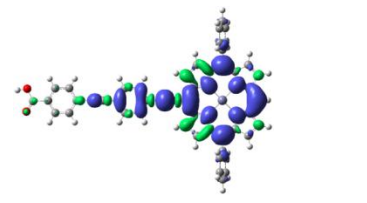
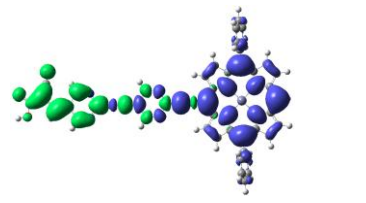
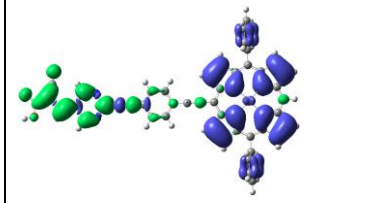
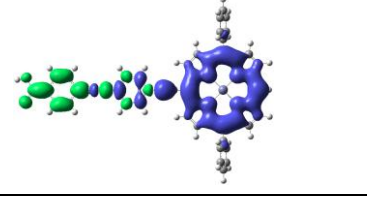
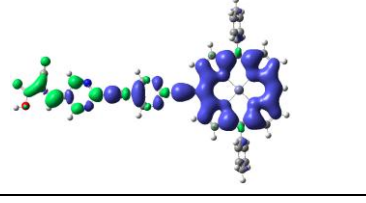
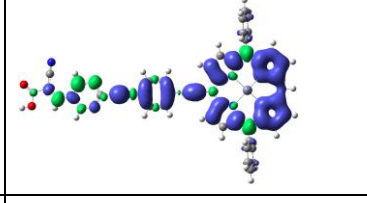
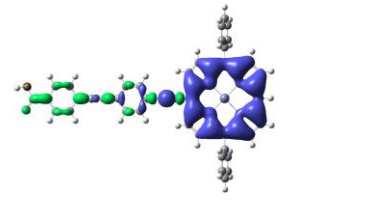
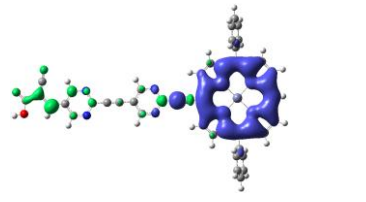
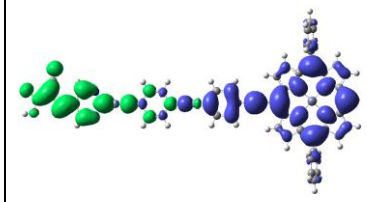
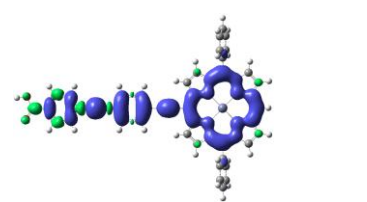
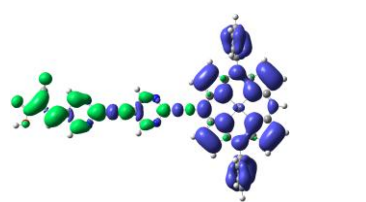
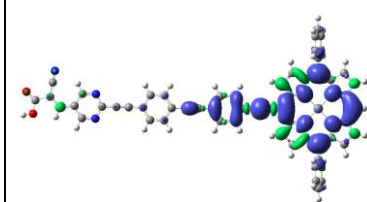
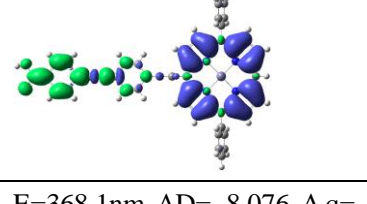
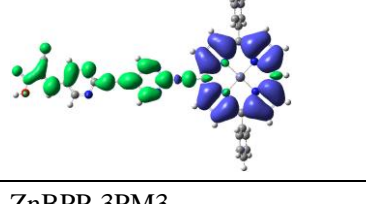
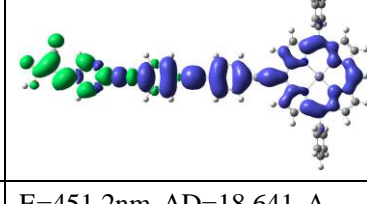
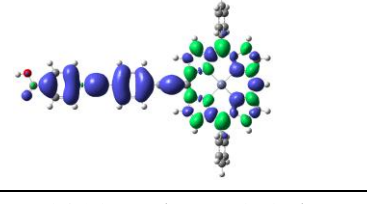
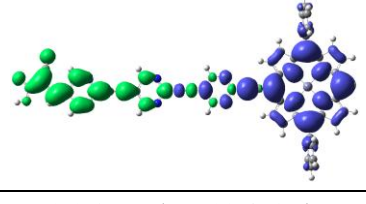
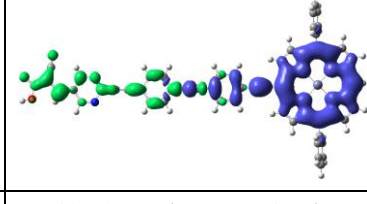
Sensitizers	Wavelength (nm)	$f$	Main Configurations (Assignment: H=HOMO, L=LUMO, L+1=LUMO+1, H-1=HOMO-1, etc.)
ZnBPP-1PM	662.5	1.0467	H-0->L+0(+95%)
	517.5	0.1840	H-0->L+1(+65%) H-1->L+2(+31%)
	422.6	1.1850	H-2->L+0(+38%) H-1->L+2(+36%) H-0->L+1(17%)
	407.2	1.3976	H-1->L+1(+56%) H-0->L+2(+37%)
	389.0	0.1240	H-2->L+0(+32%) H-4->L+0(19%) H-6->L+0(+16%) H-1->L+2(12%) H-0->L+1(+8%) H-10->L+0(7%)
ZnBPP-1PM2	715.4	1.0233	H-0->L+0(+98%)
	570.4	0.1139	H-0->L+1(+77%) H-1->L+2(+20%)
	455.0	2.1026	H-2->L+0(+60%) H-1->L+2(+28%)
	424.8	1.1397	H-1->L+1(+55%) H-0->L+2(+40%)
	413.2	0.1699	H-2->L+0(+36%) H-1->L+2(30%) H-0->L+3(+17%) H-0->L+1(+13%)
	373.9	0.0996	H-6->L+0(+82%) H-6->L+1(8%)
	349.1	0.3626	H-2->L+2(+36%) H-1->L+3(+34%) H-4->L+1(9%) H-6->L+2(6%)
ZnBPP-2PM2	702.7	1.0500	H-0->L+0(+98%)
	445.7	2.273	H-1->L+2(+41%) H-2->L+0(+31%) H-0->L+3(13%) H-0->L+1(10%)
	429.2	0.9189	H-1->L+2(+41%) H-2->L+0(+31%) H-0->L+3(13%) H-0->L+1(10%)
	381.2	0.1726	H-6->L+0(+65%) H-0->L+3(+17%) H-6->L+1(7%)
	371.1	0.5267	H-1->L+3(+86%) H-0->L+2(7%)
ZnBPP-1PM3	723.8	0.6466	H-0->L+0(+98%)
	592.8	0.6138	H-0->L+1(+82%) H-1->L+2(+15%)
	495.5	1.8347	H-2->L+0(+85%) H-1->L+2(8%)
	451.2	0.7397	H-0->L+3(+42%) H-1->L+2(+31%) H-2->L+0(+11%) H-0->L+1(9%)
	436.0	0.8872	H-1->L+1(+54%) H-0->L+2(+38%)
	426.3	0.1182	H-2->L+1(+45%) H-0->L+3(+38%) H-1->L+2(11%)
	390.6	0.1375	H-3->L+0(+50%) H-4->L+0(+18%) H-2->L+1(12%) H-1->L+2(8%)
	379.4	0.3066	H-2->L+1(+28%) H-3->L+0(+18%) H-1->L+2(+17%) H-0->L+3(13%) H-0->L+4(11%)
	368.9	0.2836	H-2->L+2(+28%) H-5->L+0(+26%) H-6->L+0(18%) H-1->L+3(11%) H-5->L+1(+6%)
	366.3	0.3069	H-5->L+0(+39%) H-2->L+2(39%) H-6->L+0(8%) H-1->L+3(+7%)
	360.7	0.1160	H-7->L+0(+76%) H-7->L+1(+6%) H-3->L+1(5%)
ZnBPP-2PM3	756.8	0.6321	H-0->L+0(+99%)
	595.1	0.6313	H-0->L+1(+83%) H-1->L+2(14%)
	486.7	1.6690	H-0->L+3(+48%) H-1->L+2(23%) H-2->L+0(20%)

