Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
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Evaluating push-pull dyes efficiency using TD-DFT and Charge Transfer indices

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Supporting Material

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Figure SI.1. λ_{theo} (in eV) *vs* λ_{exp} (in eV) together with associated linear regression. Dotted lines corresponds to fit where values for compounds **1***c*, **2***c* and **4***c* (white points) were not included.

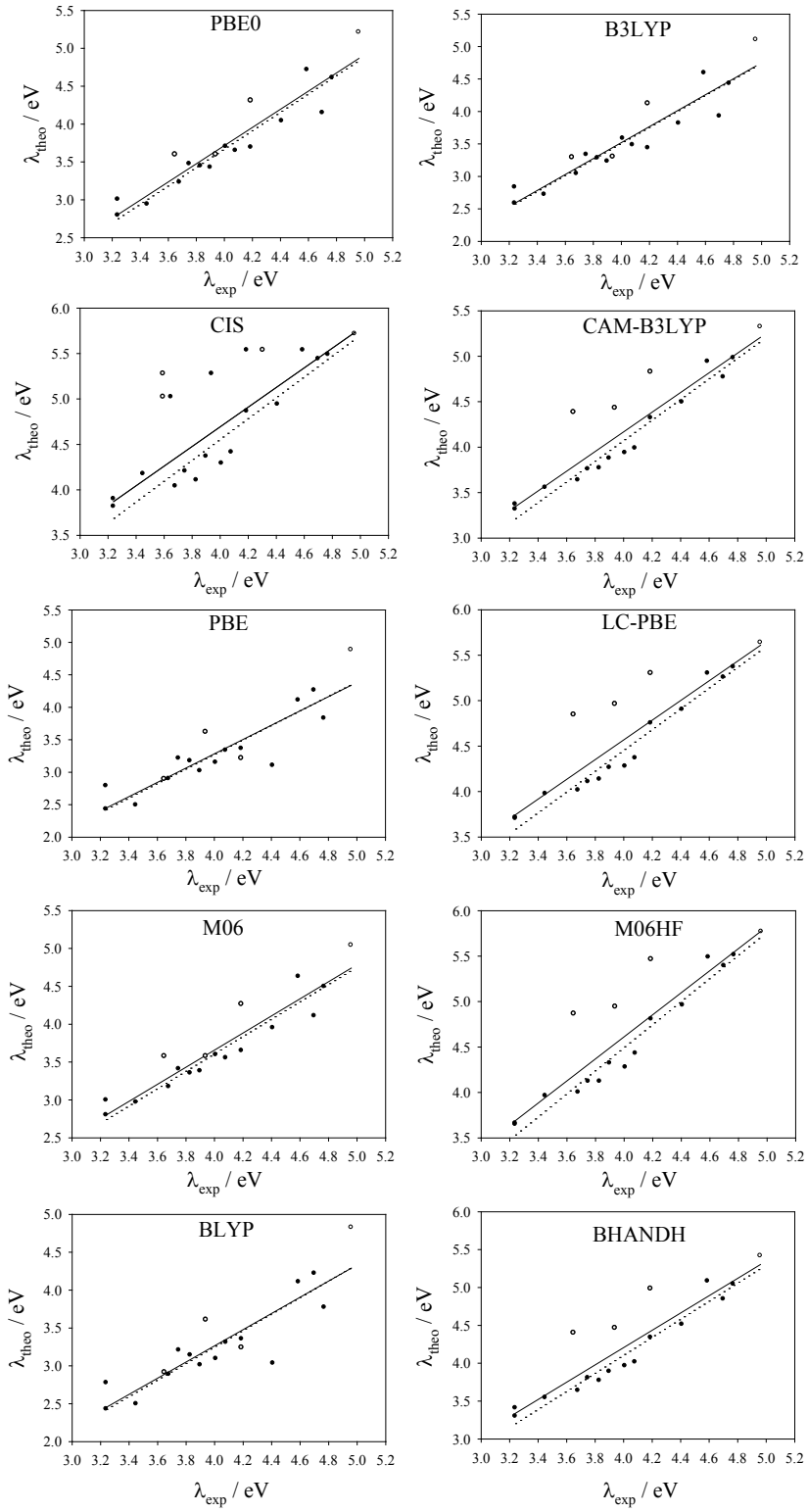
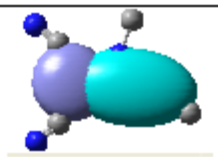
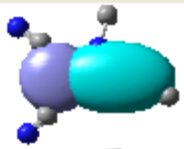
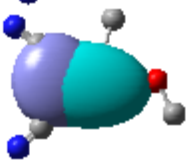
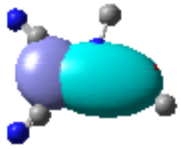
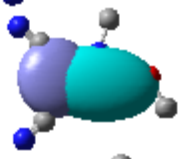
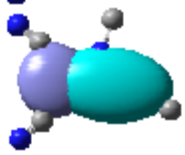
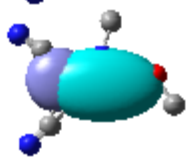
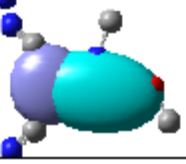


Table SI.1. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **1a**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				1a			
PBE0	238	0.3605	1.42	0.35	2.35	1.58	
B3LYP	243	0.3520	1.45	0.34	2.37	1.59	
CIS	217	0.5516	0.89	0.42	1.78	1.83	
CAM-B3LYP	233	0.3671	1.36	0.36	2.34	1.60	
PBE	254	0.3159	1.63	0.32	2.50	1.40	
LC-PBE	220	0.3790	1.30	0.37	2.33	1.61	
M06	246	0.3335	1.29	0.34	2.15	1.52	
M06-HF	215	0.4272	1.29	0.35	2.15	1.52	
BLYP	257	0.3156	1.62	0.32	2.49	1.47	
BHandH	229	0.3853	1.26	0.36	2.20	1.62	
Experimental	250						

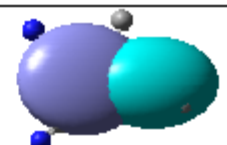
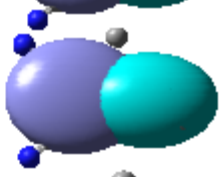
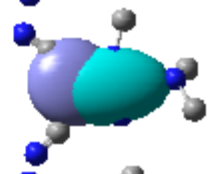
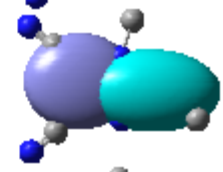
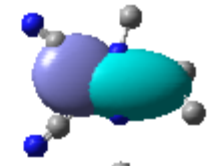
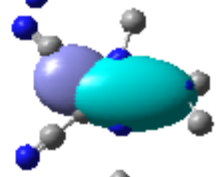
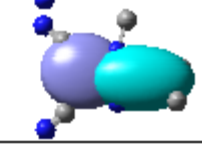
a) Isocontour value 0.001

Table SI.2. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **1b**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				1b			
PBE0	263	0.3141	2.48	0.45	5.37	1.77	
B3LYP	270	0.2977	2.56	0.46	5.56	1.84	
CIS	224	0.6180	1.22	0.44	2.57	0.78	
CAM-B3LYP	251	0.3605	2.12[a]	0.43	4.38	1.47	
PBE	302	0.1891	3.06	0.53	7.87	2.19	
LC-PBE	234	0.3990	1.87	0.43	3.84	1.21	
M06	268	0.3092	2.32	0.43	4.83	1.67	
M06-HF	226	0.4364	1.83	0.42	3.72	1.12	
BLYP	302	0.1965	3.02	0.53	7.64	2.17	
BHandH	244	0.3889	1.96	0.42	3.99	1.37	
Experimental	270						

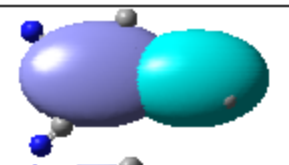
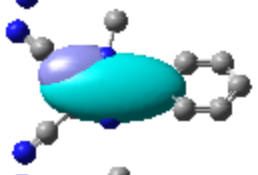
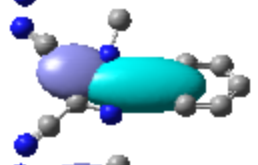
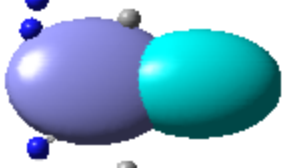
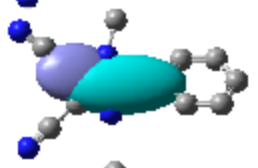
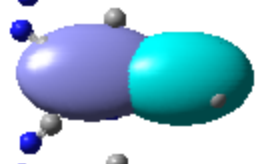
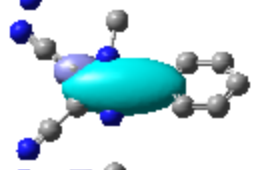
a) Isocontour value 0.001

