Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Conformational Effects, Molecular Orbitals, and Reaction Activities of Bis(phthalocyaninato) Lanthanum Double-deckers: Density Functional Theory Calculations

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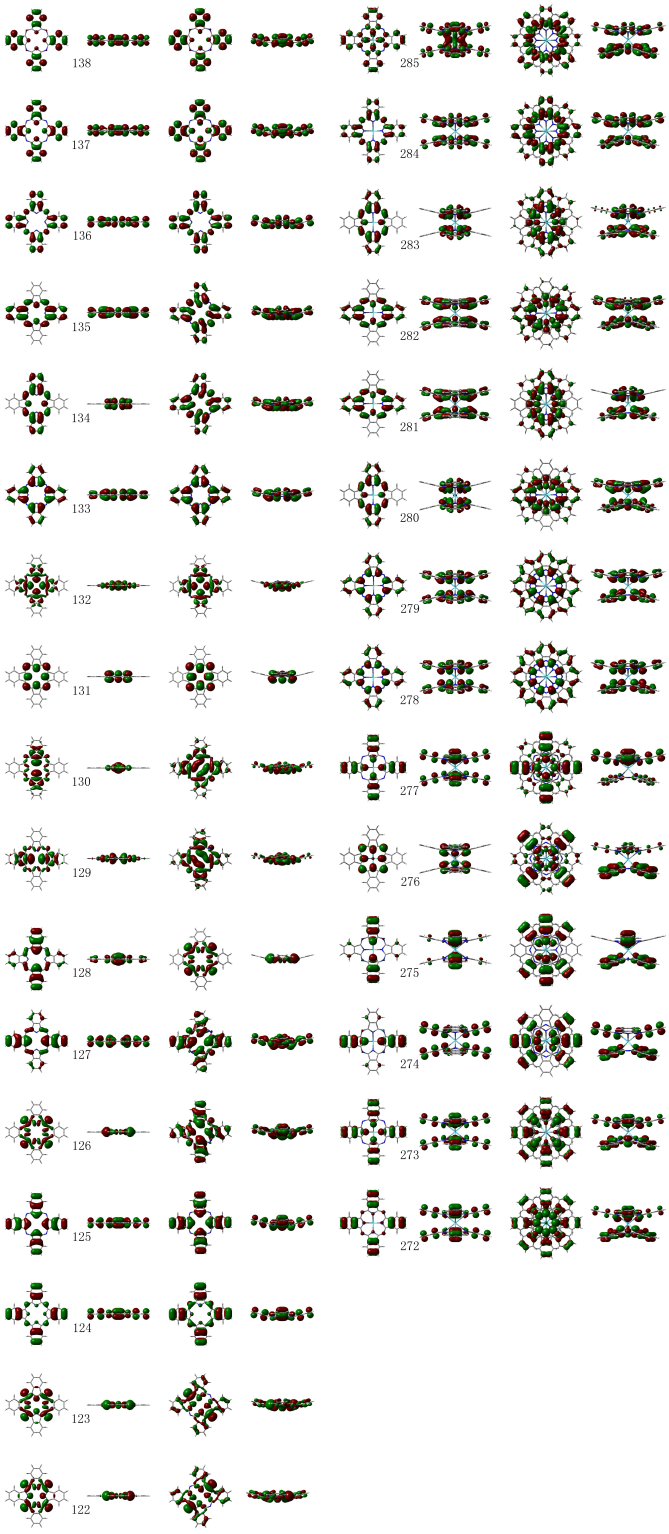

Figure S1. The orbital distributions of the bis(phthalocyaninato) lanthanum double-decker.

Table S1. Molecular orbital energy of the bis(phthalocyaninato) lanthanum double-decker.