	465.9	0.4682	H-2->L+0(+69%) H-0->L+3(+26%)
	448.2	0.4831	H-1->L+1(+49%) H-0->L+2(28%) H-1->L+3(21%)
	420.2	0.5455	H-1->L+2(+39%) H-2->L+1(+28%) H-0->L+3(+18%) H-2->L+0(7%) H-0->L+1(+6%)
	404.7	0.7462	H-1->L+3(+72%) H-0->L+2(17%) H-1->L+1(+5%)
	389.6	0.4269	H-5->L+0(+81%) H-7->L+0(+5%)
	366.8	0.2288	H-7->L+0(+52%) H-8->L+0(+13%) H-2->L+1(+10%)
ZnBPP-3PM3	717.3	0.7406	H-0->L+0(+98%)
	592.0	0.5129	H-0->L+1(+83%) H-1->L+2(+13%)
	483.0	1.2466	H-0->L+3(+56%) H-1->L+2(+28%) H-0->L+1(7%) H-2->L+0(5%)
	461.8	0.2691	H-1->L+1(33%) H-1->L+3(+33%) H-0->L+2(32%)
	444.2	1.4889	H-2->L+0(+77%) H-0->L+3(+14%)
	408.7	0.2158	H-1->L+2(+40%) H-0->L+3(21%) H-2->L+1(15%) H-2->L+0(+11%) H-0->L+1(5%)
	402.8	1.0806	H-1->L+3(+63%) H-0->L+2(+28%) H-1->L+1(+6%)
	387.3	0.2800	H-6->L+0(+77%) H-6->L+1(+7%) H-5->L+0(+7%)
ZnBPP-1PE	591.2	0.3820	H-0->L+0(+81%) H-1->L+1(19%)
	436.6	1.6593	H-1->L+1(+59%) H-0->L+2(+21%) H-0->L+0(+15%)
	432.5	1.1525	H-1->L+0(+53%) H-0->L+1(42%)
	360.7	0.2107	H-5->L+0(+56%) H-1->L+2(+30%)
	341.8	0.2300	H-2->L+1(+68%) H-4->L+0(+16%)
ZnBPP-2PE	604.9	0.7785	H-0->L+0(+85%) H-1->L+1(+14%)
	472.0	1.3615	H-0->L+2(+58%) H-1->L+1(+31%) H-0->L+0(7%)
	443.9	0.7879	H-1->L+0(+54%) H-0->L+1(+35%) H-1->L+2(9%)
	432.2	0.6455	H-2->L+0(+46%) H-0->L+2(+29%) H-1->L+1(21%)
	396.6	0.3003	H-1->L+2(+80%) H-2->L+1(+11%) H-0->L+1(+6%)
	368.1	0.5164	H-2->L+1(+72%) H-1->L+2(8%) H-4->L+0(+8%)
	345.3	0.1589	H-0->L+3(+70%) H-2->L+2(18%)
	336.7	0.2267	H-2->L+2(+60%) H-6->L+1(+12%) H-4->L+1(+10%) H-0->L+3(+6%) H-8->L+0(6%)
	333.7	0.1728	H-6->L+1(+31%) H-4->L+1(+22%) H-2->L+2(17%) H-0->L+3(10%) H-9->L+0(6%)
ZnBPP-3PE	609.4	1.0569	H-0->L+0(+86%) H-1->L+1(12%)
	494.6	1.1262	H-0->L+2(+72%) H-1->L+1(+19%)
	453.9	1.1268	H-2->L+0(+57%) H-1->L+1(+21%) H-0->L+2(17%)
	449.0	0.5952	H-1->L+0(+54%) H-0->L+1(30%) H-1->L+2(+13%)
	414.4	0.3005	H-1->L+2(+74%) H-2->L+1(+13%)

