Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Theoretical design of porphyrin sensitizers with different acceptors for its application in dye-sensitized solar cells

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Table S1. Geometric parameters of all dyes calculated using B3LYP functional

Geometric parameters	YD2-o-C8	Dye1	Dye2	Dye3
r(Zn-N1) /Å	2.049	2.050	2.050	2.050
r(N1-C2) /Å	1.369	1.369	1.368	1.368
r(C2-C3) /Å	1.443	1.443	1.443	1.443
r(C3-C4) /Å	1.362	1.362	1.362	1.362
r(C5-C6) /Å	1.402	1.402	1.401	1.401
r(C6-C7) /Å	1.500	1.500	1.500	1.500
α(C2-N1-C5) /degree	106.5	106.5	106.5	106.5
α(Zn-N1-C2) /degree	126.9	127.0	127.0	127.0
α(C4-C5-C6) /degree	124.6	124.6	124.6	124.6
α(N1-C5-C6) /degree	125.9	125.9	125.9	125.9
α(C5-C6-C7) /degree	117.5	117.5	117.5	117.5

Table S2. The calculated absorption energies (λ), oscillator strength (*f*), and electron transition configurations for all designed dyes and reference dye YD2-o-C8.

System	λ(nm)	*f* (>= 0.1)	Composition (> =5%)
YD2-o-C8	637	0.5030	H->L (89%), H-1->L+1 (8%)
	489	0.1462	H-2->L+1 (50%), H-1->L (29%), H->L+1 (21%)
	436	1.6862	H-1->L+1 (49%), H->L+2 (30%), H-2->L (9%), H->L (8%)
	422	0.6264	H-2->L+1 (40%), H-1->L (26%), H->L+1 (12%), H-4->L (9%), H-3->L (6%), H-1->L+2 (5%)
	418	0.1159	H-4->L (71%), H-3->L (14%), H-2->L+1 (6%)
	404	0.3167	H-7->L (12%), H-1->L+1 (16%), H->L+2 (62%)
	366	0.2417	H-1->L+2 (88%), H-7->L+1 (5%)
	333	0.1674	H-7->L+1 (72%), H-11->L+1 (6%), H-9->L (7%)
	318	0.1245	H-14->L (68%), H-11->L (10%), H-16->L (6%), H-8->L+1 (5%)
Dye1	665	0.9613	H->L (91%), H-1->L+1 (5%)
	548	0.2044	H-2->L (92%)
	500	0.4499	H-1->L+1 (18%), H->L+2 (78%)
	495	0.1540	H-2->L+1 (48%), H-1->L (32%), H->L+1 (18%)
	457	0.9566	H-3->L (43%), H-1->L+1 (36%), H->L+2 (11%)
	455	0.2681	H-2->L+1 (46%), H-1->L (25%), H-1->L+2 (15%), H->L+1 (11%)
	410	0.2848	H-3->L+1 (14%), H-1->L+2 (72%), H-2->L+1 (5%), H->L+1 (7%)
	378	0.2669	H-3->L (37%), H-2->L+2 (12%), H-1->L+1 (32%), H->L+2 (7%)
	368	0.1432	H-8->L (57%), H-3->L+1 (24%)， H-10->L (5%)
	363	0.2034	H-10->L (69%), H-3->L+1 (16%)
	356	0.3402	H-10->L (18%), H-8->L (36%), H-3->L+1 (35%)
	343	0.1889	H-3->L+2 (82%), H->L+3 (7%)
Dye2	742	1.3262	H->L (96%)
	592	0.2201	H-2->L (65%), H->L+1 (25%)， H-2->L+1 (7%)
	581	0.1833	H-2->L (27%), H->L+1 (60%)， H-1->L+2 (9%)
	491	0.4454	H-2->L+1 (60%), H-1->L+2 (23%)， H-3->L (6%), H-2->L (7%)
	473	0.6922	H-3->L (60%), H-2->L+1 (22%), H-1->L+2 (13%)
	429	0.6223	H-2->L+2 (26%), H-1->L+1 (45%), H->L+2 (18%), H-3->L+2 (8%)
	409	0.1224	H-3->L (29%), H-3->L+1 (20%), H-1->L+2 (31%), H-2->L+1 (8%), H->L+1 (9%)
	395	0.1851	H-3->L+1 (28%), H->L+3 (64%)
	369	0.1758	H-9->L (22%), H-6->L+1 (13%), H-3->L+1 (20%), H->L+3 (16%), H-13->L (7%), H-1->L+2 (7%)

