Electronic Supplementary Material (ESI) for RSC Advances.
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Supporting materials

Table S1HOMO, LUMO and gap energies (in eV) of dyescalculated by DFT

	WS-2			WS-92			WS-95		
	Gas		Solvent	Gas		Solvent	Gas		Solvent
		+TiO_2			+TiO_2			+TiO_2	
L+1	-2.18	-3.68	-2.28	-2.14	-3.67	-2.26	-2.27	-3.60	-2.35
L	-2.95	-3.70	-3.02	-2.91	-3.69	-3.00	-2.85	-3.62	-2.92
H	-5.16	-5.21	-5.12	-4.81	-4.99	-4.78	-4.89	-5.01	-4.89
H-1	-5.88	-6.14	-5.92	-5.59	-5.80	-5.61	-5.31	-5.51	-5.35
Gap	2.21	1.51	2.1	1.90	1.3	1.78	2.04	1.39	1.97

Table S2. Optimized structure (Cartesian x, y, z coordinates) for WS-2/TiO_2.

	WS-2/TiO_2 (Angstroms)		
Atom	X	Y	Z
C	-14.5003	10.50439	-1.09841
O	-15.3014	11.498	-0.92884
O	-15.0846	9.37175	-1.32004
Ti	-16.903	10.23774	-1.07478
O	-17.6925	9.21659	-2.36676
O	-18.0173	11.80238	-1.35125
O	-17.4669	9.60043	0.47103
Ti	-19.2764	8.46449	-1.88066
Ti	-19.6537	12.10559	-0.86914
Ti	-18.5831	8.0742	1.04562
O	-20.8466	8.55117	-2.88571
O	-20.0012	9.84953	-0.88119
O	-19.0278	7.25877	-0.62361
O	-19.9873	13.93382	-0.66248
O	-21.084	11.69417	-2.10038
O	-19.51	11.48059	1.02468
O	-17.8379	7.08159	2.08523
O	-20.2558	8.82984	1.73405
Ti	-21.6853	9.92979	-2.048
Ti	-21.6909	14.20594	-0.12252
Ti	-21.0656	10.21058	1.09038
H	-18.6494	11.02004	1.15702
Ti	-23.1338	11.92918	-1.11667
O	-23.3952	10.78521	-2.43138
O	-22.3838	9.9726	-0.30328
O	-22.8961	13.81393	-1.36412
O	-22.4875	14.25372	1.553
O	-21.7171	12.32495	0.25524
O	-22.1631	11.02087	2.38147
O	-24.1987	12.0682	0.46247
Ti	-22.9846	12.46989	1.69562
C	5.30769	6.08539	-2.01657
C	5.42631	7.45389	-2.27261
C	4.34183	8.31612	-2.10838
C	3.06365	7.86477	-1.7184
C	2.98498	6.49196	-1.42262
C	4.06773	5.62254	-1.57215
C	6.47433	5.15188	-2.2178

N	1.93141	8.73564	-1.59106
C	2.14323	10.19202	-1.86592
C	0.87747	10.97454	-1.44062
C	-0.08089	9.84562	-1.23349
C	0.54934	8.59599	-1.29245
C	2.31753	10.58423	-3.34578
C	1.78497	12.02192	-3.41486
C	0.50624	11.94096	-2.57353
C	-1.45256	9.98324	-1.03051
C	-2.25816	8.84978	-0.84146
C	-1.61419	7.60095	-0.81206
C	-0.24745	7.46453	-1.06137
C	-3.72741	8.98206	-0.69374
C	-4.27565	10.05628	-0.05236
C	-5.70067	10.26897	0.04536
C	-6.63317	9.41196	-0.47759
C	-6.10163	8.19987	-1.10177
C	-4.66417	8.00457	-1.23771
N	-6.82288	7.23201	-1.59704
S	-5.76227	6.14428	-2.21567
N	-4.30382	6.92939	-1.88007
C	-8.07101	9.73263	-0.4054
C	-8.64601	10.80798	0.24537
C	-10.0475	10.92169	0.07825
C	-10.5811	9.93172	-0.71857
S	-9.32065	8.8477	-1.16659
C	-11.9564	9.69258	-1.13513
C	-13.0457	10.49629	-0.95176
C	-12.9869	11.7834	-0.31755
N	-12.9482	12.84582	0.19541
H	6.3949	7.86105	-2.60712
H	4.5478	9.37514	-2.3136
H	2.06171	6.04214	-1.04322
H	3.93969	4.55486	-1.32936
H	6.13913	4.10393	-2.38655
H	7.13352	5.16955	-1.3206
H	7.07742	5.45073	-3.10488
H	2.99327	10.56914	-1.24763
H	1.03384	11.50517	-0.47162
H	1.68206	9.92345	-3.98239
H	3.36122	10.5191	-3.72215
H	1.59631	12.36531	-4.45726
H	2.51456	12.71929	-2.93739