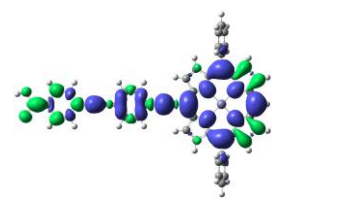
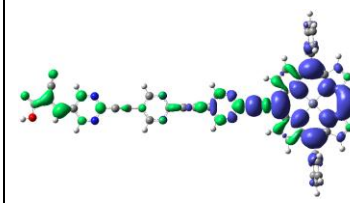
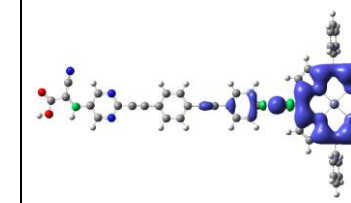
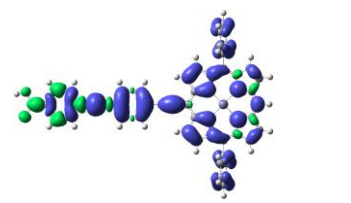
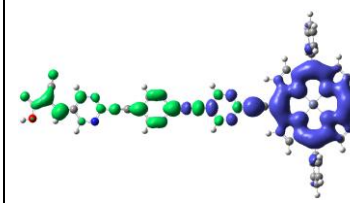
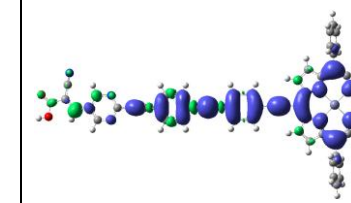
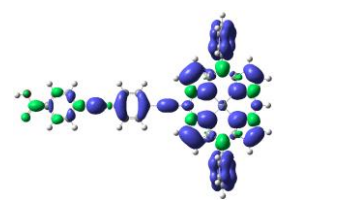
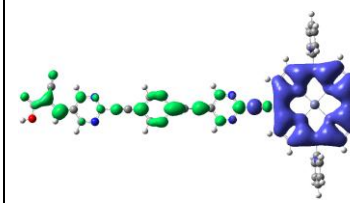
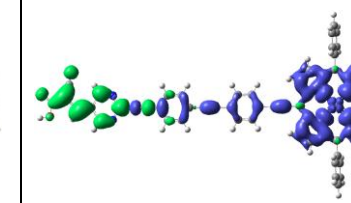
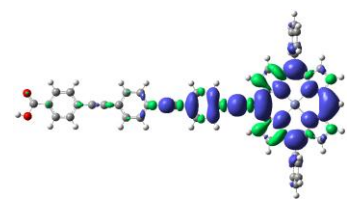
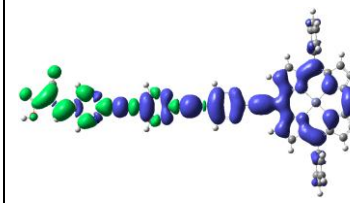
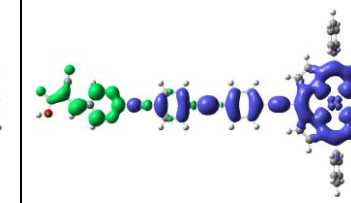
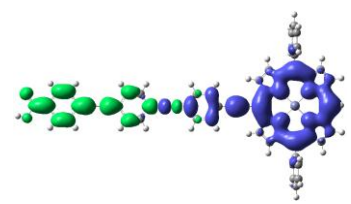
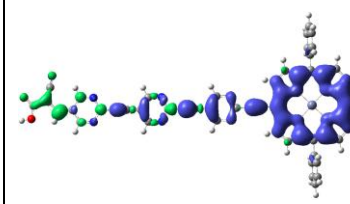
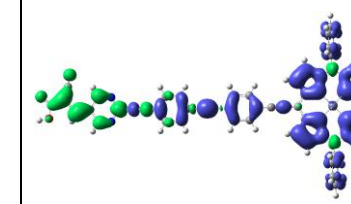
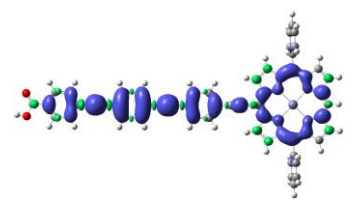
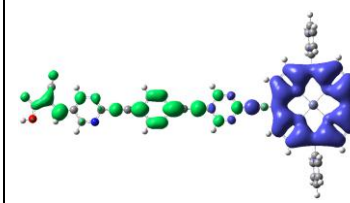
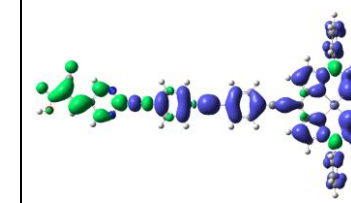



			H-0->L+1(+9%)
	405.2	0.1285	H-2->L+0(+33%) H-1->L+1(31%) H-0->L+3(20%) H-0->L+2(+9%)
	385.0	0.7559	H-2->L+2(+71%) H-0->L+3(+21%)
	384.1	0.5714	H-2->L+1(+78%) H-1->L+2(10%) H-1->L+0(+5%)
	371.2	0.1287	H-0->L+3(+41%) H-2->L+2(23%) H-3->L+0(+21%) H-1->L+1(5%) H-2->L+0(+5%)
	341.7	0.1161	H-1->L+3(+87%)