Table SI.3. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **1c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					1c		
PBE0	288	0.1247	3.06	0.83	12.15	1.68	
B3LYP	301	0.1027	3.07	0.86	12.74	1.71	
CIS	224	0.5835	1.30	0.46	2.85	2.40	
CAM-B3LYP	257	0.2671	2.70	0.58	7.59	1.84	
PBE	386	0.0341	3.18	0.93	14.24	1.77	
LC-PBE	234	0.3546	2.13	0.48	4.88	2.10	
M06	291	0.1386	2.99	0.79	11.36	1.63	
M06-HF	227	0.392	2.07	0.46	4.65	2.11	
BLYP	383	0.0361	3.16	0.94	14.22	1.77	
BHandH	249	0.3004	2.58	0.56	6.87	1.94	
Experimental	296						

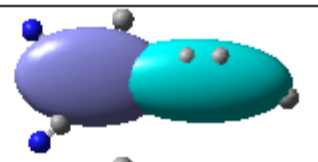
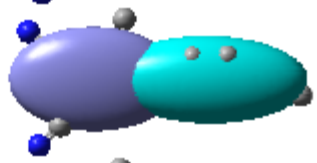
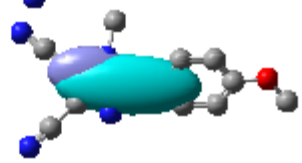
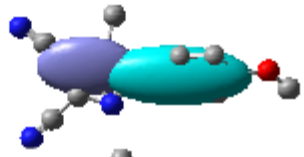
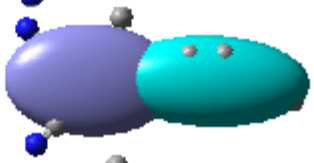
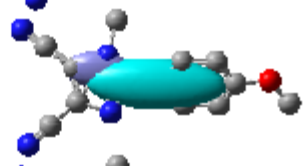
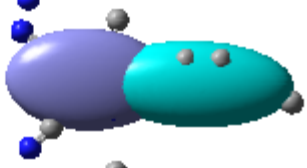
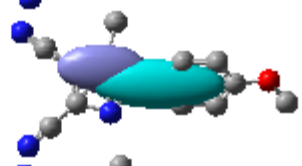
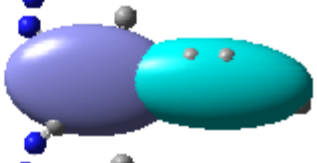
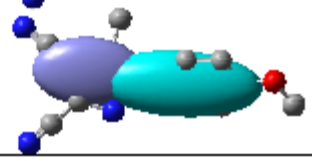
a) Isocontour value 0.001

Table SI.4. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **2a**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					2a		
PBE0	269	0.2945	3.84	0.93	17.08	2.13	
B3LYP	280	0.2424	3.97	1.07	20.34	2.17	
CIS	226	0.6691	1.31	0.45	2.84	2.01	
CAM-B3LYP	249	0.4353	2.67	0.47	5.97	2.63	
PBE	324	0.0913	4.14	1.10	21.85	2.23	
LC-PBE	231	0.4751	1.91	0.42	3.86	2.70	
M06	276	0.3027	3.64	0.85	14.931	2.06	
M06-HF	225	05477	1.92	0.42	3.84	2.61	
BLYP	329	0.0890	4.13	1.11	21.92	2.22	
BHandH	246	0.4458	1.72	0.31	2.60	1.24	
Experimental	260						

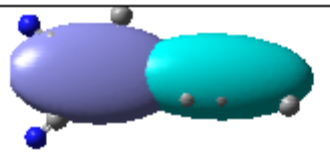
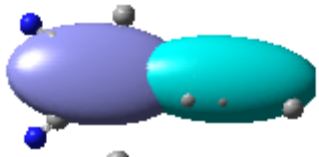
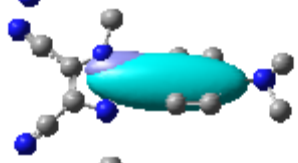
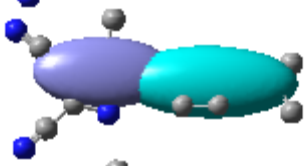
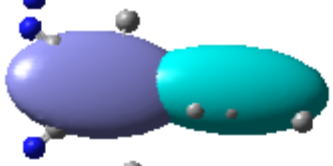
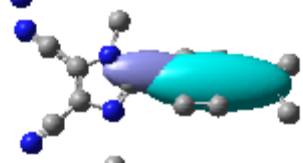
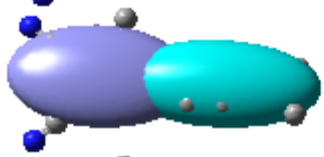
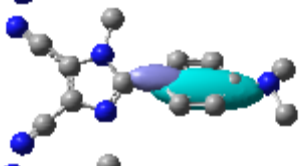
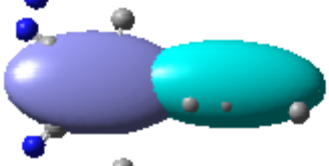
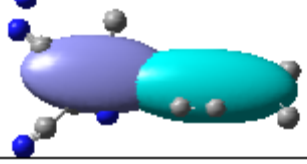
a) Isocontour value 0.001

Table SI.5. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **2b**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				2b			
PBE0	299	0.2016	4.47	0.93	20.98	3.02	
B3LYP	316	0.1555	4.53	0.98	21.29	2.95	
CIS	228	0.7661	1.61	0.48	3.68	8.60	
CAM-B3LYP	260	0.5171	3.59	0.59	10.21	4.08	
PBE	291	0.3000	4.84	1.04	24.09	2.74	
LC-PBE	236	0.6688	2.39	0.46	5.26	6.27	
M06	302	0.2247	4.32	0.91	18.91	3.08	
M06-HF	230	0.7564	2.30	0.45	4.94	8.19	
BLYP	294	0.1860	4.79	1.04	23.95	2.75	
BHandH	256	0.4903	3.64	0.63	11.06	3.93	
Experimental	264						

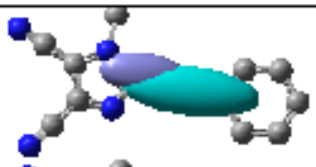
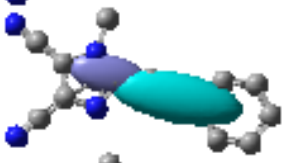
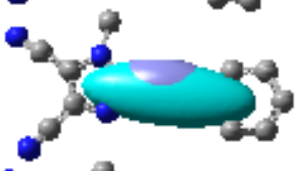
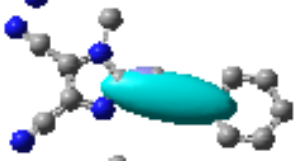
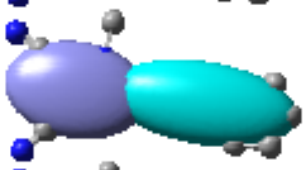
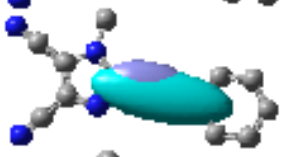
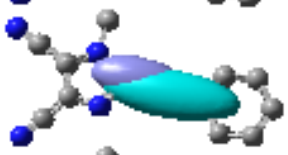
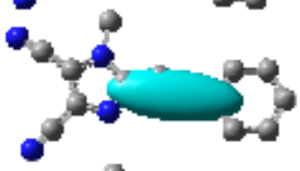
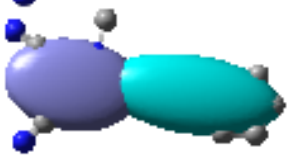
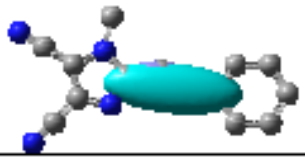
a) Isocontour value 0.001

Table SI.6. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **2c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				2c			
PBE0	345	0.1418	5.01	1.09	26.12	3.07	
B3LYP	376	0.1087	5.04	1.10	26.73	3.12	
CIS	235	0.9455	1.72	0.54	4.48	1.93	
CAM-B3LYP	280	0.6173	4.16	0.54	14.73	2.88	
PBE	343	0.1095	5.27	0.74	27.56	3.27	
LC-PBE	250	0.9053	2.63	0.55	6.95	3.50	
M06	347	0.1602	4.86	1.08	25.21	2.99	
M06-HF	251	0.7621	1.94	0.54	5.02	3.86	
BLYP	344	0.0592	5.23	1.10	27.51	3.29	
BHandH	278	0.5962	4.33	0.82	17.02	2.79	
Experimental	315						

