Supplementary Information (SI) for Nanoscale.

Supporting Information

Tuning Optical and Charge Transfer Properties of Tetrathiafulvalene-Based D-A′-π-A Dyes for DSSCs: A DFT and TDDFT Investigation

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Table S1: Coordinates of the designed dye molecules studied at HSEH1PBE/6-31G(d) level of theory in the angstrom unit.

1. Dye A1:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-1.022501	-2.292941	0.167939
C	-2.424598	-2.212925	0.089636
C	-3.110165	-1.052161	-0.235823
C	-2.282966	0.095462	-0.443017
C	-0.841362	0.016100	-0.353722
C	-0.176050	-1.214167	-0.050111
H	-0.596681	-3.254973	0.433408
H	-2.988268	-3.110897	0.322551
N	-0.240325	1.183529	-0.576739
N	-2.721739	1.319895	-0.729625
S	-1.412883	2.275302	-0.867205
C	1.264641	-1.330741	0.038363
C	1.993999	-2.485618	0.277595
C	3.379802	-2.284416	0.314087
C	3.743052	-0.966810	0.101070
S	2.339192	0.026604	-0.148149
H	1.536908	-3.458169	0.417852
H	4.097793	-3.079264	0.488020
C	-5.333707	-2.101777	-0.540444
C	-7.035562	-0.219549	-0.176375
C	-4.560676	-1.007513	-0.353527
C	-8.143811	0.451938	0.200432
C	-9.760383	2.163114	1.273620
C	-10.495057	1.062570	1.093817
H	-10.114355	3.071762	1.746286
H	-11.528900	0.951227	1.398675
H	-4.941285	-3.100796	-0.69041

S	-8.118049	2.158251	0.668866
S	-9.750806	-0.287099	0.264413
S	-5.441469	0.536402	-0.293959
S	-7.053711	-1.925125	-0.631569
C	5.060788	-0.398878	0.067870
C	5.420962	0.924813	-0.157940
S	6.467839	-1.370672	0.327657
C	6.800299	1.147785	-0.121128
H	4.692151	1.706149	-0.345170
C	7.537908	-0.003056	0.134286
H	7.258093	2.117380	-0.275369
C	8.937332	-0.220721	0.255595
H	9.266553	-1.238869	0.459865
C	9.967656	0.671558	0.154689
C	11.338290	0.142966	0.332241
O	11.603680	-1.017835	0.557165
C	9.784141	2.055134	-0.106140
N	9.598725	3.183445	-0.320912
O	12.271288	1.101370	0.216388
H	13.127626	0.660500	0.347865

2. Dye A2:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-0.869767	1.965745	0.147357
C	0.533058	2.016271	0.069712
C	1.325476	0.913181	-0.214445
C	0.610088	-0.314719	-0.377088
C	-0.832253	-0.368357	-0.289211
C	-1.609710	0.804294	-0.030237
H	-1.385263	2.892435	0.376316
H	1.007677	2.972232	0.266858
N	-1.320560	-1.594244	-0.469082
N	1.162993	-1.501919	-0.618639
S	-0.049695	-2.580772	-0.720556
C	2.773047	0.998643	-0.335830
C	3.442724	2.158603	-0.532078
S	3.790799	-0.458068	-0.276435
S	5.168079	2.140810	-0.637001
C	5.313697	0.438200	-0.196197
C	6.487787	-0.134047	0.144401
S	6.625903	-1.839091	0.596736
S	8.023973	0.744398	0.171199
C	8.287581	-1.711716	1.129518

C	8.916715	-0.549130	0.940216
H	8.737992	-2.593415	1.570050
H	9.949210	-0.353103	1.204228
H	2.960600	3.117877	-0.679827
C	-3.055444	0.789131	0.053621
C	-3.886615	1.888815	0.255084
C	-5.245850	1.576816	0.295632
C	-5.492472	0.218664	0.123647
S	-3.999651	-0.653878	-0.089906
H	-3.514449	2.900620	0.365174
H	-6.028852	2.310631	0.442336
C	-6.708374	-0.520599	0.093749
C	-7.994853	-0.082678	0.232069
C	-9.068516	-1.099028	0.155170
C	-8.341956	1.278488	0.441749
O	-8.882783	-2.283299	-0.019957
O	-10.289187	-0.559699	0.302322
N	-8.593598	2.401411	0.612475
H	-10.918879	-1.297455	0.237445
H	-6.630828	-1.596413	-0.060401