Table S2. Electron density difference plots of electronic transition  $S_0 \rightarrow S_1$  for each porphyrin.  $\Delta D$  is the electron transfer distance ( $\text{\AA}$ )<sup>a</sup>;  $\Delta q$  is the fraction of electron exchange ( $e^-$ )<sup>b</sup>,  $\Omega$  is overlaps between the regions of density depletion and increment. (Isovalue:  $4 \times 10^{-4} e \cdot \text{au}^{-3}$ )

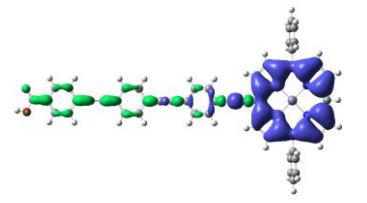
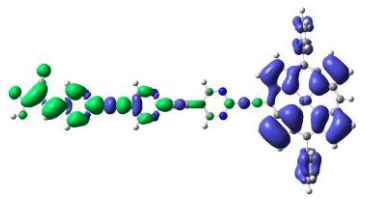
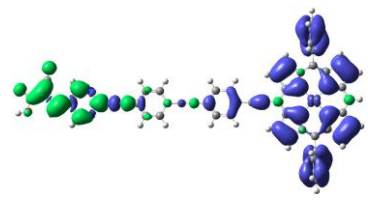
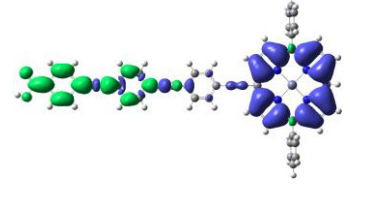
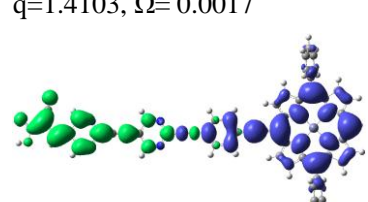
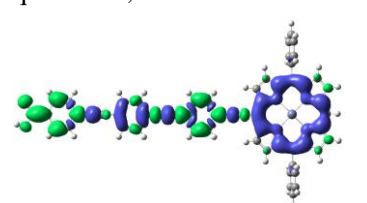
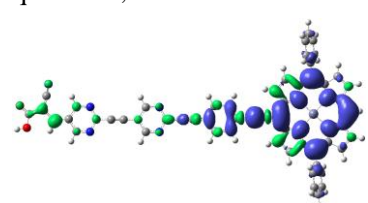
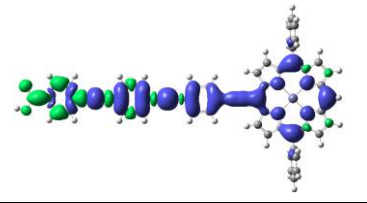
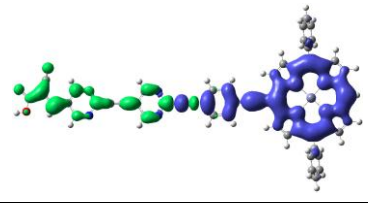
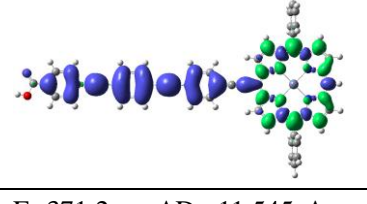
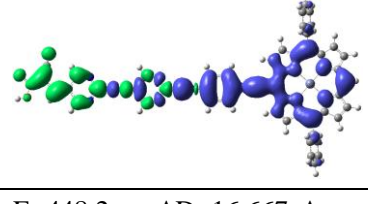
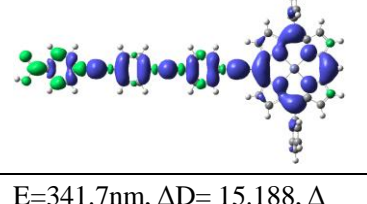
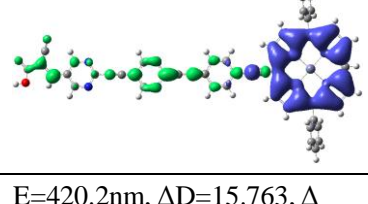
ZnBPP-1PE	ZnBPP-1PM	ZnBPP-1PM2
E=591.2nm, $\Delta D= 2.141$ $\Delta q=0.656$ , $\Omega=0.383$ 	E=662.5nm, $\Delta D=8.038$ , $\Delta q=1.049$ , $\Omega= 0.243$ 	E=715.4nm, $\Delta D=15.076$ , $\Delta q=1.3091$ , $\Omega= 0.0146$ 
E=436.6nm, $\Delta D= 7.417$ $\Delta q=0.6237$ , $\Omega=0.1353$ 	E=517.5nm, $\Delta D= 9.118$ , $\Delta q=0.6548$ , $\Omega= 0.0907$ 	E=570.4nm, $\Delta D=6.944$ , $\Delta q=0.6533$ , $\Omega= 0.2890$ 
E=432.5nm, $\Delta D= 6.478$ $\Delta q= 0.5194$ , $\Omega= 0.0752$ 	E=422.6nm, $\Delta D= 8.554$ , $\Delta q=0.6537$ , $\Omega= 0.1167$ 	E=455.0nm, $\Delta D=11.060$ , $\Delta q=0.8423$ , $\Omega= 0.2685$ 
E=360.7nm, $\Delta D= 4.608$ $\Delta q= 0.9235$ , $\Omega= 0.3488$ 	E=407.2nm, $\Delta D= 10.837$ , $\Delta q=0.6130$ , $\Omega= 0.007$ 	E=424.8nm, $\Delta D=14.217$ , $\Delta q=0.5438$ , $\Omega= 0.0340$ 
E=341.8nm, $\Delta D= -3.194$ $\Delta q= 0.7366$ , $\Omega= 0.4245$ 	E=389.0nm, $\Delta D= 9.992$ , $\Delta q=0.8319$ , $\Omega= 0.0408$ 	E=413.2nm, $\Delta D=13.995$ , $\Delta q=0.7828$ , $\Omega= 0.0339$ 
ZnBPP-2PE	ZnBPP-2PM2	E=373.9nm, $\Delta D=15.530$ , $\Delta q=1.1052$ , $\Omega= 0.0283$
E=604.9nm, $\Delta D= 2.924$ , $\Delta q=0.7046$ , $\Omega= 0.4381$	E=702.7nm, $\Delta D= 14.632$ , $\Delta q=1.3209$ , $\Omega= 0.0236$	