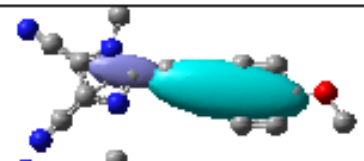
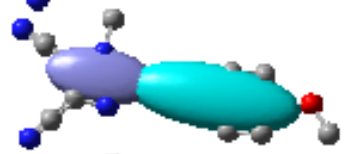
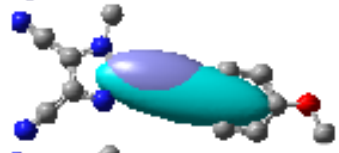
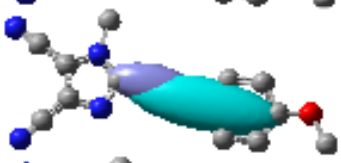
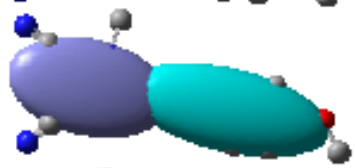
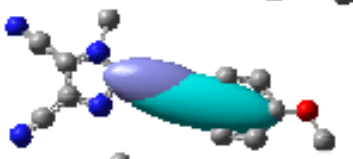
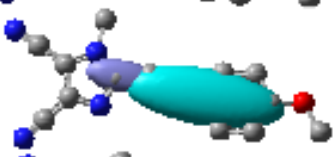
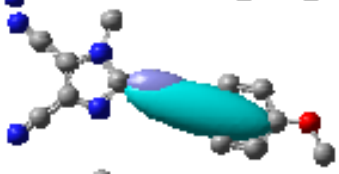
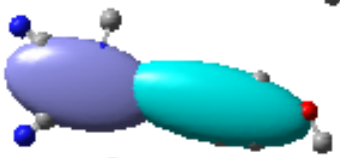
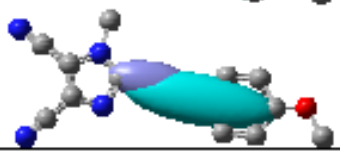
a) Isocontour value 0.001

Table SI.7. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **3a**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					3a		
PBE0	335	1.1802	1.90	0.38	3.44	2.49	
B3LYP	346	1.0613	2.99	0.42	6.05	2.73	
CIS	289	1.4308	0.34	0.50	0.82	2.55	
CAM-B3LYP	315	1.2393	0.78	0.40	1.50	2.27	
PBE	394	0.2653	5.02	0.79	19.00	3.22	
LC-PBE	290	1.2439	0.70	0.43	1.43	2.11	
M06	345	1.1374	1.60	0.39	3.02	2.56	
M06-HF	290	1.1871	0.57	0.41	1.11	2.50	
BLYP	401	0.2479	5.01	0.80	19.28	3.26	
BHandH	313	1.2661	0.66	0.41	1.31	2.25	
Experimental	309						

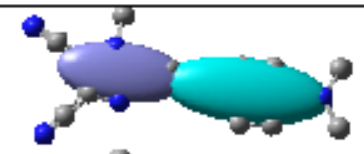
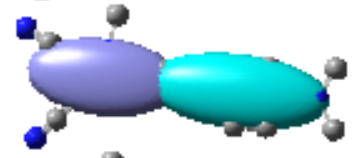
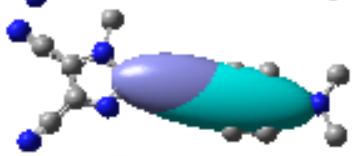
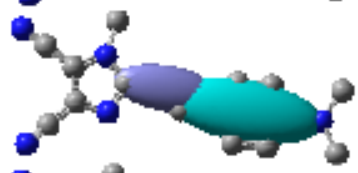
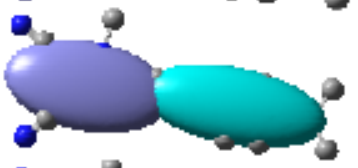
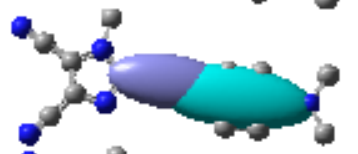
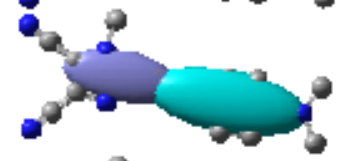
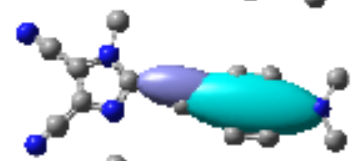
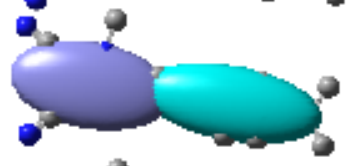
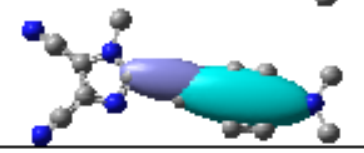
a) Isocontour value 0.001

Table SI.8. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **3b**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT} /Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					3b		
PBE0	357	1.1200	4.23	0.56	11.45	3.10	
B3LYP	372	0.8464	4.84	0.67	15.69	3.09	
CIS	295	1.5403	0.97	0.55	2.54	2.25	
CAM-B3LYP	330	1.3737	2.26	0.47	5.12	2.93	
PBE	386	1.1014	5.66	0.91	24.83	3.58	
LC-PBE	302	1.3955	1.87	0.49	4.35	2.90	
M06	364	1.1503	3.63	0.54	9.37	3.07	
M06-HF	301	1.3092	1.74	0.46	3.84	2.84	
BLYP	387	1.0987	5.60	0.92	24.72	3.60	
BHandH	326	1.4011	2.10	0.48	4.82	2.81	
Experimental	331						

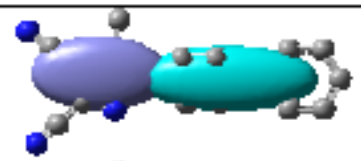
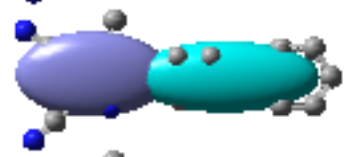
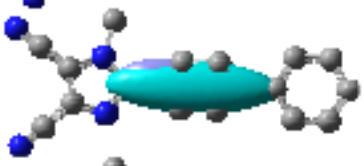
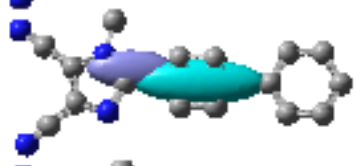
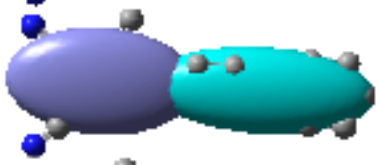
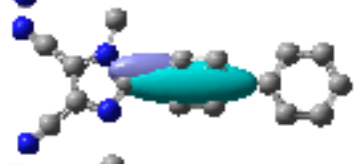
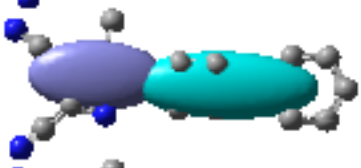
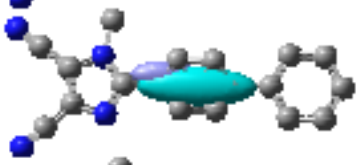
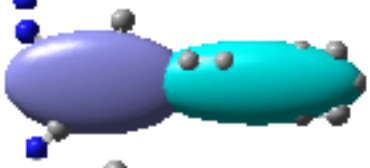
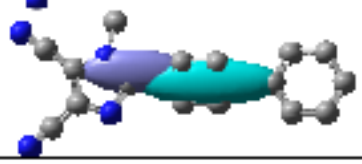
a) Isocontour value 0.001

Table SI.9. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **3c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT} / e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				3c			
PBE0	413	0.8697	5.35	0.76	19.57	3.98	
B3LYP	438	0.5526	5.67	0.87	23.82	3.98	
CIS	318	1.6423	1.71	0.63	5.16	3.52	
CAM-B3LYP	368	1.4425	3.30	0.56	8.99	3.15	
PBE	445	1.0851	6.11	0.96	28.18	3.73	
LC-PBE	334	1.4978	2.83	0.58	7.89	2.80	
M06	414	0.9914	4.79	0.71	16.45	3.91	
M06-HF	339	1.4106	3.02	0.56	8.20	2.68	
BLYP	447	1.0838	6.07	0.97	28.12	3.73	
BHandH	364	1.4737	3.25	0.58	9.03	3.29	
Experimental	383						