3. Dye A3:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	1.001215	-2.270272	0.233909
C	-0.399075	-2.225403	0.133365
C	-1.099740	-1.076342	-0.202786
C	-0.295415	0.090682	-0.398207
C	1.148877	0.055488	-0.287241
C	1.820812	-1.169317	0.031447
H	1.453386	-3.219217	0.505324
H	-0.946771	-3.135229	0.356793
N	1.717671	1.240944	-0.509469
N	-0.768968	1.298895	-0.697048
S	0.515564	2.289094	-0.820798
C	-2.548603	-1.060338	-0.343641
C	-3.295177	-2.173873	-0.529664
S	-3.463404	0.464691	-0.320173
S	-5.014971	-2.036707	-0.652741
C	-5.042540	-0.325537	-0.220111
C	-6.172164	0.325275	0.128743
S	-6.192010	2.037080	0.576399
S	-7.763378	-0.448273	0.173375
C	-7.847222	2.015810	1.144023

C	-8.554375	0.897289	0.964957
H	-8.230521	2.923486	1.595195
H	-9.592083	0.768065	1.248892
H	-2.879151	-3.166131	-0.659603
C	3.251701	-1.288342	0.153730
C	4.065637	-2.386985	0.387686
C	5.383875	-1.916601	0.410884
C	5.320571	-0.550213	0.188750
H	3.745069	-3.410405	0.519245
H	6.285512	-2.491521	0.566639
C	6.257831	0.504079	0.090941
C	7.616801	0.441023	0.207974
C	8.377206	1.701071	0.064346
C	8.305641	-0.775179	0.458927
O	7.878192	2.783731	-0.149356
O	9.700115	1.512118	0.198817
N	8.823251	-1.796597	0.664788
H	10.109367	2.387137	0.090103
H	5.847013	1.493108	-0.101247
O	4.011761	-0.185853	0.033737

4. Dye A4:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-0.413962	1.663175	-0.040898
C	0.990608	1.751113	-0.084401
C	1.824191	0.676058	-0.348687
C	1.153069	-0.573848	-0.528370
C	-0.288848	-0.672301	-0.475990
C	-1.111825	0.476943	-0.238515
H	-0.969923	2.566467	0.173806
H	1.432655	2.719810	0.127648
N	-0.732072	-1.913286	-0.663502
N	1.749473	-1.742871	-0.753200
S	0.574843	-2.860964	-0.880704
C	3.271684	0.810441	-0.432365
C	3.904869	1.985543	-0.650528
S	4.338121	-0.604959	-0.284351
S	5.635492	2.026065	-0.694539
C	5.820313	0.351935	-0.164820
C	6.994084	-0.156696	0.264587
S	7.172903	-1.832471	0.805005
S	8.491992	0.784090	0.332039
C	8.784769	-1.602243	1.446491

C	9.378363	-0.424679	1.235931
H	9.238075	-2.438334	1.965953
H	10.380679	-0.169619	1.559193
H	3.392982	2.919050	-0.853026
C	-2.554496	0.395197	-0.195393
C	-3.460267	1.445788	-0.083224
C	-4.811683	1.036949	-0.045828
C	-4.972099	-0.339173	-0.111140
S	-3.416357	-1.115524	-0.277003
C	-6.135468	-1.154139	-0.084700
C	-7.395069	-0.902063	0.384520
C	-8.386770	-1.990337	0.206225
C	-7.790138	0.253200	1.113068
O	-8.159427	-3.046449	-0.343658
O	-9.585483	-1.681073	0.725843
N	-8.124286	1.163811	1.754387
H	-10.154017	-2.451825	0.559810
H	-6.023183	-2.165119	-0.477360
O	-3.107146	2.755842	-0.027469
O	-5.833257	1.909265	-0.026279
C	-4.191635	3.642221	-0.310046
C	-5.445359	3.206532	0.415371
H	-3.866340	4.631103	0.019711
H	-4.368934	3.661776	-1.392832
H	-5.284600	3.188005	1.500019
H	-6.284588	3.866950	0.190911

