Supporting information for

Third order NLO properties of corannulene and its Li-doped dimers: effect of the concave-convex and convex-convex stuctures

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Table S1 BSSE estimated by B97-D and M06-2X calculations for the eclipsed concave-convex model of corannulene dimer with various basis sets (energy in kcal/mol).

Basis set	B97-D	M06-2X	
6-31+G*	15.2	13.3	Ref. 32
6-31+G**	15.5	13.8	Our work
cc-pVTZ	16.1	12.3	Ref. 34
cc-pVQZ	16.6	13.3	Ref. 29

Table S2 Simulated wavelengths (nm), energies (eV), oscillator strengths (*f*), major contribution for the studied dimers.

Dimers	State	λ_{gm}	E_{gm}	f	MO transitions
1a	23	252.4	4.91	0.3951	H-7→L (29%), H-6→L+1 (29%)
	37	221.6	5.60	0.6299	H-2→L+4 (31%), H-2→L+7 (11%) H-2→L+10 (4%)
2a	7	299.4	4.14	0.1137	H→ L (49%), H-1→L+1 (48%)
	16	253.4	4.89	0.5323	H-5→L+1 (38%), H-4→L (38%)
	35	216.6	5.72	0.9036	H→L+13 (34%), H-6→L+4 (20%)
1b	19	254.1	4.88	0.6421	H-1→L+2 (24%), H→L+3 (22%) H-5→L+1 (14%), H-4→L (12%)
	37	221.6	5.60	0.6299	H-2→L+4 (31%), H-2→L+7(11%) H-2→L+10 (14%)
2b	16	266.6	4.65	0.6503	H-5→L+1 (46%), H-4→L (46%)
	35	215.2	5.76	0.5444	H-3→L+5 (34%), H-6→L+4(20%)

[a] assignment: H = HOMO, L = LUMO, H-1= HOMO-1, L+1 = LUMO+1, *etc*.

Table S3 The orbital overlap integral (S_{ij}, a.u.) and electronic coupling (V_{ij}, a.u.) between HOMOs of two monomers of the studied dimers.

Dimers	S_{ij}	V_{ij}
1a	0.013	-0.009
2a	0.112	-0.080
1b	-0.004	0.003
2b	-1.361	0.975

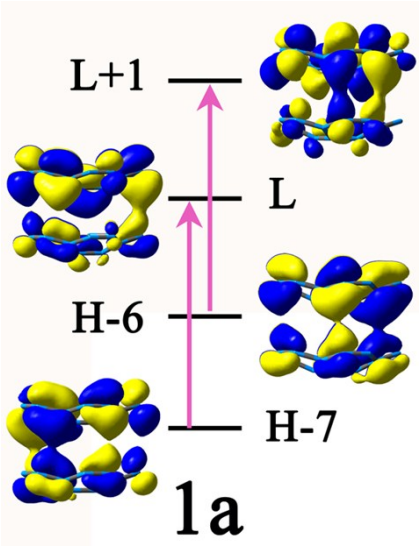

Fig. S1 Orbital diagrams of **1a** involved in the dominant electron transition (H = HOMO, H-1 = HOMO-1, L = LUMO, L+1 = LUMO, etc.).

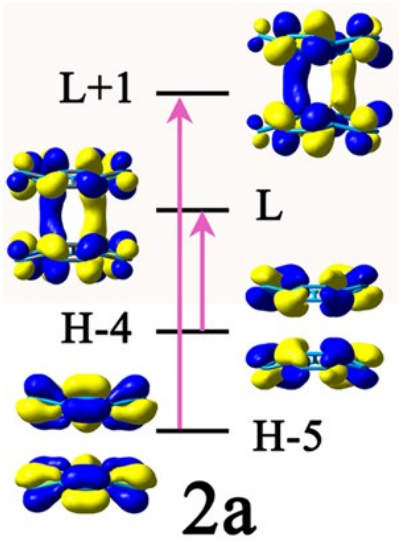

Fig. S2 Orbital diagrams of **2a** involved in the dominant electron transition.

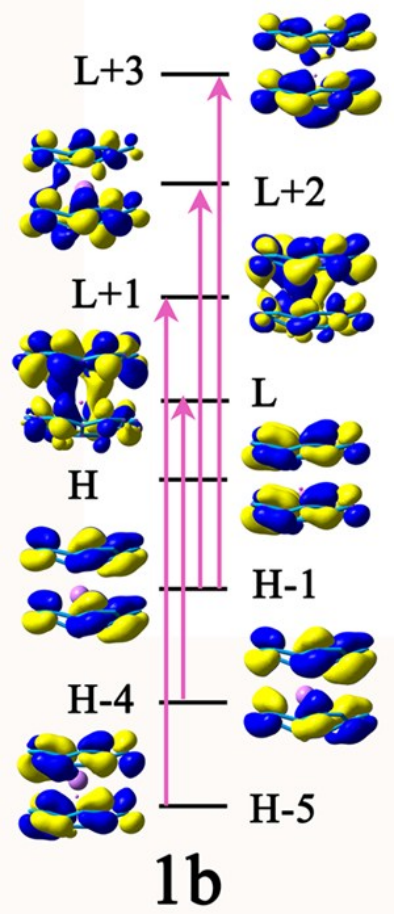

Fig. S3 Orbital diagrams of **1b** involved in the dominant electron transition.

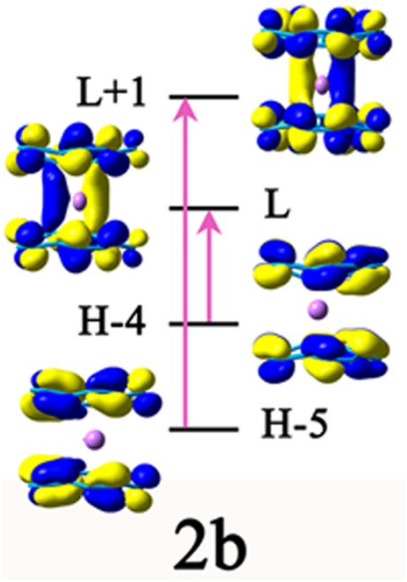

Fig. S4 Orbital diagrams of **2b** involved in the dominant electron transition.