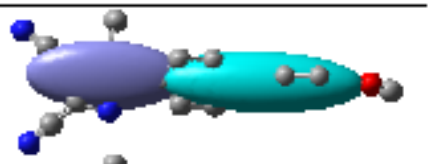
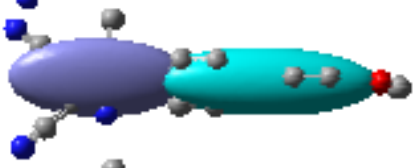
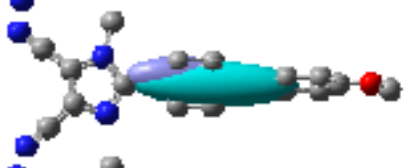
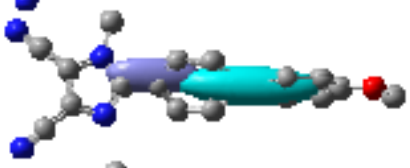
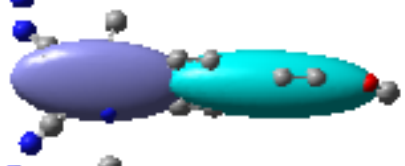
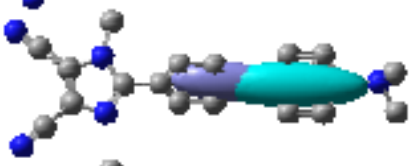
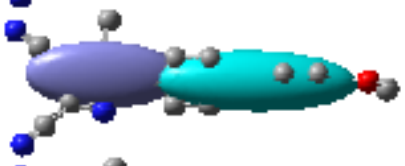
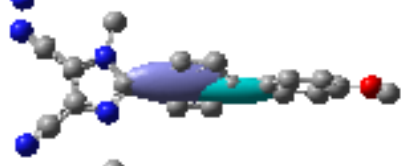
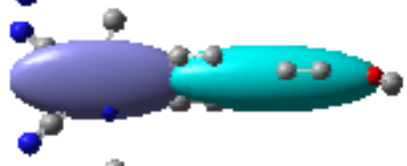
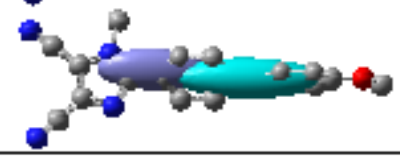
a) Isocontour value 0.001

Table SI.10. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **4a**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT} / e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				4a			
PBE0	307	0.5479	5.30	0.78	19.79	2.78	
B3LYP	325	0.3674	5.58	0.90	23.97	2.96	
CIS	251	1.2050	0.93	0.49	2.17	2.11	
CAM-B3LYP	276	1.0907	2.73	0.46	6.06	2.19	
PBE	400	0.0979	6.14	1.06	31.14	3.17	
LC-PBE	253	1.1750	1.47	0.43	3.07	1.84	
M06	314	0.6043	4.99	0.75	17.71	2.74	
M06-HF	250	0.3375	1.28	0.42	2.58	2.38	
BLYP	409	0.0927	6.13	1.06	31.24	2.28	
BHandH	275	1.0871	2.96	0.49	6.99	2.43	
Experimental	281						

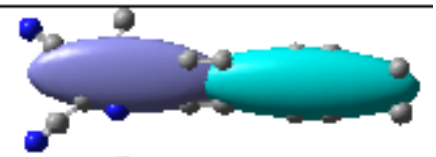
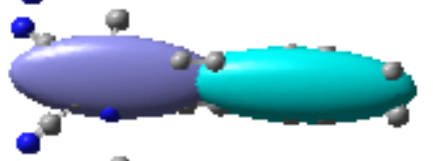
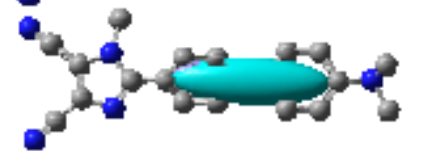
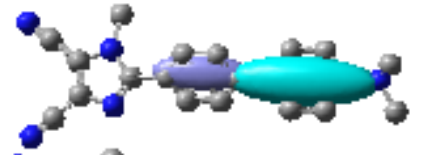
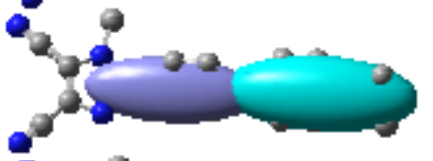
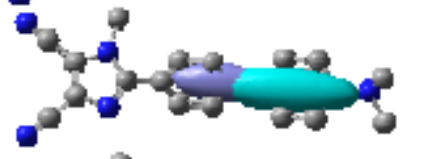
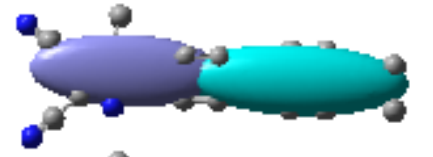
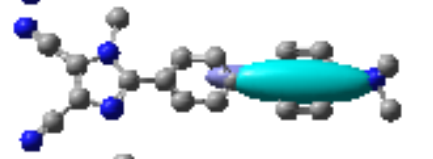
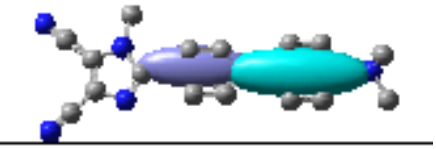
a) Isocontour value 0.001

Table SI.11. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **4b**

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				4b			
PBE0	336	0.4142	6.34	0.97	29.67	4.58	
B3LYP	361	0.2617	6.49	1.06	33.01	4.51	
CIS	255	1.3844	1.48	0.52	3.67	7.76	
CAM-B3LYP	287	1.2224	3.84	0.54	10.02	4.71	
PBE	369	0.6350	7.01	1.15	38.54	4.17	
LC-PBE	261	1.3616	2.34	0.48	5.40	5.02	
M06	340	0.4818	6.03	0.94	27.13	4.64	
M06-HF	258	1.2658	2.01	0.46	4.41	2.26	
BLYP	370	0.6380	6.03	1.15	38.34	4.19	
BHandH	286	1.1745	4.11	0.59	11.57	4.79	
Experimental	296						

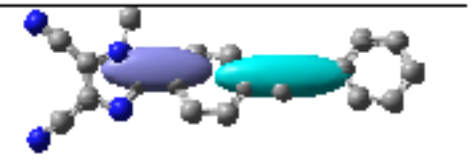
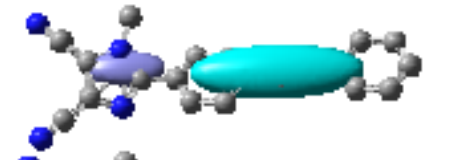
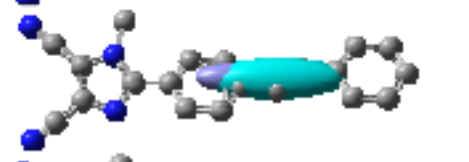
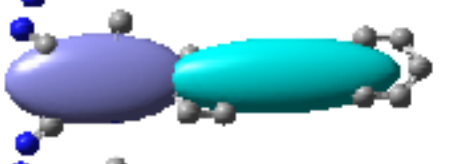
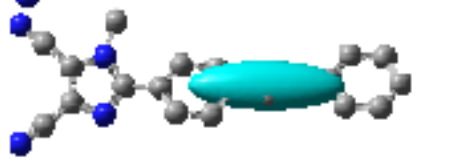
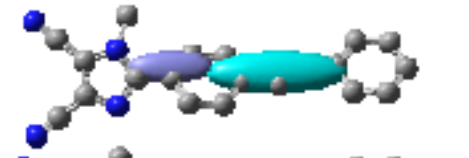
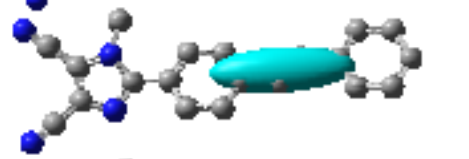
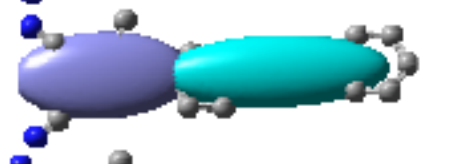
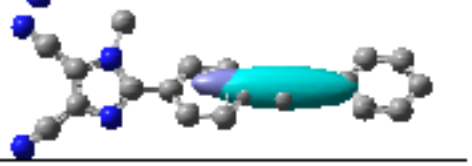
a) Isocontour value 0.001

Table SI.12. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **4c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					4c		
PBE0	345	0.2574	7.31	1.12	39.14	4.40	
B3LYP	377	0.1438	7.45	1.19	42.54	4.46	
CIS	247	1.3232	1.55	0.51	3.80	3.55	
CAM-B3LYP	283	1.1816	4.13	0.61	12.02	2.59	
PBE	429	0.3145	6.10	0.99	28.97	3.37	
LC-PBE	256	1.3218	2.63	0.52	6.60	1.95	
M06	347	0.3234	6.99	1.08	36.26	4.47	
M06-HF	255	1.3459	2.59	0.53	6.56	1.41	
BLYP	426	0.3272	7.87	1.25	47.22	4.22	
BHandH	282	1.1446	4.48	0.65	13.96	3.11	
Experimental	340						