5. Dye B1:

Atom	Coordinates (Angstroms)		
	X	Y	Z
C	-1.076839	-2.273126	0.235989
C	-2.477244	-2.185123	0.148082
C	-3.153034	-1.030370	-0.230601
C	-2.304304	0.078954	-0.487390
C	-0.888190	-0.006993	-0.389776
C	-0.219809	-1.208095	-0.027177
H	-0.658209	-3.224931	0.546566
H	-3.051643	-3.065876	0.418116
N	-0.373822	1.198167	-0.691965
N	-2.623659	1.335048	-0.848134
C	1.220232	-1.322716	0.073799
C	1.957018	-2.458963	0.366829
C	3.341727	-2.243232	0.396988
C	3.695856	-0.934130	0.125449

S	2.283202	0.033259	-0.171678
H	1.506076	-3.427112	0.550711
H	4.066351	-3.022454	0.609921
C	-5.397696	-2.053888	-0.510159
C	-7.060370	-0.122034	-0.203626
C	-4.603664	-0.973133	-0.347942
C	-8.154544	0.583438	0.149982
C	-9.732205	2.347481	1.193343
C	-10.489108	1.258358	1.037841
H	-10.065481	3.271095	1.651832
H	-11.522889	1.172933	1.351211
H	-5.025590	-3.064264	-0.633534
S	-8.094910	2.300418	0.575363
S	-9.777330	-0.119723	0.225868
S	-5.448095	0.590666	-0.322683
S	-7.115416	-1.838652	-0.617905
C	5.008390	-0.356247	0.070748
C	5.356144	0.963417	-0.194814
S	6.424864	-1.307718	0.353017
C	6.733473	1.199619	-0.169288
H	4.619624	1.732760	-0.400667
C	7.482377	0.063521	0.117224
H	7.182127	2.168426	-0.352663
C	8.883825	-0.137472	0.240342
H	9.223152	-1.145824	0.474511
C	9.905756	0.760799	0.108544
C	11.281622	0.250831	0.297150
O	11.559146	-0.899885	0.556887
C	9.708332	2.133900	-0.193957
N	9.511323	3.253281	-0.442654
O	12.205392	1.213827	0.148033
H	13.066067	0.784814	0.289911
N	-1.449048	1.911108	-0.940528
H	-1.372953	2.884880	-1.199494

6. Dye B2:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-0.859697	1.913887	0.201802
C	0.542314	1.962781	0.117141
C	1.329667	0.869975	-0.230991
C	0.595127	-0.324294	-0.458402
C	-0.822583	-0.376344	-0.364130
C	-1.606165	0.762608	-0.034060

H	-1.371345	2.827700	0.485309
H	1.025436	2.903182	0.363191
N	-1.214608	-1.633436	-0.634746
N	1.038146	-1.551716	-0.785468
C	2.778541	0.951221	-0.347898
C	3.464348	2.103625	-0.516338
S	3.770200	-0.523319	-0.320595
S	5.192453	2.056009	-0.630335
C	5.307444	0.342258	-0.217260
C	6.468160	-0.254448	0.124639
S	6.577377	-1.969142	0.548883
S	8.016878	0.600774	0.183464
C	8.224206	-1.864877	1.132750
C	8.871724	-0.708405	0.970082
H	8.651987	-2.755177	1.578508
H	9.898783	-0.527038	1.264142
H	2.996240	3.073190	-0.640553
C	-3.050762	0.738107	0.061121
C	-3.892648	1.813518	0.331112
C	-5.247888	1.481078	0.361683
C	-5.480595	0.132245	0.113010
S	-3.977278	-0.705703	-0.159365
H	-3.530438	2.821235	0.497524
H	-6.039566	2.194408	0.555631
C	-6.687247	-0.618960	0.048647
C	-7.978212	-0.206631	0.221789
C	-9.039037	-1.230554	0.092892
C	-8.340616	1.135082	0.514029
O	-8.840023	-2.400031	-0.153777
O	-10.265485	-0.717518	0.281329
N	-8.604881	2.242641	0.752653
H	-10.885726	-1.458783	0.177553
H	-6.598062	-1.682829	-0.168796
N	-0.073170	-2.242992	-0.863680
H	-0.052188	-3.226116	-1.096783

