

## Supporting Information

# Optoelectronic performance of Anthracene-Based dyes with modified Hagfeldt donors in dye-sensitized solar cells

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Table S1. Contribution data of dye fragments to HOMO and LUMO.

Dyes	MO	Donor	$\pi$ -bridge	Auxiliary acceptor	Benzoic acid
LC1	HOMO	75.77 %	21.74 %	-	2.50 %
	LUMO	5.01 %	70.70 %	-	24.29 %
LC4	HOMO	71.25 %	24.05 %	3.79 %	0.91 %
	LUMO	3.791 %	51.68 %	31.34 %	13.19 %
LC4N	HOMO	75.16 %	21.25 %	2.84 %	0.75 %
	LUMO	3.79 %	45.67 %	38.69 %	11.85 %
LC4NN	HOMO	77.07 %	20.02 %	2.31 %	0.61 %
	LUMO	3.12 %	34.33 %	46.23 %	16.32 %

Table S2. The calculation results of  $E$ ,  $\lambda$ ,  $f$ , and transition modes for the excited-states from S1 to S12.

Dyes	States	$E$ (eV)	$\lambda$ (nm)	$f$	Transition mode
LC1	1	2.6207	473.10	0.6732	H→L(0.655)
	2	3.1685	391.30	0.2204	H-1→L(0.632)
	3	3.8166	324.85	0.0143	H-6→L(0.462)
	4	3.9884	310.86	0.3766	H→L+1(0.501)
	5	4.1353	299.82	1.1026	H→L+2(0.414)
	6	4.2770	289.89	0.0403	H-2→L(0.610)
	7	4.4603	277.97	0.1214	H-7→L(0.596)
	8	4.4799	276.75	0.2012	H→L+6(0.446)
	9	4.6654	265.75	0.2238	H-11→L(0.386)
	10	4.7020	263.69	0.0547	H-3→L(0.474)
	11	4.7220	262.57	0.3554	H→L+6(0.290)
	12	4.7427	261.42	0.0114	H-15→L(0.582)
LC4	1	2.5554	485.19	1.0584	H→L(0.625)
	2	3.0909	401.13	0.3135	H-1→L(0.593)
	3	3.5517	349.09	0.2965	H→L+1(0.426)
	4	3.8107	325.36	0.0131	H-7→L(0.419)
	5	4.0012	309.87	0.1171	H-4→L(0.534)
	6	4.1272	300.41	1.0668	H→L+3(0.413)
	7	4.2512	291.65	0.0466	H-2→L(0.594)
	8	4.4487	278.70	0.0051	H-1→L+1(0.447)
	9	4.4734	277.16	0.1712	H→L+7(0.444)
	10	4.5495	272.52	0.0837	H-11→L(0.406)
	11	4.6461	266.85	0.1645	H-12→L(0.323)
	12	4.6569	266.24	0.1195	H-4→L+1(0.319)
LC4N	1	2.4712	501.72	1.0414	H→L(0.615)
	2	3.0190	410.68	0.3214	H-1→L(0.585)
	3	3.5177	352.45	0.2207	H→L+1(0.440)
	4	3.7904	327.10	0.0196	H-7→L(0.428)
	5	3.9049	317.51	0.2096	H-4→L(0.555)
	6	4.0976	302.58	0.4445	H-2→L(0.524)
	7	4.1740	297.04	0.6670	H→L+3(0.429)

LC4NN	8	4.3330	286.14	0.0087	H-1→L+1(0.456)
	9	4.3754	283.37	0.0021	H-17→L(0.397)
	10	4.4777	276.89	0.1973	H→L+8(0.358)
	11	4.5459	272.74	0.1130	H-11→L(0.370)
	12	4.5684	271.40	0.0539	H-13→L(0.331)
	1	2.4371	508.74	0.9886	H→L(0.588)
	2	2.9982	413.53	0.2955	H-1→L(0.563)
	3	3.4519	359.17	0.0940	H→L+1(0.472)
	4	3.5264	351.59	0.0001	H-11→L(0.643)
	5	3.7793	328.06	0.0233	H-7→L(0.400)
	6	3.9281	315.64	0.4145	H-6→L(0.571)
	7	4.0354	307.24	0.1702	H-2→L(0.590)
8	4.1682	297.45	0.9267	H→L+3(0.457)	
9	4.1890	295.97	0.0960	H-1→L+1(0.423)	
10	4.4757	277.02	0.1712	H→L+8(0.411)	
11	4.4921	276.00	0.1000	H-3→L(0.312)	
12	4.5093	274.95	0.0119	H-14→L(0.353)	

Table S3. The polarizability ( $\alpha$  in a.u.) of dye monomers.

Dyes	$\alpha_{xx}$	$\alpha_{yy}$	$\alpha_{zz}$	$\alpha$
LC1	1239.26	918.05	842.36	969.45
LC4	1733.87	1002.14	1045.96	1169.64
LC4N	1814.24	1132.69	1051.43	1184.94
LC4NN	1789.89	774.69	686.52	1194.33

Table S4. Estimated reorganization energies ( $\lambda$  in eV), electron recombination distance ( $r$  in Å), attenuation factor ( $\beta$  in Å<sup>-1</sup>), electron recombination rate ( $k_{rec}$  in s<sup>-1</sup>), and recombination resistance ( $R_0$  in Ω) for all dyes.

Dye	$\lambda$	$r$	$\beta$	$k_{rec}$	$R_0$
LC1	0.80	13.41	0.7	2558	2152
LC4	0.71	17.77	0.7	1042	2294
LC4N	0.61	17.71	0.7	397	2123
LC4NN	0.60	17.62	0.7	327	2318