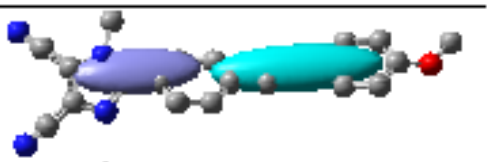
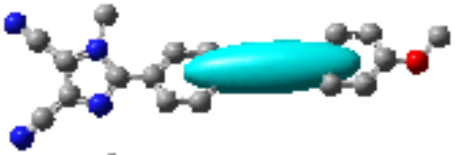
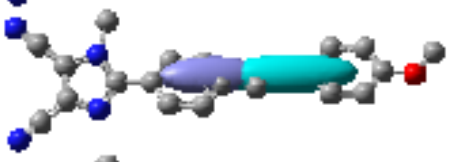
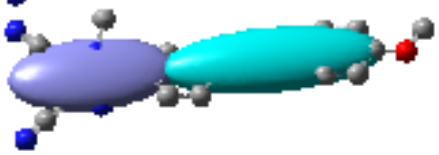
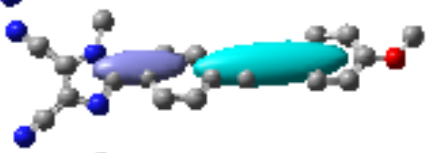
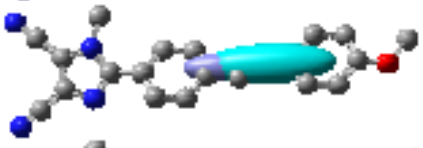
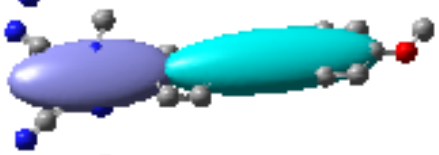
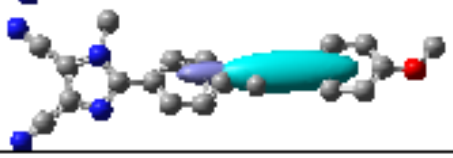
a) Isocontour value 0.001

Table SI.13. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **5a.**

Method	λ/nm	*f*	D_{CT}/Å	q_{CT} / e	μ_{CT} /Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					5a		
PBE0	360	1.2961	5.02	0.55	13.14	5.48	
B3LYP	378	0.8982	6.12	0.74	21.59	4.43	
CIS	302	1.6677	0.72	0.48	1.67	6.10	
CAM-B3LYP	329	1.5865	1.83	0.41	3.61	6.19	
PBE	391	1.3183	6.98	1.06	35.49	3.83	
LC-PBE	300	1.5823	1.14	0.42	2.31	5.81	
M06	370	1.6123	4.30	0.51	10.64	5.88	
M06-HF	301	1.5429	1.19	0.40	2.31	5.69	
BLYP	395	1.3137	6.93	1.07	35.66	3.82	
BHandH	329	1.6075	1.99	0.42	4.09	6.31	
Experimental	324						

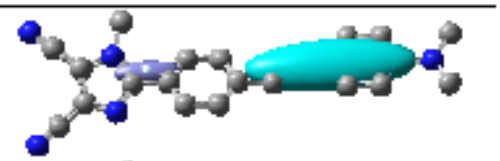
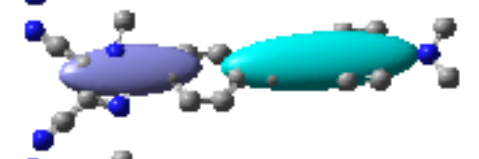
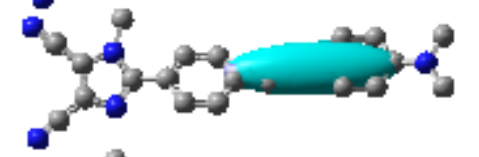
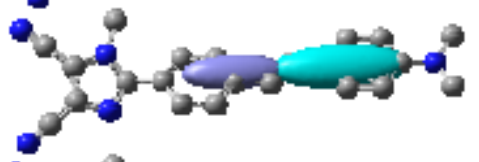
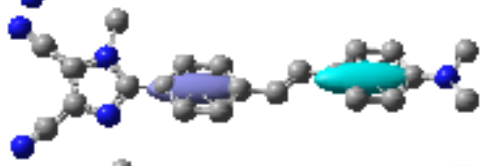
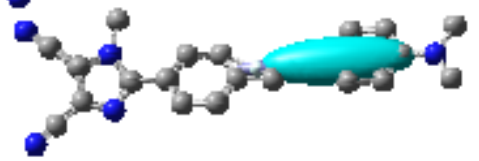
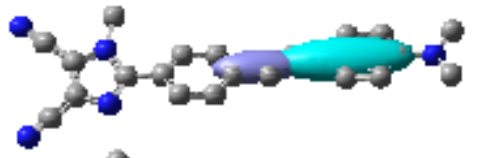
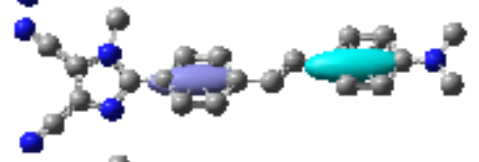
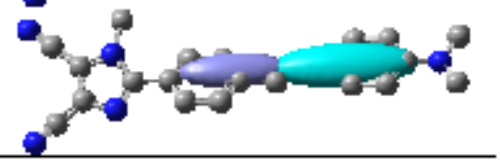
a) Isocontour value 0.001

Table SI.14. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **5b**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				5b			
PBE0	384	1.1445	6.40	0.71	21.88	5.40	
B3LYP	408	0.6954	7.02	0.90	30.31	4.22	
CIS	307	1.7428	1.45	0.51	3.57	5.27	
CAM-B3LYP	341	1.677'	3.21	0.48	7.40	5.79	
PBE	428	1.1815	7.68	0.47	40.80	4.19	
LC-PBE	309	1.7071	2.27	0.47	5.13	5.42	
M06	391	1.2307	5.72	0.66	18.15	5.66	
M06-HF	310	1.6392	2.29	0.45	4.97	5.40	
BLYP	430	1.1843	7.60	1.11	40.66	4.15	
BHandH	341	1.6911	3.33	0.50	7.95	5.88	
Experimental	337						

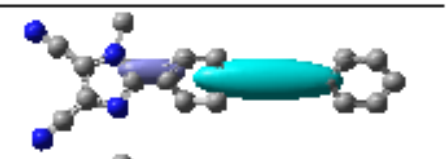
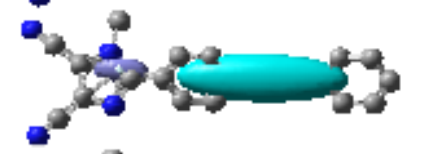
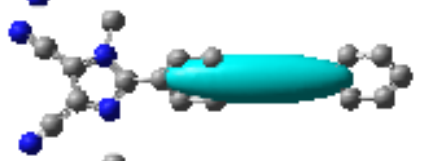
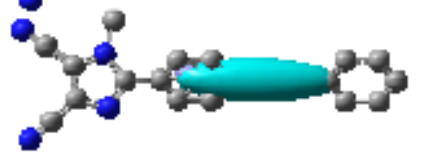
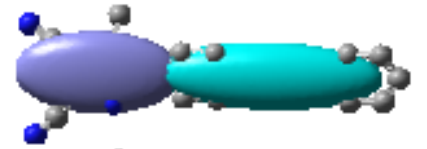
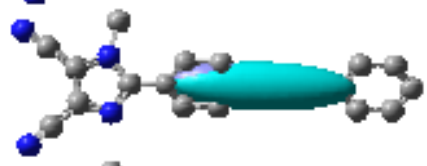
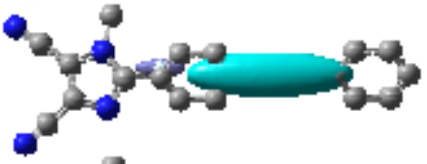
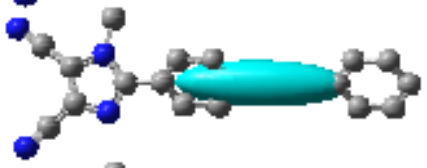
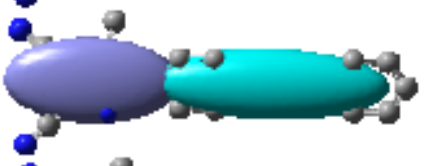
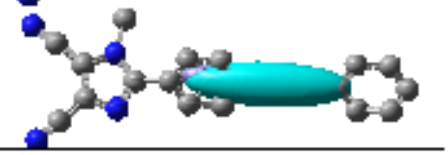
a) Isocontour value 0.001

Table SI.15. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **5c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
					5c		
PBE0	444	0.8960	7.55	0.88	32.01	5.61	
B3LYP	480	0.4962	7.98	1.04	39.70	4.92	
CIS	325	1.8516	2.19	0.58	6.11	5.71	
CAM-B3LYP	374	1.7097	4.29	0.59	12.16	6.30	
PBE	511	1.0096	6.52	0.67	20.86	3.19	
LC-PBE	335	1.7955	3.27	0.57	8.88	6.08	
M06	443	1.0292	6.90	0.84	27.67	5.82	
M06-HF	340	1.7116	3.54	0.56	9.45	6.32	
BLYP	511	1.0122	6.44	0.68	20.85	5.61	
BHandH	376	1.7223	4.47	0.61	13.18	6.38	
Experimental	381						