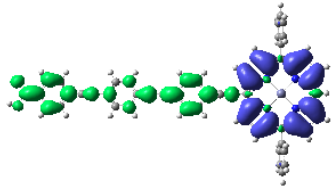
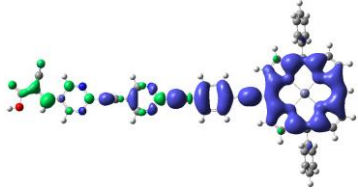
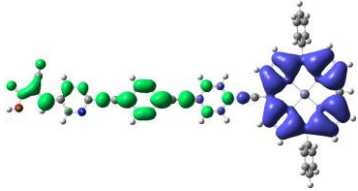
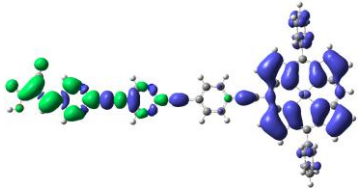
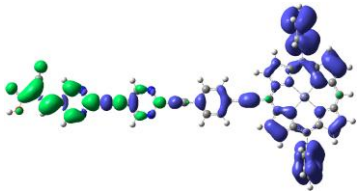
		
E=472.0nm, $\Delta D= 13.730$ , $\Delta q= 0.86279$ , $\Omega= 0.0129$	E=445.7nm, $\Delta D= 13.4888$ , $\Delta q= 0.7098$ , $\Omega= 0.0744$	E=349.1nm, $\Delta D=6.737$ , $\Delta q=0.6592$ , $\Omega= 0.3811$
		
E=443.9nm, $\Delta D= 12.175$ , $\Delta q= 0.6217$ , $\Omega= 0.0334$	E=429.2nm, $\Delta D= 13.845$ , $\Delta q= 0.6298$ , $\Omega= 0.0378$	ZnBPP-1PM3 E=723.8nm, $\Delta D=21.219$ , $\Delta q=1.4155$ , $\Omega= 0.0010$
		
E=432.2nm, $\Delta D= 6.706$ , $\Delta q= 0.6050$ , $\Omega= 0.2806$	E=381.2nm, $\Delta D=14.795$ , $\Delta q=0.9860$ , $\Omega= 0.0278$	E=592.8nm, $\Delta D=3.929$ , $\Delta q=0.6769$ , $\Omega= 0.3853$
		
E=396.6nm, $\Delta D= 14.170$ , $\Delta q= 1.0130$ , $\Omega= 0.0215$	E=371.1nm, $\Delta D= 11.957$ , $\Delta q= 1.1080$ , $\Omega= 0.0922$	E=495.5nm, $\Delta D=14.902$ , $\Delta q=1.0896$ , $\Omega= 0.1080$
		
E=368.1nm, $\Delta D= -8.076$ , $\Delta q= 0.7939$ , $\Omega= 0.2621$	ZnBPP-3PM3 E=717.3nm, $\Delta D=20.343$ , $\Delta q=1.3825$ , $\Omega= 0.0031$	E=451.2nm, $\Delta D=18.641$ , $\Delta q=0.7677$ , $\Omega= 0.0181$
		
E=345.3nm, $\Delta D= 6.073$ , $\Delta q=$	E=592.0nm, $\Delta D=12.478$ , $\Delta$	E=436.0nm, $\Delta D=12.749$ , $\Delta$



0.8065, $\Omega= 0.5066$ 	$q=0.7803, \Omega= 0.2062$ 	$q=0.5148, \Omega= 0.0808$ 
$E=336.7\text{nm}, \Delta D= 7.813, \Delta q= 0.7154, \Omega= 0.3245$ 	$E=483.0\text{nm}, \Delta D=17.042, \Delta q=0.8245, \Omega= 0.0282$ 	$E=426.3\text{nm}, \Delta D=8.143, \Delta q=0.6445, \Omega= 0.3410$ 
$E=333.7\text{nm}, \Delta D= 2.971, \Delta q= 0.6771, \Omega= 0.4316$ 	$E=461.8\text{nm}, \Delta D=16.723, \Delta q=0.7977, \Omega= 0.0300$ 	$E=390.6\text{nm}, \Delta D=21.608, \Delta q=0.9967, \Omega= 0.0043$ 
ZnBPP-3PE $E=609.4\text{nm}, \Delta D= 3.818, \Delta q= 0.7222, \Omega= 0.4439$ 	$E=444.2\text{nm}, \Delta D=15.478, \Delta q=0.9654, \Omega= 0.1162$ 	$E=379.4\text{nm}, \Delta D=18.821, \Delta q=0.7222, \Omega= 0.0266$ 
$E=494.6\text{nm}, \Delta D= 18.314, \Delta q= 0.9636, \Omega= 0.0059$ 	$E=408.7\text{nm}, \Delta D=16.815, \Delta q=0.6207, \Omega= 0.0870$ 	$E=368.9\text{nm}, \Delta D=18.895, \Delta q=0.8763, \Omega= 0.0968$ 
$E=453.9\text{nm}, \Delta D= -1.530, \Delta q= 0.5939, \Omega= 0.3367$ 	$E=402.8\text{nm}, \Delta D=17.028, \Delta q=0.8908, \Omega= 0.0185$ 	$E=366.3\text{nm}, \Delta D=16.301, \Delta q=0.9189, \Omega= 0.2733$ 
$E=449.0\text{nm}, \Delta D= 15.914, \Delta q= 0.6716, \Omega= 0.0356$ 	$E=387.3\text{nm}, \Delta D=20.264, \Delta q=1.0804, \Omega= 0.0148$ 	$E=360.7\text{nm}, \Delta D=21.100, \Delta q=1.04559, \Omega= 0.0215$ 