H	0.17573	12.9362	-2.19906
H	-0.31243	11.51572	-3.2009
H	-1.88423	10.99514	-1.06107
H	-2.1866	6.68363	-0.60363
H	0.15485	6.44556	-1.08546
H	-3.62417	10.82062	0.40209
H	-6.00732	11.20505	0.53629
H	-8.09578	11.55539	0.83254
H	-10.6155	11.7386	0.53813
H	-12.1195	8.73472	-1.66021

Table S3. Optimized structure (Cartesian x, y, z coordinates) for WS-92/TiO_2.

	WS-92/TiO_2 (Angstroms)		
Atom	X	Y	Z
C	2.94985	-0.16183	-1.95246
C	2.39861	-1.40647	-1.85257
C	0.9796	-1.64149	-1.96575
C	0.06196	-0.64906	-2.1877
C	0.60424	0.70172	-2.34208
C	2.03377	0.9443	-2.19922
C	4.42063	0.00237	-1.87572
C	5.09569	0.88405	-2.73629
C	6.48599	0.99408	-2.72685
C	7.23905	0.18315	-1.86568
C	6.57084	-0.66206	-0.97443
C	5.18096	-0.76081	-0.97421
N	-0.09896	1.76842	-2.60138
S	0.95428	3.08759	-2.58624
N	2.40937	2.18897	-2.30326
N	8.6304	0.06921	-1.70637
C	8.86002	-0.75251	-0.48039
C	7.52115	-1.44669	-0.11775
C	9.23128	0.06923	0.77177
C	7.96849	0.12269	1.64324
C	7.31525	-1.23909	1.38607
C	9.77038	0.49957	-2.45784
C	9.5957	0.92091	-3.80822
C	10.6398	1.33069	-4.61778
C	11.93867	1.31438	-4.07311
C	12.14544	0.88854	-2.75668
C	11.07214	0.45588	-1.95244
N	13.19081	1.6373	-4.59018
C	14.20592	1.46297	-3.65117
C	13.56016	0.98858	-2.4928
C	15.60654	1.65429	-3.63571
C	16.30362	1.3675	-2.47328
C	15.64438	0.89017	-1.31677
C	14.27409	0.69529	-1.31298
C	13.31245	2.08432	-5.98645
C	14.66899	2.13184	-6.69906
C	14.51328	2.37533	-8.2123
C	15.86687	2.45469	-8.93875

C	15.6974	2.64112	-10.4564
C	17.04551	2.73272	-11.1843
C	-1.36808	-0.98204	-2.3179
C	-1.89638	-2.25146	-2.45925
C	-3.30952	-2.30051	-2.49659
C	-3.89979	-1.06112	-2.37246
S	-2.66114	0.1369	-2.30269
C	-5.31056	-0.69952	-2.37477
C	-6.38796	-1.53798	-2.29276
C	-6.28024	-2.96088	-2.13648
N	-6.20347	-4.13164	-1.9988
H	3.04535	-2.28828	-1.71313
H	0.66338	-2.68945	-1.85041
H	4.54004	1.49061	-3.46858
H	6.95718	1.72937	-3.39291
H	4.69986	-1.46091	-0.27454
H	9.62564	-1.53384	-0.7029
H	7.48247	-2.51826	-0.42144
H	9.60578	1.08952	0.53114
H	10.03277	-0.46555	1.33702
H	7.29462	0.9397	1.29114
H	8.19377	0.29437	2.72051
H	7.87297	-2.0284	1.94544
H	6.24902	-1.28134	1.70001
H	8.60912	0.86722	-4.2875
H	10.46009	1.6281	-5.66202
H	11.30187	0.10901	-0.93594
H	16.16048	2.0306	-4.50454
H	17.39551	1.51918	-2.44511
H	16.2281	0.67564	-0.40663
H	13.75746	0.32865	-0.41293
H	12.84064	3.09462	-6.03667
H	12.66999	1.38899	-6.57899
H	15.19892	1.16142	-6.54614
H	15.28509	2.95672	-6.27064
H	13.94965	3.32441	-8.37861
H	13.91031	1.54853	-8.65869
H	16.4455	1.51989	-8.74609
H	16.45872	3.30519	-8.52398
H	15.11047	3.56955	-10.6562
H	15.11583	1.78462	-10.8747
H	16.89826	2.85861	-12.2818
H	17.65107	1.81077	-11.028