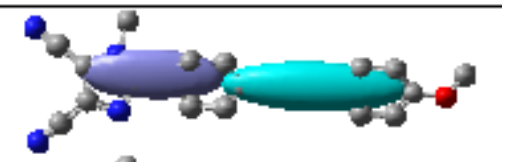
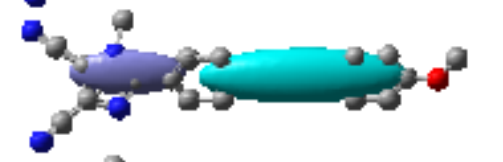
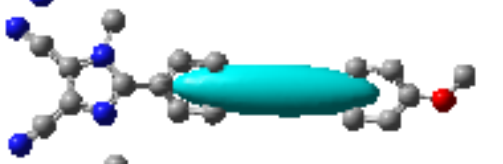
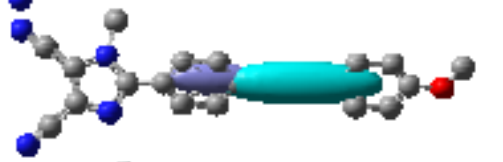
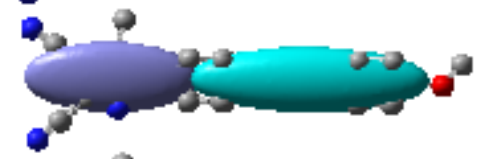
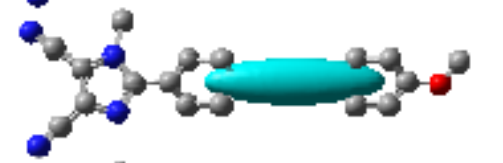
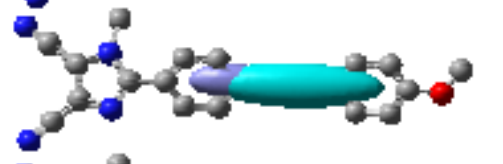
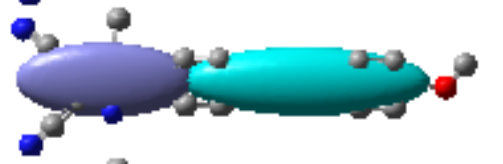
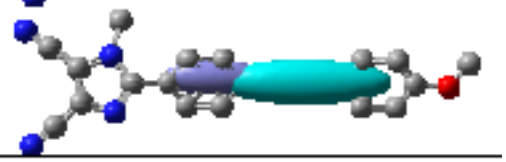
a) Isocontour value 0.001

Table SI.16. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **6a**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				6a			
PBE0	340	1.3926	4.99	0.54	13.03	3.94	
B3LYP	356	1.0288	6.08	0.70	20.33	3.52	
CIS	281	1.7163	0.79	0.49	1.85	4.66	
CAM-B3LYP	311	1.6838	1.98	0.43	4.11	4.50	
PBE	372	1.3423	7.13	1.04	35.75	3.92	
LC-PBE	284	1.6502	1.19	0.44	2.50	4.60	
M06	349	1.3800	4.30	0.51	10.58	4.12	
M06-HF	280	1.8232	1.28	0.43	2.62	4.71	
BLYP	375	1.3398	7.11	1.06	36.00	3.92	
BHandH	309	1.7092	2.15	0.45	4.62	4.51	
Experimental	304						

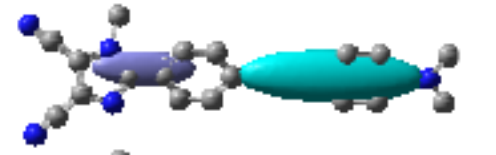
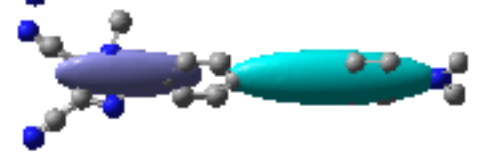
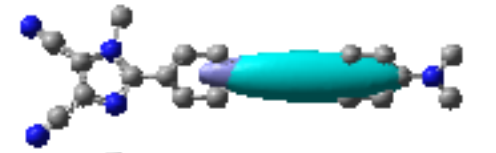
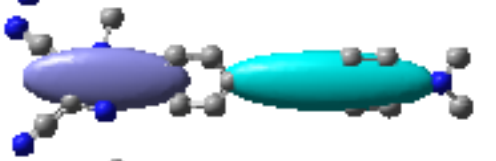
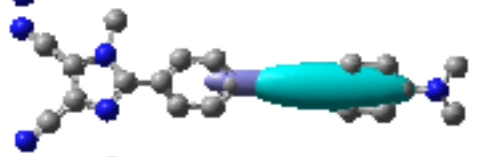
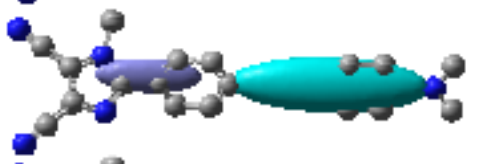
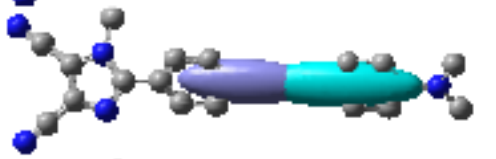
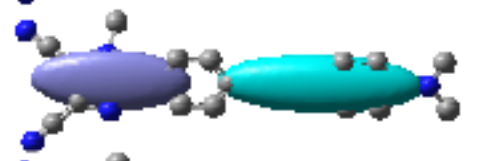
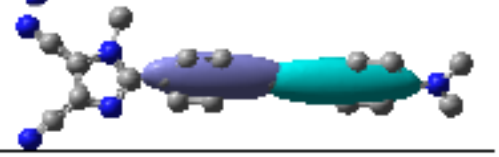
a) Isocontour value 0.001

Table SI.17. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **6b**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT}/ e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				6b			
PBE0	362	1.1989	6.61	0.73	23.03	4.14	
B3LYP	384	0.7701	7.27	0.88	30.79	3.70	
CIS	284	1.8056	1.49	0.52	3.71	4.37	
CAM-B3LYP	320	1.7818	3.41	0.50	8.20	4.81	
PBE	411	1.1007	8.06	1.10	42.53	4.28	
LC-PBE	291	1.7941	2.27	0.48	5.27	4.92	
M06	367	1.2660	5.96	0.67	19.30	4.23	
M06-HF	287	1.9411	2.43	0.47	5.51	5.06	
BLYP	412	1.1093	7.98	1.11	42.44	4.24	
BHandH	319	1.7905	3.59	0.52	8.99	4.74	
Experimental	318						

a) Isocontour value 0.001

Table SI.18. Computed charge transfer excitation energies (λ), oscillator strength (*f*), charge transfer excitation length (D_{CT}), transferred charge (q_{CT}), dipole moment (μ_{CT}), overlap between centroids (H) and the plot as centroids of charge for compound **6c**.

Method	λ/nm	*f*	D_{CT}/Å	q_{CT} / e	μ_{CT}/Debye	H / Å	Centroides of charge (C+(r)/C-(r))[a]
				6c			
PBE0	422	0.8417	7.88	0.94	35.73	4.99	
B3LYP	456	0.4839	8.30	1.06	42.32	4.67	
CIS	297	2.0377	2.26	0.60	6.50	5.66	
CAM-B3LYP	349	1.8505	4.64	0.63	14.07	6.00	
PBE	498	0.8933	8.80	1.14	48.14	4.59	
LC-PBE	312	1.9712	3.33	0.58	9.28	6.28	
M06	418	0.9545	7.32	0.91	32.08	5.04	
M06-HF	313	2.0532	3.73	0.58	10.47	6.61	
BLYP	497	0.8977	8.72	1.15	48.11	4.59	
BHandH	350	1.8327	4.92	0.67	15.82	5.93	
Experimental	359						

a) Isocontour value 0.001

Table SI.19. Computed excitation energies using an electrostatic model w_{CT} and w^0_{CT} (in eV)

