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Supporting Information

Porphyrin Dimers: A Theoretical Understanding of the Impact of Electronic Coupling Strength on the Two-Photon Absorption Properties

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Content:

Table S1. Lowest 4 OPA-active states with significant transition dipole moments in porphyrin dimers, computed at the INDO/CIS level.

	State 1			State 2			State 3			State 4		
	E / eV	μ_{01} / D	f	E / eV	μ_{02} / D	f	E / eV	μ_{03} / D	f	E / eV	μ_{04} / D	f
1-0	1.86	1.2	0.0	1.86	1.2	0.01	2.93	2.4	0.1	2.93	2.4	0.07
1-1	1.71	6.8	0.30	2.65	19.5	3.82	3.17	9.7	1.13	3.35	11.1	1.57
1-2	1.74	6.8	0.30	2.62	18.2	3.31	3.27	15.3	2.92	3.37	10.5	1.42
1-3	1.76	6.5	0.29	2.54	14.5	2.02	3.12	19.0	4.25	3.29	16.9	3.56
1-4	1.78	6.5	0.29	2.42	9.5	0.84	2.95	19.1	4.10	3.11	13.5	2.16
1-6	1.79	6.8	0.31	2.18	4.3	0.15	2.61	4.1	0.16	2.87	20.0	4.35
1-2(0)	1.74	6.8	0.30	2.62	18.2	3.31	3.27	15.3	2.92	3.37	10.5	1.42
1-2(30)	1.74	5.9	0.23	2.68	19.0	3.68	3.11	4.1	0.20	3.19	9.2	1.03
1-2(45)	1.77	5.7	0.22	2.66	16.1	2.61	3.12	17.1	3.45	3.24	7.4	0.68
1-2(60)	1.78	5.3	0.19	2.69	14.6	2.17	3.04	18.4	3.89	3.26	9.1	1.04
1-2(80)	1.80	4.5	0.14	2.92	23.4	6.10	3.31	13.4	2.28	3.32	13.4	2.27
1-2(90)	1.80	4.8	0.16	2.75	8.1	0.69	2.93	22.0	5.38	3.30	12.1	1.84
2	1.81	6.0	0.25	2.51	19.0	3.45	3.13	3.3	0.13	3.19	4.5	0.24
3	1.81	5.8	0.23	2.42	17.7	2.89	3.20	14.8	2.66	3.25	5.9	0.43
4	1.38	8.1	0.34	2.51	21.3	4.34	2.73	5.1	0.27	2.92	5.0	0.27
5	1.53	16.8	1.65	2.28	9.1	0.71	2.66	6.6	0.45	3.26	9.6	1.14
6	1.49	16.8	1.59	2.25	8.5	0.62	2.60	6.7	0.44	3.20	7.8	0.74
7	1.73	7.3	0.35	2.07	8.2	0.53	2.88	2.9	0.09	3.06	20.2	4.76

Table S2. Lowest 4 OPA-active states with significant transition dipole moments in porphyrin dimers, computed at the INDO/MRDCI level.