H	17.64059	3.60157	-10.821
H	-1.30705	-3.17573	-2.52451
H	-3.84417	-3.2509	-2.60551
H	-5.51431	0.38233	-2.45902
C	-7.82103	-1.7076	-2.33387
O	-8.67147	-0.74674	-2.22784
O	-8.3471	-2.88062	-2.47751
Ti	-10.2071	-2.09341	-2.28373
O	-10.9441	-3.23705	-3.50201
O	-11.3994	-0.60912	-2.6596
O	-10.7375	-2.65404	-0.69689
Ti	-12.4876	-4.03434	-2.96113
Ti	-13.049	-0.35772	-2.19274
Ti	-11.7746	-4.19316	-0.01794
O	-14.0605	-4.09445	-3.96396
O	-13.2815	-2.62426	-2.05338
O	-12.1778	-5.13948	-1.62757
O	-13.4749	1.46097	-2.10694
O	-14.4569	-0.92217	-3.38862
O	-12.8733	-0.84706	-0.26207
O	-10.9796	-5.07527	1.08267
O	-13.4833	-3.479	0.62482
Ti	-14.9678	-2.70732	-3.21676
Ti	-15.1901	1.68184	-1.58005
Ti	-14.3623	-2.18701	-0.10631
H	-11.9903	-1.25359	-0.10254
Ti	-16.5158	-0.72625	-2.41521
O	-16.7191	-1.96705	-3.64992
O	-15.6671	-2.58378	-1.47621
O	-16.3741	1.14745	-2.78838
O	-15.9876	1.80076	0.0915
O	-15.1206	-0.1687	-1.07787
O	-15.4992	-1.34912	1.13203
O	-17.5859	-0.53641	-0.84492
Ti	-16.3934	0.00752	0.35431

Table S4. Optimized structure (Cartesian x, y, z coordinates) for WS-95/TiO_2.

	WS-95/TiO_2 (Angstroms)		
Atom	X	Y	Z
C	2.95539	2.03886	4.31421
C	2.84133	2.06823	2.95619
C	1.57574	1.86676	2.28671
C	0.39649	1.67734	2.95624
C	0.48716	1.53682	4.40943
C	1.76157	1.72384	5.08405
C	4.23526	2.37586	4.98268
C	4.23118	3.29731	6.04328
C	5.41198	3.72588	6.65108
C	6.63398	3.22739	6.18508
C	6.62837	2.2845	5.14756
C	5.45828	1.86068	4.52657
N	-0.49791	1.22235	5.20481
S	0.1576	1.15542	6.67531
N	1.75701	1.56754	6.3778
N	7.96857	3.50043	6.60506
C	8.75956	2.35933	6.06947
C	8.03718	2.02775	4.74516
C	10.20139	2.24512	5.56233
C	10.14558	0.99936	4.63242
C	8.65235	0.69436	4.34896
C	8.56255	4.50752	7.41184
C	7.83798	5.71735	7.62372
C	8.31894	6.76416	8.38881
C	9.59992	6.62476	8.95833
C	10.34236	5.45722	8.75207
C	9.82892	4.39187	7.98452
N	10.38411	7.46583	9.74433
C	11.6119	6.88907	10.06346
C	11.59631	5.62279	9.44583
C	12.74857	7.28526	10.8049
C	13.81946	6.41112	10.89751
C	13.79369	5.14404	10.26999
C	12.68901	4.73715	9.54204
C	9.87261	8.79223	10.12282
C	10.75292	9.83816	10.8161
C	10.01612	11.181	10.98464