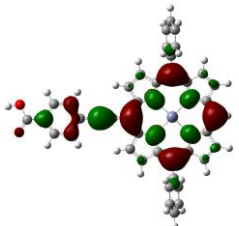
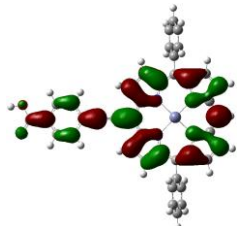
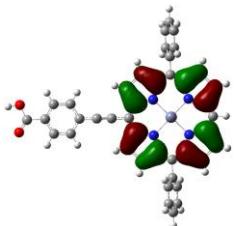
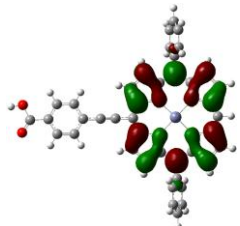
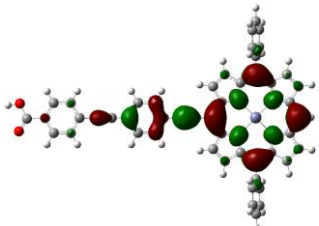
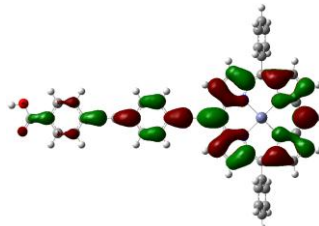
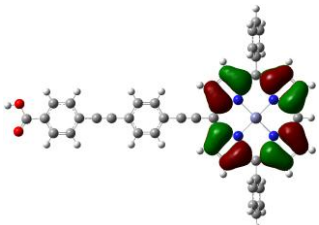
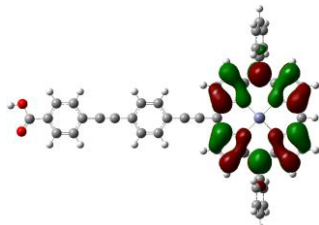
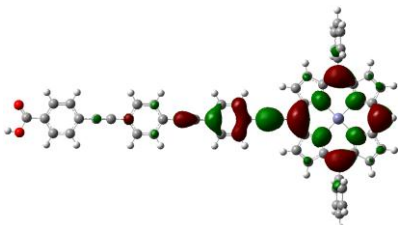
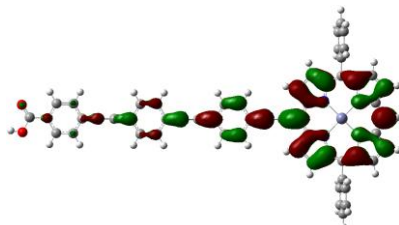


