

Supporting Information

N719 Derivatives for Application in a Dye-Sensitized Solar Cell (DSSC): A Theoretical Study

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Table S1. HOMO, LUMO and HOMO-LUMO gap values of N719 neutral derivatives calculated by different level of theory approximations.

System	M06/LANL2DZ/ Double-Zeta			M06/LANL2DZ 6-311+G(2d,p)			BPW91/LANL2DZ 6-311+G(2d,p)		
	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]
N719	-5.50	-2.89	2.61	-5.67	-3.01	2.66	-4.81	-3.66	1.14
N719-2	-5.59	-2.89	2.70	-5.76	-3.01	2.75	-4.84	-3.66	1.18
N719-3	-3.88	-2.77	1.11	-4.04	-2.91	1.14	-3.56	-3.40	0.17
N719-4	-3.88	-2.78	1.10	-4.05	-2.92	1.13	-3.56	-3.41	0.16
N719-5	-3.86	-2.73	1.13	-4.03	-2.88	1.15	-3.54	-3.35	0.19
N719-6	-3.89	-2.74	1.15	-4.05	-2.89	1.16	-3.57	-3.36	0.21
N719-7	-5.59	-2.84	2.75	-5.78	-2.97	2.81	-4.87	-3.63	1.23
N719-8	-5.86	-2.82	3.04	-6.07	-2.96	3.12	-5.13	-3.62	1.51
N719-9	-3.90	-2.78	1.12	-4.07	-2.92	1.15	-3.58	-3.40	0.18
N719-10	-3.90	-2.77	1.13	-4.07	-2.91	1.16	-3.57	-3.40	0.17

Table S2. HOMO, LUMO and HOMO-LUMO gap values of N719 di-anionic derivatives calculated by different level of theory approximations.

System	M06/LANL2DZ/ Double-Zeta			M06/LANL2DZ 6-311+g(2d,p)			BPW91/LANL2DZ 6-311+g(2d,p)		
	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]	E _{HOMO} [eV]	E _{LUMO} [eV]	Δ _{H-L} [eV]
N719	-5.24	-2.54	2.70	-5.41	-2.66	2.75	-4.53	-3.31	1.22
N719-2	-5.35	-2.55	2.80	-5.53	-2.67	2.86	-4.58	-3.31	1.27
N719-3	-3.68	-2.45	1.24	-3.86	-2.57	1.29	-3.19	-3.09	0.10
N719-4	-3.68	-2.46	1.22	-3.86	-2.59	1.28	-3.20	-3.10	0.09
N719-5	-3.65	-2.41	1.24	-3.83	-2.54	1.29	-3.16	-3.05	0.11
N719-6	-3.64	-2.43	1.21	-3.83	-2.57	1.25	-3.18	-3.04	0.14
N719-7	-5.32	-2.50	2.82	-5.51	-2.63	2.88	-4.57	-3.29	1.28
N719-8	-5.56	-2.48	3.08	-5.78	-2.62	3.16	-4.81	-3.28	1.53
N719-9	-3.70	-2.44	1.26	-3.88	-2.56	1.32	-3.20	-3.07	0.13
N719-10	-3.64	-2.47	1.17	-3.83	-2.60	1.22	-3.19	-3.08	0.11

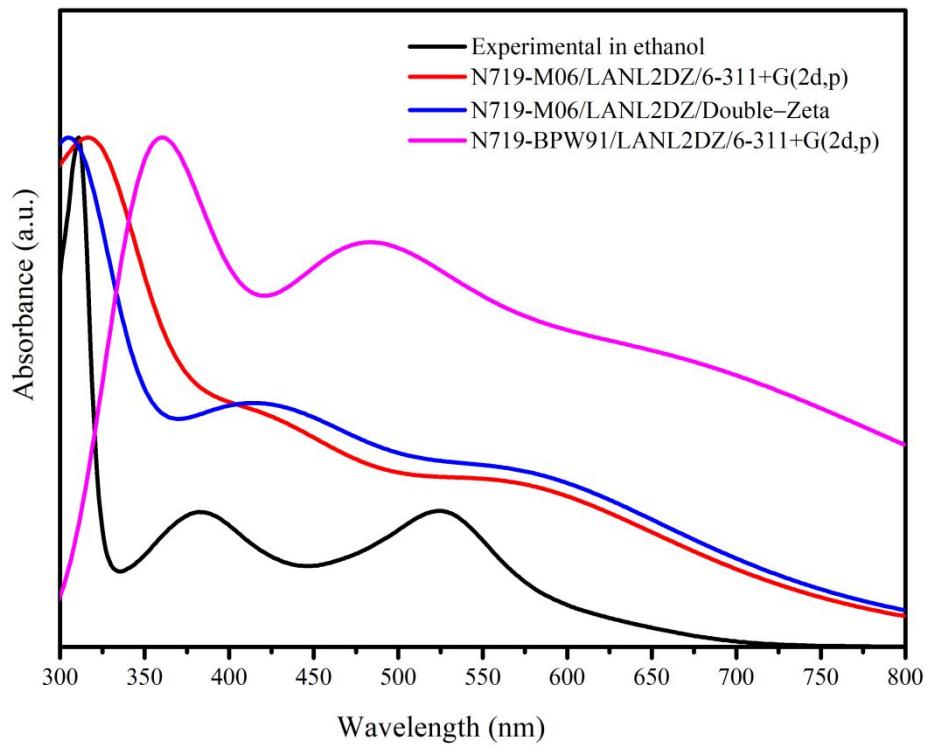


Figure S1. Comparison of theoretical UV-Visible spectra of N719 (di-anionic) obtained by different methodologies and experimental UV-Visible spectrum obtained in our laboratory.