C	10.88846	12.25403	11.65846
C	10.14511	13.59284	11.80796
C	11.01725	14.67146	12.46507
C	-0.86123	1.46879	2.2147
C	-0.95588	1.02829	0.9054
C	-2.29523	0.79324	0.51301
C	-3.18062	1.07369	1.52073
S	-2.43543	1.70591	2.90755
C	-2.91466	0.19245	-0.74086
C	-4.33943	0.16271	-0.20766
C	-4.48887	0.68152	1.05804
C	-5.57036	-0.27175	-0.74863
C	-6.61611	-0.09966	0.14678
S	-6.08006	0.67399	1.62195
C	-8.03176	-0.40524	-0.00174
C	-8.65041	-1.11488	-0.99397
C	-7.94253	-1.73693	-2.07579
N	-7.36293	-2.25667	-2.96364
C	-2.31095	-1.21082	-0.94908
C	-2.7043	-1.95552	-2.23636
C	-2.02569	-3.33593	-2.31938
C	-2.21738	-4.01586	-3.68641
C	-1.48227	-5.36604	-3.76404
C	-1.57877	-6.01231	-5.15689
C	-0.82723	-7.35298	-5.22798
C	-0.89913	-7.98615	-6.6245
C	-2.76887	1.13547	-1.94821
C	-3.33968	2.55114	-1.74301
C	-3.18178	3.42903	-2.99873
C	-3.91933	4.77336	-2.86757
C	-3.74947	5.66282	-4.1122
C	-4.58929	6.94955	-4.02527
C	-4.39373	7.86417	-5.24658
C	-5.27588	9.11886	-5.17605
H	3.71914	2.32067	2.33855
H	1.58575	1.94067	1.18751
H	3.28132	3.73078	6.39652
H	5.3548	4.4254	7.49692
H	5.51308	1.17863	3.66466
H	8.60702	1.54186	6.82143
H	8.26608	2.79105	3.95835
H	10.95676	2.1	6.36577
H	10.47162	3.16207	4.98716

H	10.62733	0.11501	5.11236
H	10.69562	1.20923	3.68475
H	8.44684	0.4188	3.2905
H	8.27377	-0.11721	5.01364
H	6.87182	5.8822	7.12568
H	7.73311	7.68712	8.51544
H	10.4336	3.48325	7.88848
H	12.81649	8.25798	11.30756
H	14.71342	6.70863	11.47055
H	14.66429	4.47391	10.36013
H	12.66712	3.75304	9.04956
H	8.97864	8.60507	10.76528
H	9.50843	9.25505	9.17374
H	11.67238	10.00658	10.20639
H	11.04529	9.46785	11.82682
H	9.09339	11.02188	11.59252
H	9.69295	11.55406	9.98331
H	11.81216	12.41184	11.05208
H	11.20739	11.89332	12.66532
H	9.22494	13.44276	12.42223
H	9.81771	13.95303	10.80308
H	10.45901	15.63114	12.56243
H	11.93169	14.87253	11.86132
H	11.33927	14.36228	13.48571
H	-0.10615	0.78781	0.25395
H	-5.65319	-0.68675	-1.75799
H	-8.67671	-0.00401	0.79987
H	-2.55486	-1.84707	-0.06503
H	-1.19938	-1.1026	-0.96866
H	-2.3861	-1.35985	-3.12386
H	-3.81007	-2.08106	-2.29034
H	-2.42605	-3.99451	-1.51221
H	-0.93086	-3.21587	-2.13602
H	-1.82634	-3.34314	-4.48692
H	-3.3058	-4.16741	-3.87986
H	-1.90688	-6.0605	-3.00047
H	-0.40548	-5.21316	-3.512
H	-1.15295	-5.31422	-5.91682
H	-2.652	-6.17405	-5.41656
H	-1.25847	-8.06251	-4.48166
H	0.24433	-7.1963	-4.956
H	-0.3521	-8.95678	-6.65127
H	-0.44259	-7.32055	-7.39247