	State 1			State 2			State 3			State 4		
	E / eV	μ_{01} / D	f	E / eV	μ_{02} / D	f	E / eV	μ_{03} / D	f	E / eV	μ_{04} / D	f
1-0	2.24	1.8	0.03	2.30	1.4	0.02	3.10	1.6	0.03	3.12	1.0	0.01
1-1	2.07	9.0	0.64	3.00	13.6	2.12	3.27	3.7	0.17	3.49	5.6	0.41
1-2	2.10	9.3	0.69	2.98	14.5	2.37	3.39	2.1	0.06	3.59	2.6	0.09
1-3	2.12	8.8	0.63	2.96	14.7	2.43	3.45	3.1	0.13	3.60	2.7	0.10
1-4	2.15	9.1	0.68	2.93	13.4	1.99	3.42	6.8	0.60	3.52	4.7	0.30
1-6	2.17	9.7	0.77	2.91	8.8	0.86	3.23	5.8	0.41	3.37	14.2	2.57
1-2(0)	2.10	9.3	0.69	2.98	14.5	2.37	3.39	2.1	0.06	3.59	2.6	0.09
1-2(30)	2.12	8.9	0.64	2.99	13.6	2.10	3.43	3.0	0.12	3.43	2.3	0.07
1-2(45)	2.14	8.0	0.52	2.99	12.4	1.76	3.27	2.3	0.07	3.51	3.4	0.16
1-2(60)	2.18	7.5	0.46	3.01	11.2	1.43	3.40	3.5	0.16	3.50	3.9	0.20
1-2(80)	2.24	7.5	0.48	3.06	4.9	0.28	3.32	2.2	0.06	3.47	18.3	4.40
1-2(90)	2.24	7.0	0.42	3.09	3.1	0.11	3.33	3.1	0.12	3.46	17.1	3.82
2	2.16	9.1	0.68	2.89	15.2	2.53	3.40	4.1	0.22	3.49	6.8	0.61
3	2.19	8.7	0.63	2.80	14.8	2.31	3.14	3.4	0.14	3.43	3.3	0.14
4	1.57	8.2	0.40	2.56	2.4	0.05	2.74	14.2	2.09	3.15	2.4	0.07
5	1.07	15.2	0.94	2.10	4.8	0.18	2.34	4.3	0.17	2.84	6.1	0.40
6	1.03	15.3	0.91	2.06	5.1	0.20	2.31	3.7	0.12	2.78	5.4	0.31
7	2.01	10	0.76	2.33	7.2	0.46	3.10	4.4	0.23	3.36	21	5.63

Table S3. Lowest 2 TPA-active states with significant transition dipole moments in porphyrin dimers, computed at the INDO/MRDCI–SOS level.

	State 5						State 6					
	E / eV	μ_{15} / D	μ_{25} / D	μ_{35} / D	μ_{45} / D	δ / GM	E / eV	μ_{16} / D	μ_{26} / D	μ_{36} / D	μ_{46} / D	δ / GM
1-0	3.55	2.2	0.0	2.6	0.7	5.3E+01				N/A		
1-1	2.39	2.3	1.7	0.7	2.3	2.0E+01	2.89	12.5	11.3	1.4	0.3	2.0E+03
1-2	2.32	3.6	3.6	0.2	0.8	2.1E+01	2.99	14.7	17.2	1.2	0.2	2.0E+03
1-3	2.28	3.1	3.5	3.3	1.5	4.5E+01	3.07	12.6	19.3	3.4	1.7	3.7E+03
1-4	2.26	3.8	3.8	5.9	0.4	6.0E+01	3.21	14.9	19.9	12.6	0.7	7.1E+03
1-6	2.24	2.5	1.9	5.5	0.6	2.4E+01	3.41	12.8	19.3	12.3	6.1	1.1E+04
1-2(0)	2.32	3.6	3.6	0.2	0.8	2.1E+01	2.99	14.7	17.2	1.2	0.2	2.0E+03
1-2(30)	2.32	3.3	3.4	2.9	1.7	2.1E+01	3.01	14.6	19.6	1.5	1.9	2.2E+03
1-2(45)	2.31	2.5	3.1	0.9	2.3	1.5E+01	3.03	13.3	23.6	3.0	2.2	2.0E+03
1-2(60)	2.31	2.2	2.9	1.0	2.2	7.1E+00	3.07	11.9	26.8	5.7	4.7	7.0E+02
1-2(80)	2.33	0.9	1.0	2.8	0.5	1.1E+00	3.09	6.9	35.9	4.2	9.6	3.0E+02
1-2(90)	2.33	0.8	0.6	2.1	0.9	1.0E+00	3.14	4.0	38.1	3.8	6.3	7.3E+01
2	2.31	4.7	4.1	2.1	1.2	9.2E+01	3.09	15.2	16.6	5.3	1.2	4.9E+03
3	2.29	3.1	3.5	5.6	0.2	4.1E+01	3.011	14.8	20.2	7.3	2.8	4.3E+03
4	2.48	3.5	0.5	0.0	0.0	1.6E+02	2.89	2.6	1.2	6.0	5.1	3.8E+02
5	2.10					1.7E+06[a]	2.22					6.4E+04[a]
6	2.06					7.1E+07[a]	2.17					1.4E+04[a]
7	2.58	17.3	16.7	19.4	2.4	3.6E+03	3.40	7.3	4.4	1.0	3.9	5.0E+03

[a]TPA is mainly due to double resonance effects.