7. Dye B3:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-1.010430	2.243534	0.291640
C	0.388302	2.194792	0.177381
C	1.082499	1.050423	-0.201236
C	0.259898	-0.085198	-0.428964

C	-1.158160	-0.047508	-0.305216
C	-1.836491	1.148769	0.059941
H	-1.457681	3.185001	0.595721
H	0.944890	3.093206	0.424405
N	-1.636466	-1.273876	-0.588736
N	0.617333	-1.331844	-0.785040
C	2.531395	1.027290	-0.347144
C	3.293640	2.128656	-0.527098
S	3.417036	-0.513813	-0.338944
S	5.012377	1.958918	-0.670686
C	5.011515	0.242810	-0.250681
C	6.130736	-0.431164	0.085633
S	6.124757	-2.147182	0.518390
S	7.735078	0.315452	0.129144
C	7.775602	-2.150004	1.100708
C	8.500094	-1.041725	0.927414
H	8.142636	-3.063538	1.553570
H	9.537657	-0.928282	1.218587
H	2.892935	3.128873	-0.643626
C	-3.266167	1.247197	0.197414
C	-4.100316	2.311727	0.501441
C	-5.408934	1.813183	0.496829
C	-5.319472	0.464779	0.189470
H	-3.797917	3.329988	0.699434
H	-6.321867	2.358069	0.690622
C	-6.235057	-0.599701	0.027322
C	-7.595351	-0.573229	0.147520
C	-8.328188	-1.837504	-0.074172
C	-8.309521	0.610179	0.472825
O	-7.806651	-2.894423	-0.354497
O	-9.655059	-1.686425	0.070801
N	-8.848188	1.605919	0.741201
H	-10.044552	-2.561875	-0.092748
H	-5.804287	-1.566405	-0.225152
O	-4.003091	0.137859	0.009716
N	-0.539538	-1.946511	-0.850502
H	-0.586917	-2.924768	-1.100073

8. Dye B4:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	-0.385758	1.629015	-0.021677
C	1.017980	1.712417	-0.071377
C	1.846682	0.638594	-0.373338

C	1.155037	-0.582289	-0.593638
C	-0.262407	-0.674555	-0.536270
C	-1.090424	0.448488	-0.253231
H	-0.938071	2.526210	0.226235
H	1.468214	2.670871	0.168656
N	-0.608354	-1.949025	-0.786347
N	1.643792	-1.802577	-0.878743
O	3.295852	0.762996	-0.450889
O	3.949236	1.927287	-0.655707
S	4.332599	-0.673891	-0.311919
S	5.683208	1.931811	-0.705386
C	5.835235	0.247874	-0.192401
C	6.998593	-0.288732	0.230014
S	7.146411	-1.973438	0.752502
S	8.514226	0.622933	0.307562
C	8.754062	-1.772862	1.415521
C	9.369414	-0.604391	1.217157
H	9.187659	-2.618851	1.935769
H	10.372290	-0.368002	1.552711
H	3.454024	2.872076	-0.847129
C	-2.532181	0.361315	-0.200232
C	-3.447757	1.394750	-0.037062
C	-4.794310	0.967899	-0.011681
C	-4.941274	-0.406245	-0.138975
S	-3.375753	-1.153774	-0.341762
C	-6.093197	-1.236344	-0.147138
C	-7.361216	-1.021550	0.319376
C	-8.331121	-2.119999	0.093451
C	-7.785646	0.100160	1.082894
O	-8.080133	-3.152781	-0.490081
O	-9.540615	-1.850569	0.610710
N	-8.146900	0.980432	1.751356
H	-10.092828	-2.625320	0.411685
H	-5.963397	-2.231258	-0.573960
O	-3.108207	2.704795	0.075399
O	-5.825302	1.826070	0.054381
C	-4.203930	3.588530	-0.166448
C	-5.448782	3.108834	0.546507
H	-3.889373	4.567253	0.201865
H	-4.387248	3.650342	-1.246742
H	-5.280984	3.047124	1.628482
H	-6.297009	3.767908	0.354257
N	0.556140	-2.529815	-0.969502
H	0.612462	-3.516961	-1.177515