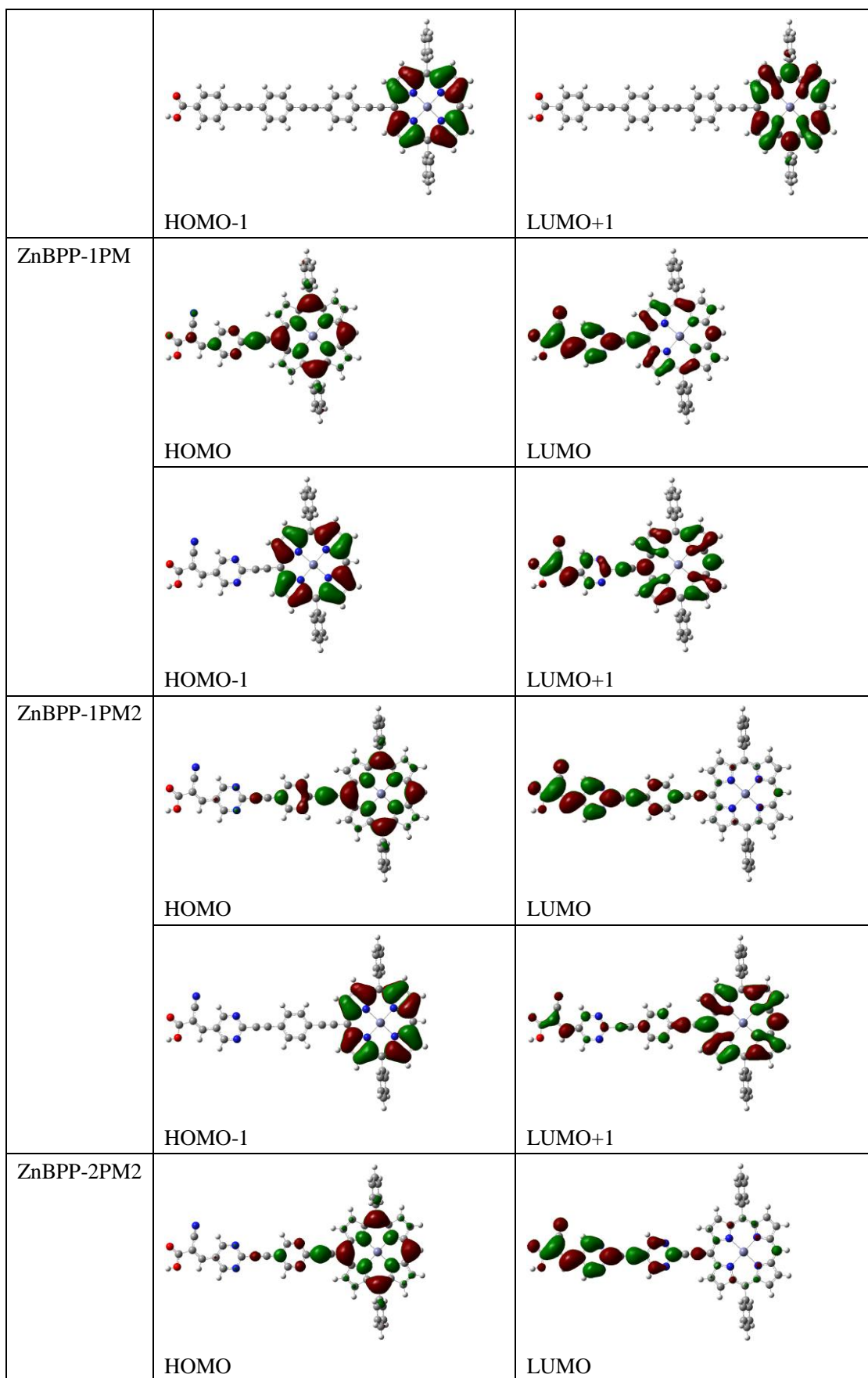
		
E=414.4nm, $\Delta D= 19.153$ , $\Delta$ q= 0.9432, $\Omega= 0.0104$		ZnBPP-2PM3 E=756.8nm, $\Delta D=20.749$ , $\Delta$ q=1.4103, $\Omega= 0.0017$
		
E=405.2nm, $\Delta D= 10.921$ , $\Delta$ q= 0.6901, $\Omega= 0.4106$		E=595.1nm, $\Delta D=10.041$ , $\Delta$ q=0.7353, $\Omega= 0.2756$
		
E=385.0nm, $\Delta D= 10.357$ , $\Delta$ q= 0.7933, $\Omega= 0.3953$		E=486.7nm, $\Delta D=18.433$ , $\Delta$ q=0.8394, $\Omega= 0.0176$
		
E=384.1nm, $\Delta D= -12.626$ , $\Delta$ q= 0.8879, $\Omega= 0.1454$		E=465.9nm, $\Delta D=17.117$ , $\Delta$ q=1.0900, $\Omega= 0.0617$
		
E=371.2nm, $\Delta D= 11.545$ , $\Delta$ q= 0.7035, $\Omega= 0.3105$		E=448.2nm, $\Delta D=16.667$ , $\Delta$ q=0.7535, $\Omega= 0.0304$
		
E=341.7nm, $\Delta D= 15.188$ , $\Delta$ q= 1.1988, $\Omega= 0.1183$		E=420.2nm, $\Delta D=15.763$ , $\Delta$ q=0.6412, $\Omega= 0.1108$