	364	0.3867	H-8->L (13%), H-3->L+2 (65%), H-1->L+1 (6%), H-1->L+3 (5%)
Dye3	742	1.3574	H->L (96%)
	592	0.2129	H-2->L (62%), H->L+1 (27%) H-2->L+1 (6%)
	581	0.1967	H-2->L (30%), H->L+1 (58%) H-1->L+2 (8%)
	492	0.4851	H-2->L+1 (57%), H-1->L+2 (24%) H-3->L (8%), H-2->L (6%)
	474	0.6253	H-3->L (60%), H-2->L+1 (24%), H-1->L+2 (11%)
	430	0.6108	H-2->L+2 (26%), H-1->L+1 (45%), H->L+2 (18%)， H-3->L+2 (8%)
	412	0.1236	H-3->L (27%), H-3->L+1 (22%), H-1->L+2 (31%)，H-2->L+1 (8%), H->L+1 (8%)
	396	0.1895	H-3->L+1 (27%), H->L+3 (65%)

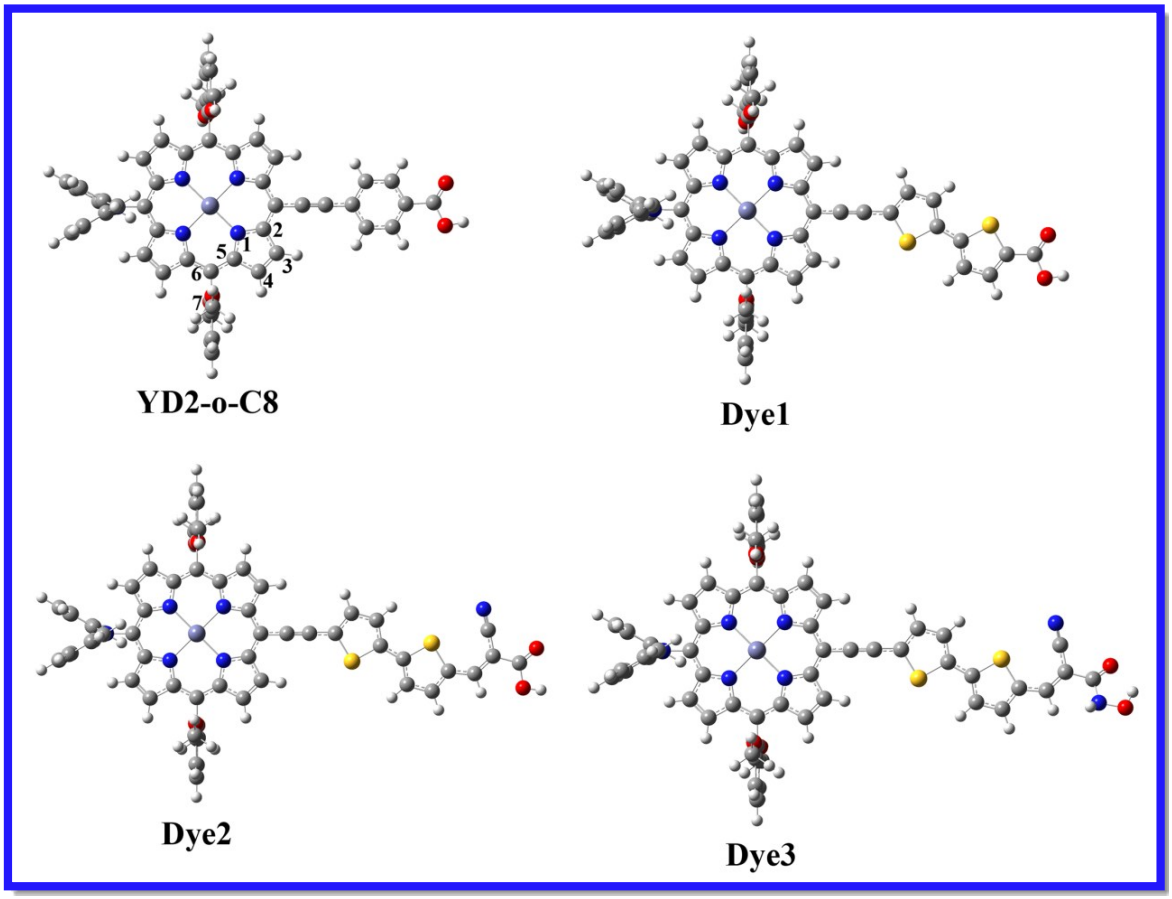

Figure S1. Molecular geometries of all investigated dyes optimized using B3LYP functional.