9. Dye C1:

Atoms	Coordinates (Angstroms) X	Y	Z
C	-1.036226	-2.388753	0.145770
C	-2.435633	-2.300034	0.060854
C	-3.112928	-1.124716	-0.249764
C	-2.267858	-0.000469	-0.436090
C	-0.854202	-0.087459	-0.341585
C	-0.183068	-1.305274	-0.052492
H	-0.613921	-3.355937	0.398493
H	-3.008697	-3.196598	0.276084
N	-0.346061	1.135833	-0.574678
N	-2.587185	1.274282	-0.725374
C	1.257454	-1.420661	0.043052
C	1.998660	-2.566888	0.281099
C	3.382803	-2.348225	0.318947
C	3.732307	-1.026742	0.108692
S	2.315512	-0.050812	-0.139050
H	1.551017	-3.543913	0.420777
H	4.110387	-3.134276	0.493406
C	-5.356615	-2.134319	-0.590153
C	-7.022082	-0.223871	-0.179614
C	-4.563767	-1.063918	-0.366745
C	-8.117599	0.460759	0.208884
C	-9.699111	2.165110	1.342419
C	-10.454950	1.085725	1.125797
H	-10.034208	3.062157	1.849729
H	-11.489448	0.983038	1.431560
H	-4.983560	-3.136159	-0.768006
S	-8.060109	2.152407	0.727070
S	-9.740555	-0.245879	0.241891
S	-5.410147	0.495355	-0.255410
S	-7.075021	-1.914900	-0.688123
C	5.042601	-0.442670	0.077925
C	5.385520	0.887995	-0.134691
S	6.462930	-1.399035	0.322413
C	6.761766	1.128333	-0.099841
H	4.645834	1.661778	-0.310229
C	7.515408	-0.015386	0.140830
H	7.206707	2.105362	-0.244598
C	8.917386	-0.215392	0.255141
H	9.260877	-1.230909	0.448779
C	9.936093	0.691402	0.158672
C	11.313665	0.179532	0.326187

O	11.595851	-0.979527	0.540203
C	9.733180	2.074606	-0.088917
N	9.531337	3.202200	-0.292770
O	12.234173	1.150937	0.214675
H	13.096210	0.719280	0.339063
C	-1.315101	3.293186	-1.021361
H	-2.190770	3.606003	-1.588572
H	-1.282494	3.823600	-0.065700
H	-0.399479	3.484629	-1.580282
N	-1.417607	1.869870	-0.789793

10. Dye C2:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	0.857169	-2.048804	0.115796
C	-0.543538	-2.092090	0.026197
C	-1.329084	-0.977312	-0.254231
C	-0.594939	0.227633	-0.403683
C	0.820058	0.273538	-0.304637
C	1.602732	-0.883015	-0.047067
H	1.369490	-2.978140	0.341881
H	-1.028157	-3.045435	0.212082
N	1.209741	1.545242	-0.500997
N	-1.033968	1.473882	-0.658482
C	-2.778271	-1.050319	-0.377769
C	-3.465772	-2.188371	-0.618773
S	-3.767963	0.421004	-0.256456
S	-5.194488	-2.131050	-0.729626
C	-5.306845	-0.446465	-0.209728
C	-6.467110	0.129912	0.166572
S	-6.574590	1.815290	0.696596
S	-8.017613	-0.724478	0.169548
C	-8.220493	1.675321	1.276012
C	-8.869472	0.532214	1.040721
H	-8.646661	2.535540	1.778740
H	-9.896217	0.333504	1.324521
H	-2.999342	-3.149048	-0.803248
C	3.047251	-0.863716	0.050668
C	3.890111	-1.951815	0.260811
C	5.245126	-1.620898	0.309575
C	5.477247	-0.260175	0.135928
S	3.972898	0.590752	-0.089220
H	3.528186	-2.967195	0.372126
H	6.037192	-2.343416	0.464038