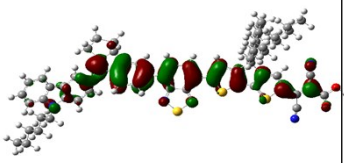
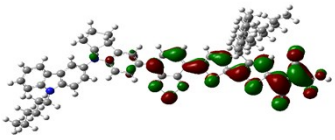
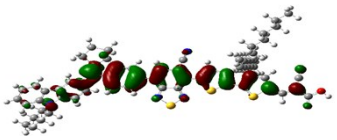
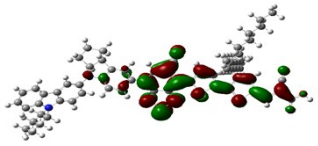
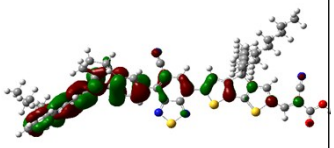
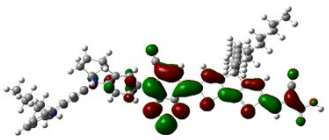
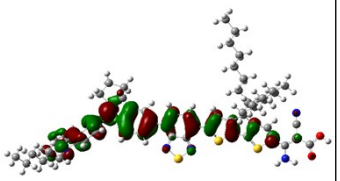
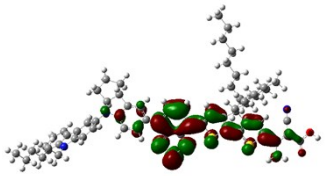
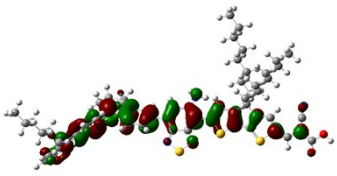
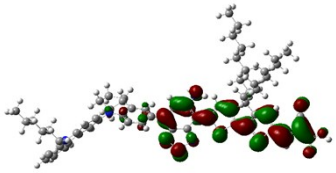
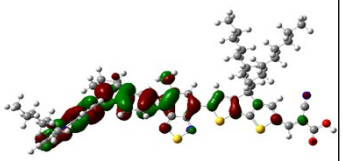
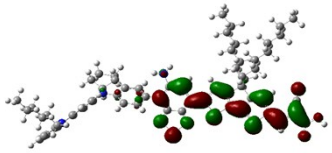
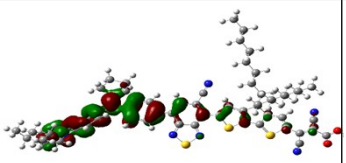
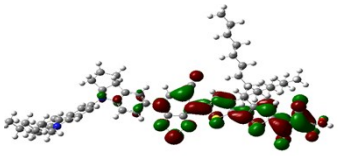
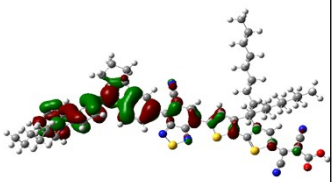
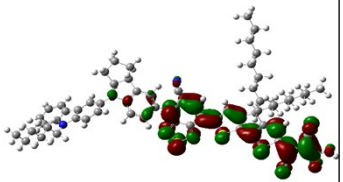
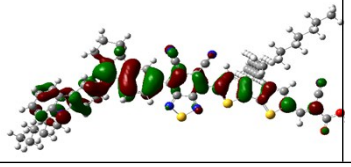
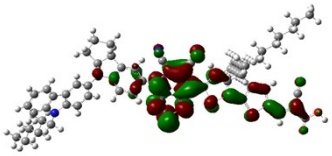
H	-1.95392	-8.18383	-6.92334
H	-3.30482	0.68676	-2.81745
H	-1.68923	1.20969	-2.22014
H	-2.83254	3.05035	-0.88397
H	-4.42477	2.47866	-1.49352
H	-3.58732	2.88436	-3.88477
H	-2.09718	3.61081	-3.18875
H	-3.54325	5.31838	-1.96921
H	-5.00612	4.57534	-2.70616
H	-4.05424	5.09136	-5.02134
H	-2.67157	5.92675	-4.23086
H	-4.315	7.50945	-3.09958
H	-5.66857	6.67659	-3.94189
H	-4.63626	7.30156	-6.17988
H	-3.32279	8.17261	-5.3133
H	-5.10858	9.77565	-6.06069
H	-5.05356	9.71766	-4.26334
H	-6.35694	8.85005	-5.15563
C	-10.0367	-1.38687	-1.37022
O	-10.5482	-2.01163	-2.37311
O	-10.9011	-0.8801	-0.5521
Ti	-12.4223	-1.48999	-1.74833
O	-13.5245	-1.87821	-0.34483
O	-13.1201	-2.86013	-2.93235
O	-13.0299	0.00938	-2.45284
Ti	-15.213	-1.21763	-0.49738
Ti	-14.5928	-2.90186	-3.84429
Ti	-14.457	1.30162	-2.00666
O	-16.7707	-2.21577	-0.25132
O	-15.4993	-1.47241	-2.31279
O	-15.1982	0.54004	-0.41932
O	-14.4396	-3.98943	-5.35761
O	-16.1556	-3.72407	-3.0617
O	-14.4921	-1.0645	-4.62646
O	-13.9226	2.81869	-1.82139
O	-15.8373	1.11192	-3.38567
Ti	-17.1788	-2.60072	-1.98074
Ti	-15.9814	-3.97598	-6.30137
Ti	-16.3108	-0.37328	-4.12489
H	-13.7692	-0.55771	-4.18948
Ti	-18.0129	-3.39863	-4.35368
O	-18.6377	-3.65811	-2.72649
O	-17.7319	-1.41643	-3.33181