Molecular orbital energy of $[La(Pc)_2]^-$ (eV)										
Rotation Angle (α)	**0**	**5**	**10**	**15**	**20**	**25**	**30**	**35**	**40**	**45**
MO(283)	-0.02	-0.03	-0.04	-0.06	-0.08	-0.11	-0.09	-0.09	-0.07	-0.09
MO(282)	-0.03	-0.03	-0.04	-0.07	-0.09	-0.11	-0.09	-0.10	-0.08	-0.09
MO(281)	-0.28	-0.27	-0.26	-0.25	-0.25	-0.26	-0.24	-0.25	-0.25	-0.25
MO(280)	-0.28	-0.28	-0.26	-0.26	-0.26	-0.25	-0.25	-0.26	-0.25	-0.25
MO(279)	-2.23	-2.25	-2.26	-2.30	-2.34	-2.36	-2.31	-2.29	-2.24	-2.25
MO(278)	-2.51	-2.51	-2.47	-2.44	-2.39	-2.42	-2.45	-2.51	-2.51	-2.52
Gap between MO(280,281) and MO(282,283)	0.26	0.24	0.22	0.19	0.17	0.15	0.16	0.16	0.17	0.16
Gap between MO(278) and MO(279)	0.28	0.26	0.21	0.14	0.05	0.06	0.15	0.21	0.27	0.28
Gap between MO(279) and MO(280)	1.95	1.97	2.00	2.04	2.09	2.11	2.05	2.03	1.99	1.99
Molecular orbital energy of $[La(Pc)_2]$ (eV)										
Rotation Angle (α)	**0**	**5**	**10**	**15**	**20**	**25**	**30**	**35**	**40**	**45**
MO(283α)	-2.43	-2.45	-2.48	-2.49	-2.38	-2.48	-2.53	-2.51	-2.47	-2.47
MO(283β)	-2.24	-2.27	-2.29	-2.31	-2.29	-2.34	-2.35	-2.33	-2.32	-2.31
MO(282α)	-2.44	-2.45	-2.48	-2.49	-2.39	-2.49	-2.53	-2.52	-2.47	-2.48
MO(282β)	-2.26	-2.27	-2.29	-2.31	-2.29	-2.34	-2.35	-2.33	-2.32	-2.31
MO(281α)	-2.75	-2.77	-2.76	-2.74	-2.85	-2.73	-2.73	-2.72	-2.77	-2.75
MO(281β)	-2.62	-2.63	-2.62	-2.60	-2.64	-2.56	-2.58	-2.58	-2.60	-2.60
MO(280α)	-2.77	-2.77	-2.76	-2.74	-2.87	-2.74	-2.73	-2.72	-2.79	-2.76
MO(280β)	-2.63	-2.63	-2.62	-2.60	-2.66	-2.56	-2.58	-2.58	-2.61	-2.60
MO(279α)	-4.70	-4.74	-4.77	-4.81	-4.60	-4.77	-4.75	-4.76	-4.68	-4.68
MO(279β)	-3.91	-3.92	-3.96	-3.99	-4.14	-4.08	-4.01	-3.93	-3.94	-3.95
MO(278α)	-5.03	-5.05	-5.02	-4.96	-5.09	-4.95	-4.98	-5.01	-5.10	-5.08

MO(278β)	-4.73	-4.73	-4.70	-4.65	-4.55	-4.58	-4.67	-4.70	-4.72	-4.75
Gap between MO(280α,281α) and MO(282α,283α)	0.37	0.37	0.33	0.29	0.36	0.22	0.23	0.25	0.29	0.29
Gap between MO(280β,281β) and MO(282β,283β)	0.32	0.32	0.28	0.25	0.47	0.25	0.20	0.20	0.31	0.28
Gap between MO(278α) and MO(279α)	0.82	0.81	0.74	0.66	0.41	0.50	0.66	0.77	0.78	0.80
Gap between MO(278β) and MO(279β)	0.33	0.32	0.25	0.16	0.48	0.17	0.24	0.25	0.42	0.40
Gap between MO(279α) and MO(280α)	1.28	1.28	1.34	1.39	1.49	1.52	1.43	1.35	1.34	1.35
Gap between MO(279β) and MO(280β)	1.93	1.96	2.00	2.06	1.73	2.03	2.02	2.04	1.89	1.92
Molecular orbital energy of $[La(Pc)_2]^+$ (eV)										
Rotation Angle (α)	**0**	**5**	**10**	**15**	**20**	**25**	**30**	**35**	**40**	**45**
MO(283)	-4.76	-4.76	-4.77	-4.80	-4.80	-4.84	-4.82	-4.81	-4.81	-4.81
MO(282)	-4.77	-4.76	-4.77	-4.80	-4.80	-4.84	-4.82	-4.81	-4.81	-4.81
MO(281)	-5.10	-5.09	-5.08	-5.06	-5.03	-5.03	-5.03	-5.04	-5.05	-5.06
MO(280)	-5.12	-5.09	-5.08	-5.07	-5.03	-5.03	-5.03	-5.04	-5.05	-5.06
MO(279)	-6.47	-6.49	-6.49	-6.54	-6.58	-6.58	-6.52	-6.50	-6.47	-6.46
MO(278)	-7.23	-7.22	-7.19	-7.15	-7.08	-7.10	-7.15	-7.19	-7.22	-7.23
Gap between MO(280,281) and MO(282,283)	0.34	0.34	0.31	0.27	0.23	0.20	0.21	0.23	0.24	0.25
Gap between MO(278) and MO(279)	0.76	0.73	0.70	0.61	0.50	0.52	0.63	0.69	0.75	0.77
Gap between MO(279) and MO(280)	1.35	1.39	1.41	1.47	1.54	1.55	1.49	1.46	1.42	1.41