Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2012**, *28* (07), 1651-1657
doi: 10.3866/PKU.WHXB201204194

D-π-A-π-D 型萘基衍生物的电子、光谱和电荷传输性质

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Electronic, Optical and Charge Transport Properties of D-π-A-π-D Type Naphthalene-Based Derivatives

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Table S1 Optical properties of OMC, BMC, and "CH"/N substituted naphthalene derivatives computed at the TD-CAM-B3LYP/6-31G(*d*)//HF/6-31G(*d*) level (absorption) and TD-CAM-B3LYP/6-31G(*d*)//TD-CAM-B3LYP/6-31G(*d*) level (emission)

	Absorption			Emission		
	E_v	λ_{abs}	f	E_v	λ_{em}	f
OMC	3.38	366.4	0.80	2.29	542.3	0.84
BMC	4.33	286.2	1.43	3.08	402.7	1.52
BMC-N1	4.09	302.8	1.10	2.94	422.3	1.36
BMC-N2	4.23	293.4	1.31	3.02	409.9	1.48
BMC-N13	3.94	314.8	0.95	2.83	437.7	1.25
BMC-N14	3.75	330.3	0.59	2.62	472.6	0.88
BMC-N145	3.44	360.6	0.75	2.40	517.6	0.88
BMC-N1456	3.29	376.5	0.75	2.25	550.5	0.85

E_v: vertical excitation energies (in eV). $\lambda_{abs}/\lambda_{em}$: the maximum absorption/emission wavelength (in nm). *f*: the oscillator strength.

Table S2 E_{HOMO}, E_{LUMO}, and E_g (in eV) of OMC, BMC, and "CH"/N substituted naphthalene derivatives computed at the PBE0/6-31G(*d*)//HF/6-31G(*d*) level (S_0) and TD-PBE0/6-31G(*d*)// TD-PBE0/6-31G(*d*) level (S_1)

	S_0			S_1		
	E_{HOMO}	E_{LUMO}	E_g	E_{HOMO}	E_{LUMO}	E_g
OMC	-5.15	-1.96	3.19	-4.87	-2.47	2.40
BMC	-5.21	-0.85	4.36	-4.82	-1.52	3.30
BMC-N1	-5.09	-1.21	3.88	-4.85	-1.75	3.10
BMC-N2	-5.27	-1.15	4.12	-4.98	-1.76	3.22
BMC-N13	-5.18	-1.52	3.66	-4.98	-2.05	2.93
BMC-N14	-5.14	-1.66	3.48	-4.88	-2.17	2.71
BMC-N145	-5.14	-1.98	3.16	-4.93	-2.53	2.40
BMC-N1456	-5.18	-2.25	2.93	-4.99	-2.85	2.14

Table S3 E_{HOMO}, E_{LUMO}, and E_g (in eV) of Donor, π-bridge, Donor-π-bridge, and acceptors computed at the PBE0/6-31G(*d*)//HF/6-31G(*d*) level (S_0) and TD-PBE0/6-31G(*d*)//TD-PBE0/6-31G (*d*) level (S_1)

	S_0			S_1		
	E_{HOMO}	E_{LUMO}	E_g	E_{HOMO}	E_{LUMO}	E_g
Donor	−5.44	0.08	5.52	−5.01	−1.07	3.94
π-bridge	−7.02	0.30	7.32	−6.90	0.07	6.97
Donor-π-bridge	−5.24	−0.11	5.13	−5.03	−0.35	4.68
OMC-acceptor	−7.00	−2.03	4.97	−6.61	−2.61	4.00
BMC-acceptor	−6.12	−0.75	5.37	−5.75	−1.22	4.53
BMC-N1-acceptor	−6.63	−1.15	5.48	−6.19	−1.50	4.69
BMC-N2-acceptor	−6.55	−1.16	5.39	−6.27	−1.41	4.86
BMC-N13-acceptor	−7.07	−1.58	5.49	−6.26	−1.89	4.37
BMC-N14-acceptor	−6.92	−1.66	5.26	−6.43	−1.94	4.49
BMC-N145-acceptor	−7.16	−2.09	5.07	−6.76	−2.42	4.34
BMC-N1456-acceptor	−6.91	−2.53	4.38	−5.73	−2.95	2.78

Table S4 Optical properties of Donor, π-bridge, Donor-π-bridge, and acceptors computed at the TD-PBE0/6-31G(*d*)//HF/6-31G(*d*) level (absorption) and TD-PBE0/6-31G(*d*)//TD-PBE0/6-31G(*d*) level (emission)

	Absorption			Emission		
	E_v	λ_{abs}	*f*	E_v	λ_{em}	*f*
Donor	4.61	269.2	0.02	2.89	429.3	0.00
π-bridge	5.71	217.0	0.00	5.39	230.1	0.00
Donor-π-bridge	4.17	297.2	0.02	3.72	332.9	0.01
OMC-acceptor	4.26	291.3	0.05	3.37	368.1	0.04
BMC-acceptor	4.72	262.6	0.06	4.00	309.7	0.08
BMC-N1-acceptor	4.43	279.7	0.00	3.13	396.0	0.00
BMC-N2-acceptor	4.46	277.9	0.00	3.33	372.3	0.00
BMC-N13-acceptor	3.92	316.1	0.00	2.79	444.7	0.00
BMC-N14-acceptor	3.65	339.3	0.00	2.92	424.7	0.00
BMC-N145-acceptor	3.51	353.3	0.00	2.77	446.9	0.00
BMC-N1456-acceptor	3.10	399.7	0.00	1.42	871.0	0.00

E_v: the vertical excitation energies (in eV). $\lambda_{abs}/\lambda_{em}$: the maximum absorption/emission wavelength (in nm). *f*: the oscillator strength.