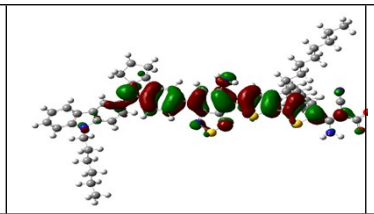
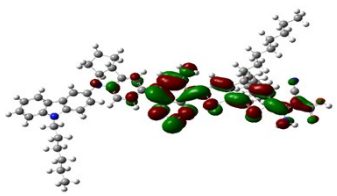
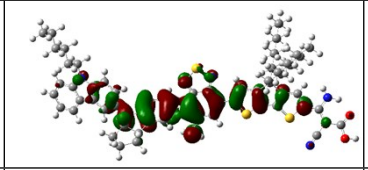
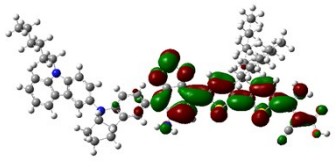
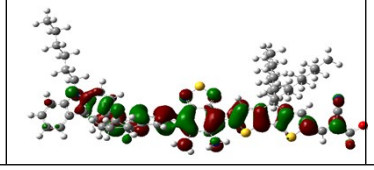
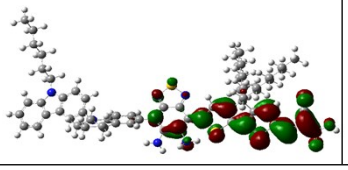
O	-17.3226	-4.79094	-5.47397
O	-16.6323	-2.85852	-7.63248
O	-16.4582	-2.46314	-5.22183
O	-17.0839	-0.07956	-5.81138
O	-18.9059	-2.44583	-5.74717
Ti	-17.554	-1.64241	-6.57377

Table S5 Maximum absorption wavelengths for dyes using different functionals

	LC-WSPBE	WB97XD	CAM-B3LYP	Exp
WS-2	440	484	505	550
WS-92	455	507	538	554
WS-95	480	522	542	574

Table S6HOMO, LUMO and gap energies (in eV) of dyescalculated by DFT

Dye	HOMO	Energy/eV	LUMO	Energy/eV
1		-5.07		-3.15
2		-5.15		-3.13
3		-4.98		-3.09
4		-4.80		-2.61
5		-4.86		-2.56
6		-4.81		-2.73
7		-5.06		-3.37
8		-5.06		-3.34
9		-5.31		-3.35