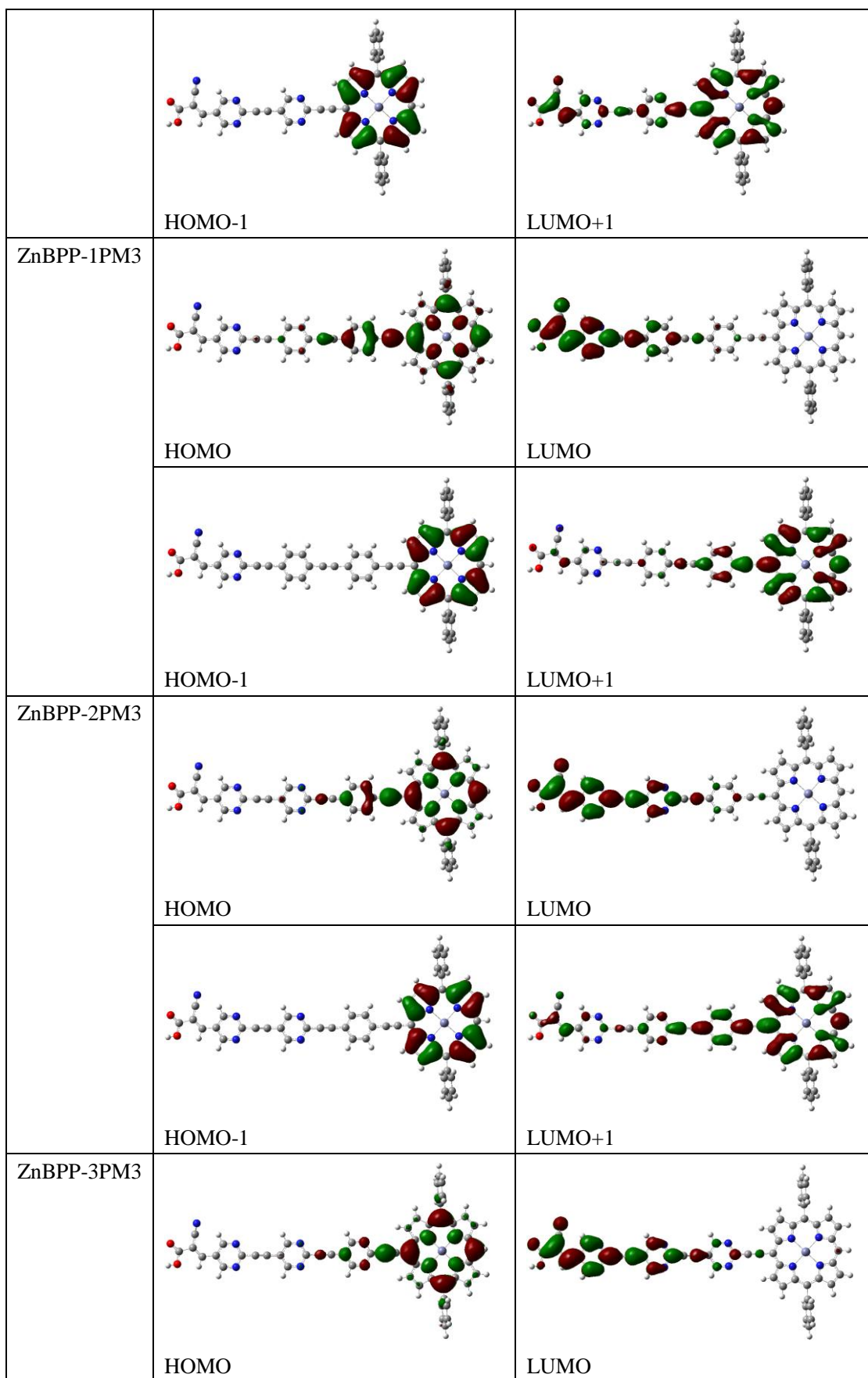
		
		<p>E=404.7nm, <math>\Delta D=17.402</math>, <math>\Delta q=0.9820</math>, <math>\Omega=0.0142</math></p> 
		<p>E=389.6nm, <math>\Delta D=20.808</math>, <math>\Delta q=1.0143</math>, <math>\Omega=0.0123</math></p> 
		<p>E=366.8nm, <math>\Delta D=20.846</math>, <math>\Delta q=0.8555</math>, <math>\Omega=0.0080</math></p> 

<sup>a</sup>calculated with Eq(10). <sup>c</sup>calculated with Eq(11)

Table S3. Molecular orbitals involved in electron transitions. (Isovalue:  $4 \times 10^{-4} e \cdot \text{au}^{-3}$ )

Molecules	HOMOs	LUMOs
ZnBPP-1PE	 HOMO	 LUMO
	 HOMO-1	 LUMO+1
ZnBPP-2PE	 HOMO	 LUMO
	 HOMO-1	 LUMO+1
ZnBPP-3PE	 HOMO	 LUMO





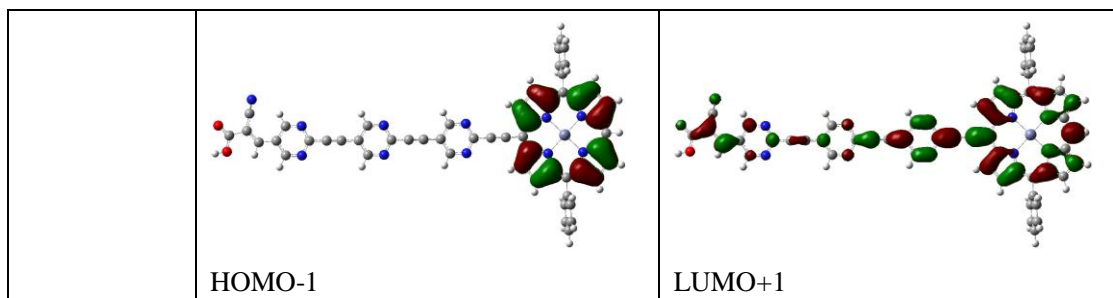


Table S4. Transition energies (in eV) of *Q* band and *B* band (two components)<sup>a</sup> for ZnBPP-PE1, ZnBPP-PE2 and ZnBPP-PE3 dyes in the tetrahydrofuran solution for the S<sub>0</sub>-S<sub>1</sub> transition. Computed for the B3LYP/6-311g(d, p) optimized geometries.

Method	ZnBPP-PE1	ZnBPP-PE2	ZnBPP-PE3
B3LYP	2.1152 (2.8628, 2.8912)	2.0652 (2.6532, 2.8131)	2.0505 (2.7517, 2.7810)
PBE0	2.1597 (2.9344, 2.9698)	2.1162 (2.7654, 2.9145)	2.1049 (2.6721, 2.8969)
CAM-B3LYP	2.1257 (3.0779, 3.1487)	2.1076 (3.0052, 3.1361)	2.1057 (2.9785, 3.1349)
LC-WPBE	1.9487 (3.2021, 3.2856)	1.9329 (3.1602, 3.2775)	1.9316 (3.1495, 3.2770)
M062X	2.1925 (3.0858, 3.1449)	2.1715 (3.0093, 3.1297)	2.1691 (2.9803, 3.1281)
WB97XD	2.0814 (3.1044, 3.1718)	2.0662 (3.0468, 3.1635)	2.0649 (3.0272, 3.1630)
WB97XD <sup>b</sup>	2.1319 (3.1530, 3.2148)	2.1190 (3.1076, 3.2085)	2.1177 (3.0947, 3.2080)
Experimental <sup>c</sup>	2.0127 (2.8242)	2.0062 (2.7987)	2.0029 (2.7987)

<sup>a</sup>There are two absorption components in *B* region for these sensitizers individually, these two components located so close that only one wide *B* absorption band could be observed.

<sup>b</sup>Transition energies (in eV) are computed for the WB97XD/6-311g(d, p) optimized geometries.

<sup>c</sup>Experimental value from Ref.6



Table S5. Electron density difference plots of electronic transition  $S_0 \rightarrow S_1$  (TDDFT/WB97XD/6-311g(d, p)) for ZnBPP-PE1, ZnBPP-PE2 and ZnBPP-PE3 dyes.  $\Delta D$  is the electron transfer distance ( $\text{\AA}$ );  $\Delta q$  is the fraction of electron exchange ( $e^-$ ),  $\Omega$  is overlaps between the regions of density depletion and increment. (Isovalue:  $4 \times 10^{-4} e \cdot \text{au}^{-3}$ ). Computed for the WB97XD/6-311g(d, p) optimized geometries.

ZnBPP-PE1	ZnBPP-PE2	ZnBPP-PE3
$\Delta D = 2.511$ , $\Delta q = 0.5655$ , $\Omega = 0.2352$	$\Delta D = 3.180$ , $\Delta q = 0.5580$ , $\Omega = 0.2306$	$\Delta D = 3.394$ , $\Delta q = 0.5511$ , $\Omega = 0.2257$