		PBE0	B3LYP	CIS	CAM-B3LYP	PBE	LC-PBE	M06	M06-HF	BLYP	BHandH
						w_{CT} / eV					
	a	5.57	4.71	10.39	7.45	3.12	10.04	5.20	10.19	3.09	6.99
1	b	4.91	4.51	10.33	7.16	2.96	9.68	5.02	9.93	2.95	6.76
	c	3.94	3.47	10.23	6.76	1.68	9.44	4.11	9.73	1.66	6.41
	a	4.14	3.43	9.84	7.04	2.05	9.52	4.30	9.65	1.97	6.70
2	b	3.82	3.33	9.57	6.49	1.85	9.03	3.88	9.28	1.81	6.02
	c	2.95	2.55	8.92	5.97	1.79	6.57	3.89	6.04	1.15	5.15
	a	3.88	3.62	5.59	5.32	2.06	7.40	3.84	7.26	2.02	4.59
3	b	3.64	3.20	7.50	5.58	1.70	7.76	3.67	7.88	1.65	5.07
	c	2.94	2.49	7.34	5.01	1.20	7.15	3.05	7.23	1.16	4.53
	a	4.04	3.50	8.37	6.34	2.06	8.52	4.07	8.56	2.00	5.84
4	b	3.45	2.94	8.43	5.93	1.55	8.22	7.99	8.38	1.36	5.43
	c	3.14	2.66	8.63	5.75	1.34	8.15	3.23	8.33	1.15	5.31
	a	3.70	3.20	7.20	5.59	1.66	7.59	3.73	7.68	1.59	5.09
5	b	3.35	2.81	7.71	5.42	2.02	7.59	3.40	7.69	1.33	4.92
	c	2.71	2.21	7.36	4.83	1.33	6.98	2.80	7.03	1.29	4.35
	a	3.94	3.47	7.64	5.82	1.90	7.81	3.98	7.89	1.82	5.34
6	b	3.54	3.05	8.04	5.63	1.58	7.81	3.62	7.92	1.52	5.17
	c	2.79	2.34	7.60	4.96	1.04	7.15	2.89	7.20	1.00	4.48
						w^0_{CT} / eV					
	a	1.31	0.90	6.93	3.59	-0.56	6.21	1.38	6.33	-0.59	3.15
1	b	1.74	1.35	7.54	4.02	-0.16	6.59	1.84	6.84	-0.17	3.63
	c	1.64	1.24	7.63	3.97	-0.39	6.57	1.73	6.83	-0.37	3.61
	a	4.33	3.93	9.69	6.53	2.57	9.06	4.36	9.18	2.52	6.06
2	b	3.90	3.50	9.40	6.10	2.08	8.60	3.95	8.85	2.05	5.69
	c	3.26	2.88	8.90	5.47	1.45	7.93	3.34	8.14	1.44	5.06
	a	3.62	3.27	8.56	5.69	2.04	8.06	3.67	8.07	2.01	5.20
3	b	3.39	3.04	8.41	5.44	1.80	7.78	3.45	7.86	1.77	4.99
	c	2.86	2.53	7.87	4.87	1.33	7.12	2.95	7.13	1.31	4.42
	a	4.10	3.71	9.13	6.21	2.45	8.63	4.11	8.73	2.39	5.73
4	b	3.69	3.30	8.83	5.81	1.98	8.21	8.21	8.40	1.94	5.36
	c	3.50	3.11	8.97	5.71	1.64	8.17	3.56	8.37	1.64	5.28
	a	3.54	3.19	8.32	5.59	2.00	7.90	3.58	7.89	1.95	5.08
5	b	3.33	2.98	8.19	5.38	1.76	7.67	3.38	7.72	1.72	4.89
	c	2.81	2.47	7.71	4.83	1.27	7.07	2.90	7.06	1.25	4.36
	a	3.78	3.42	8.69	5.84	2.20	8.17	3.84	8.16	2.15	5.36
6	b	3.54	3.18	8.54	5.60	1.93	7.91	3.60	7.98	1.89	5.14
	c	2.95	2.61	7.99	4.99	1.37	7.25	3.05	7.25	1.35	4.54

Figure SI.2 Ideal (dashed lines) and computed (full lines) transition energies (w, in eV) using different functionals

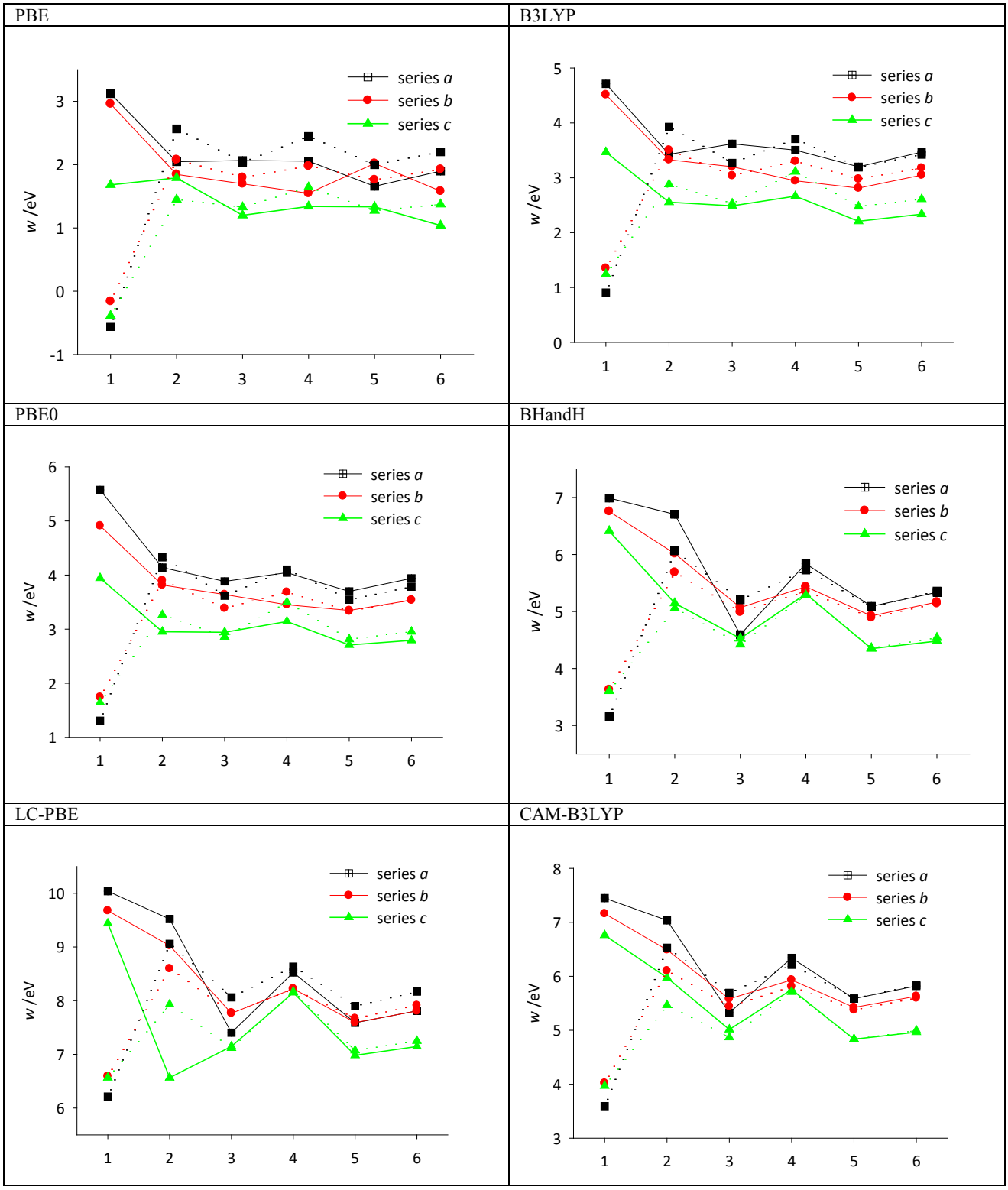


Figure SI.3 Ideal (dashed lines) and computed (full lines) coulombic contribution to transition energies (F, in eV) using different functionals