10		-4.89		-2.31
11		-4.86		-2.45
12		-5.02		-2.57

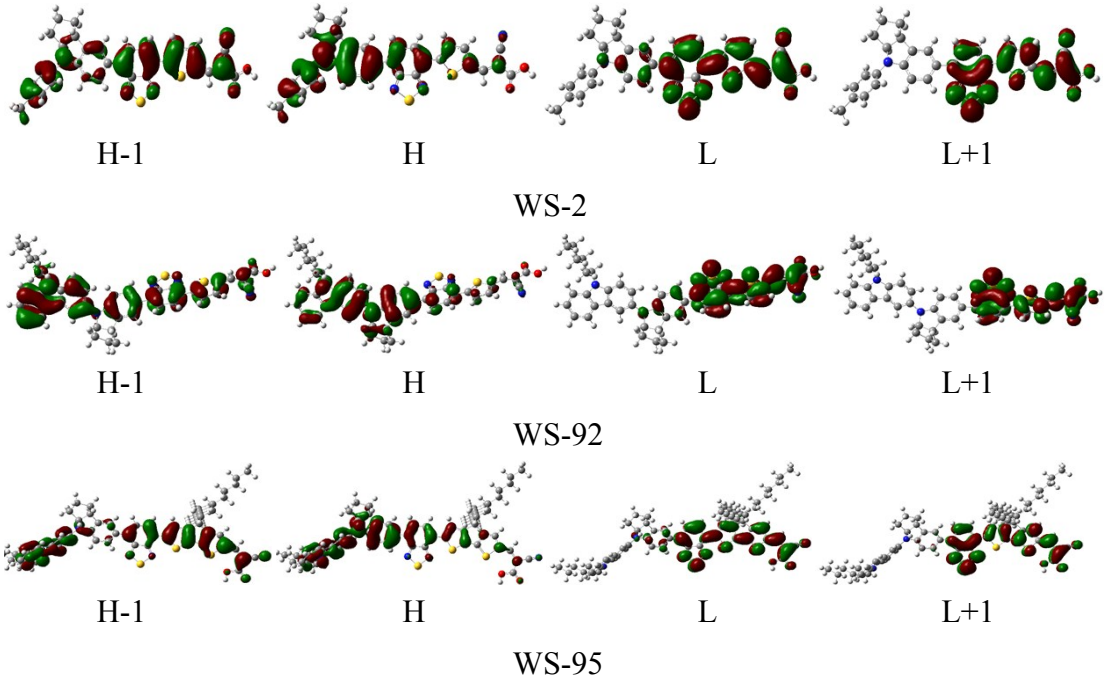


Figure S1 The plot surface of frontier orbitalof the dyes in solvent phase

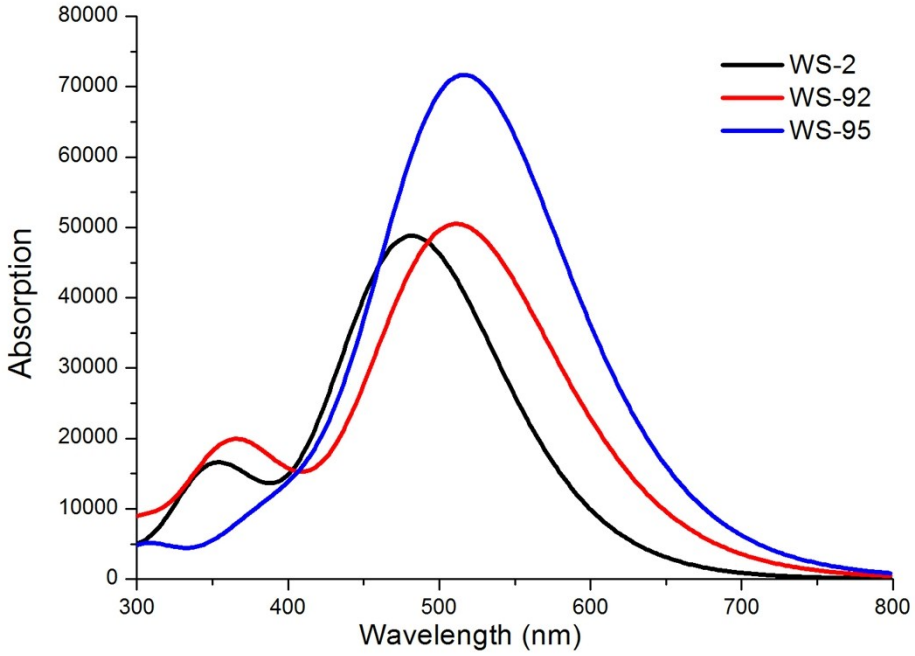


Figure S2 Absorption spectra of WS-2, WS-92 and WS-95 in gas phase