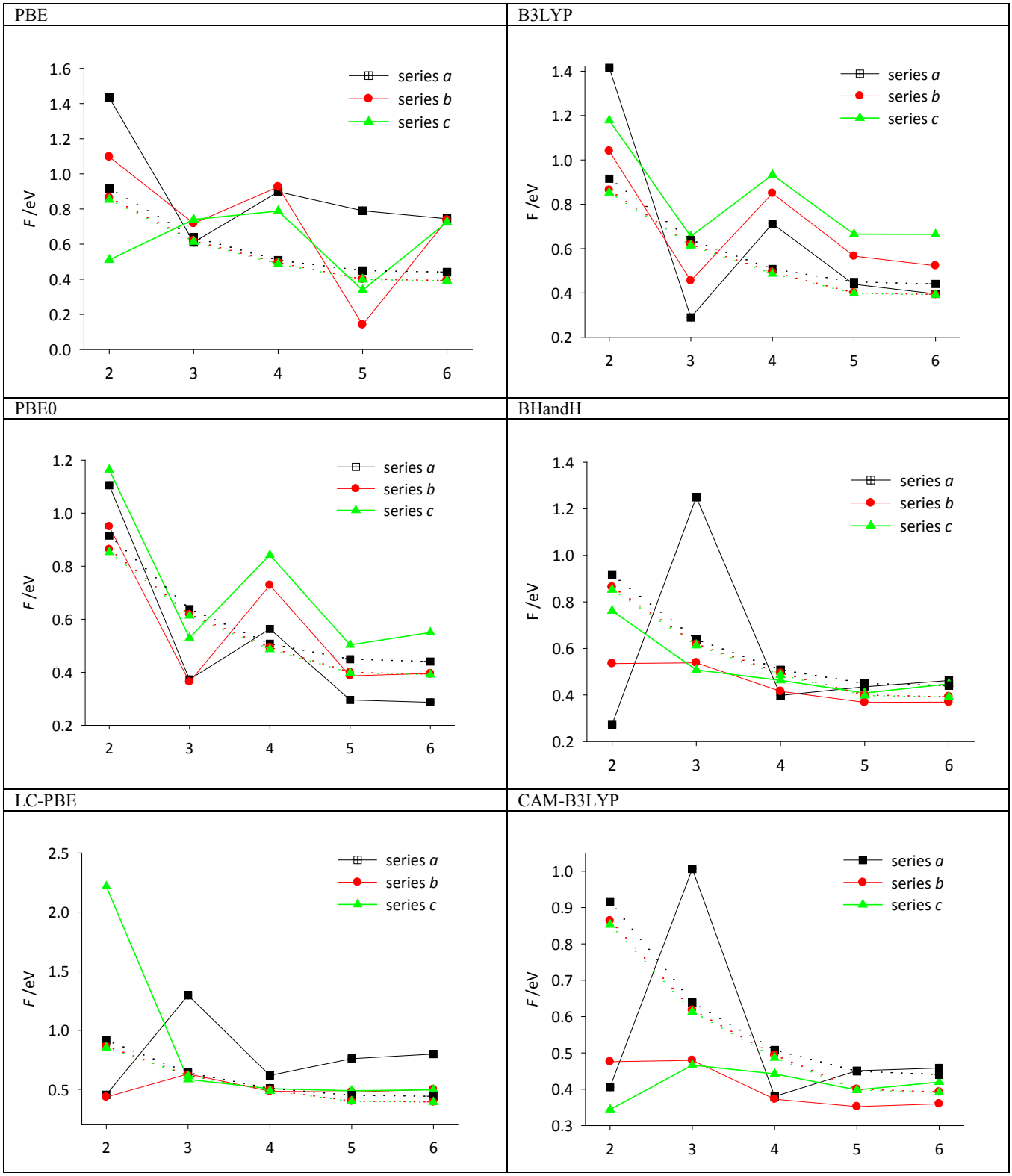
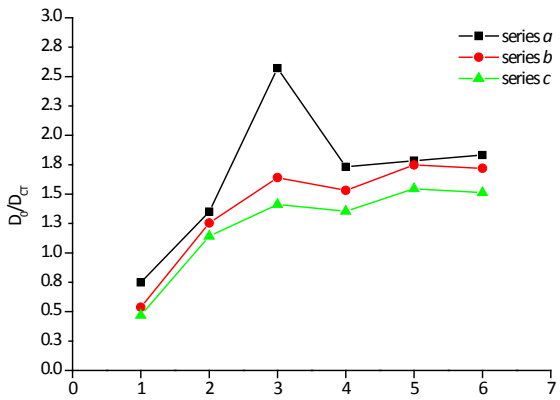
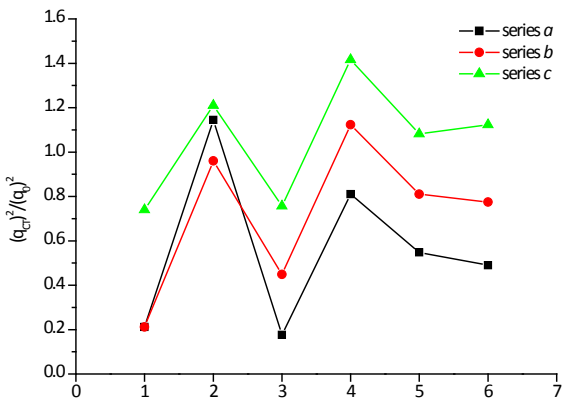


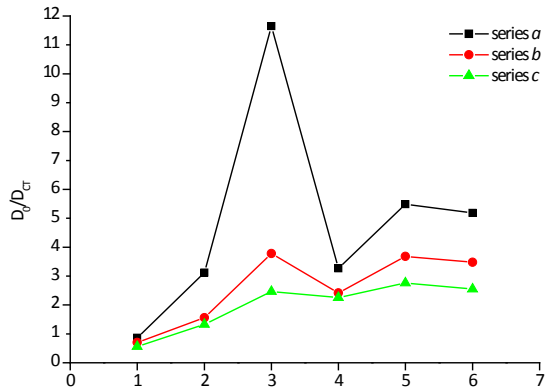
Figure SI.4 Distance and charge transfer efficiency computed using different functionals

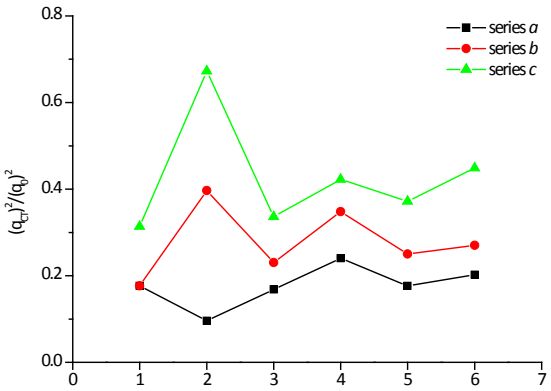
B3LYP



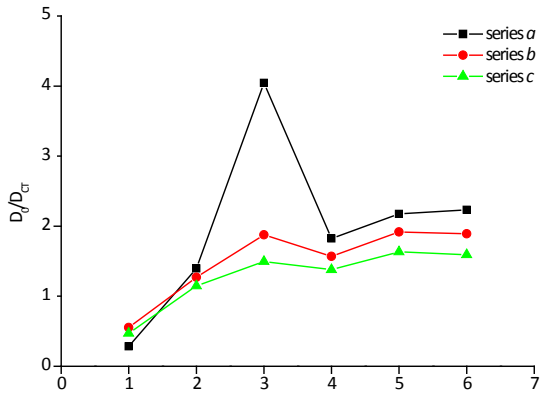


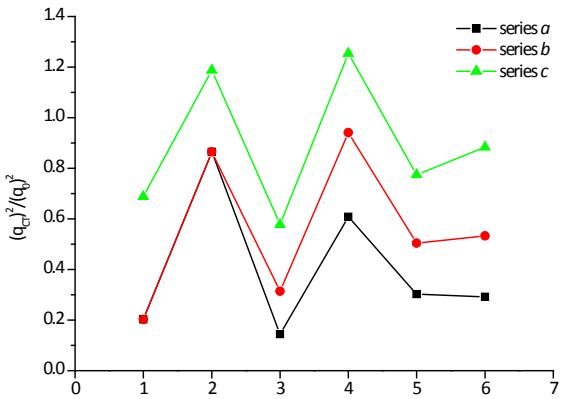
BHandH

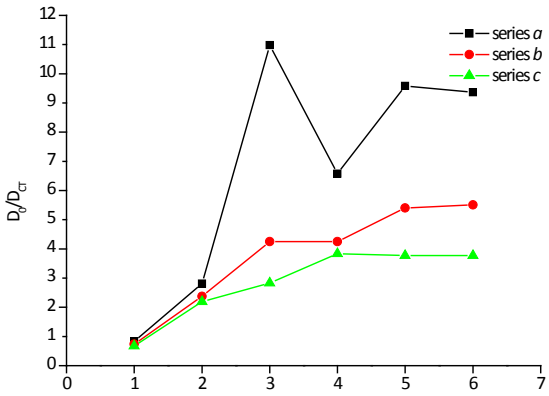
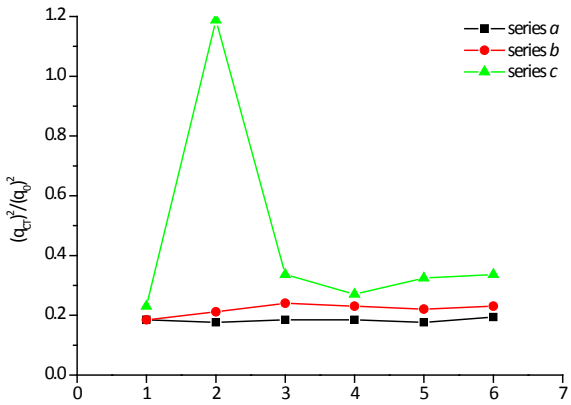




PBE0





LC-PBE	
 series a series b series c D_0/D_{CT}	 series a series b series c $(q_{CT})^2/(q_0)^2$