C	6.683013	0.493883	0.113356
C	7.975077	0.073923	0.260819
C	9.034051	1.104685	0.189761
C	8.339447	-1.281932	0.474578
O	8.833727	2.286523	0.011593
O	10.261815	0.583519	0.346078
N	8.605388	-2.401127	0.648456
H	10.880387	1.330809	0.284346
H	6.592766	1.568383	-0.042729
N	0.073211	2.179689	-0.700489
C	0.041712	3.612128	-0.894741
H	-0.874790	3.858294	-1.429093
H	0.055633	4.118143	0.074417
H	0.919835	3.900183	-1.472324

11. Dye C3:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	0.984305	-2.375649	0.205422
C	-0.412776	-2.317966	0.089407
C	-1.102341	-1.150220	-0.224829
C	-0.278094	-0.005729	-0.381078
C	1.137137	-0.052753	-0.255945
C	1.811967	-1.268741	0.039369
H	1.430141	-3.333632	0.455155
H	-0.972841	-3.227627	0.281322
N	1.615086	1.187992	-0.469500
N	-0.629247	1.260629	-0.667816
C	-2.550976	-1.115465	-0.374812
C	-3.315793	-2.201638	-0.621655
S	-3.432517	0.425248	-0.278199
S	-5.034352	-2.018395	-0.759789
C	-5.029480	-0.330179	-0.239133
C	-6.147744	0.326767	0.131994
S	-6.138050	2.014938	0.664061
S	-7.754929	-0.415512	0.126459
C	-7.790320	1.988448	1.241978
C	-8.517593	0.894520	1.001936
H	-8.155897	2.874729	1.747152
H	-9.556166	0.767423	1.283764
H	-2.917679	-3.194603	-0.794959
C	3.241084	-1.377331	0.175748
C	4.071631	-2.455851	0.439161
C	5.381671	-1.961943	0.456916

C	5.297358	-0.602030	0.202736
H	3.765410	-3.479831	0.597648
H	6.292453	-2.516914	0.631343
C	6.216090	0.464628	0.083933
C	7.576573	0.430700	0.204807
C	8.311830	1.700658	0.033157
C	8.287662	-0.765937	0.484958
O	7.793174	2.769122	-0.207030
O	9.638470	1.542017	0.174009
N	8.823883	-1.772496	0.715363
H	10.029096	2.422681	0.044980
H	5.788189	1.441553	-0.131259
O	3.982048	-0.264053	0.033624
C	0.591089	3.315434	-0.922158
H	-0.238650	3.598793	-1.568818
H	0.512657	3.841897	0.032997
H	1.547959	3.542144	-1.390799
N	0.525091	1.887861	-0.701664

12. Dye C4:

Atoms	Coordinates (Angstroms)		
	X	Y	Z
C	0.407574	-1.752722	-0.075613
C	-0.994717	-1.837816	-0.129409
C	-1.825910	-0.749695	-0.373119
C	-1.138269	0.481396	-0.531435
C	0.276237	0.574963	-0.469436
C	1.107213	-0.557251	-0.244068
H	0.963928	-2.659440	0.123898
H	-1.442596	-2.808778	0.059190
N	0.614716	1.863471	-0.649010
N	-1.627995	1.715495	-0.749008
C	-3.275392	-0.872452	-0.453626
C	-3.929614	-2.025814	-0.709883
S	-4.312118	0.556609	-0.246554
S	-5.664215	-2.028170	-0.755965
C	-5.815040	-0.368909	-0.168211
C	-6.978115	0.149134	0.277421
S	-7.125032	1.809313	0.874168
S	-8.494688	-0.763813	0.313958
C	-8.731918	1.579549	1.529792
C	-9.348004	0.421454	1.279546
H	-9.164532	2.401175	2.088485
H	-10.350518	0.170611	1.605568

H	-3.435355	-2.961290	-0.944371
C	2.548689	-0.466792	-0.185647
C	3.469982	-1.502032	-0.073352
C	4.814131	-1.070008	-0.026859
C	4.954384	0.309622	-0.086979
S	3.384301	1.057816	-0.252338
C	6.100602	1.145965	-0.054900
C	7.373595	0.917041	0.392186
C	8.331842	2.034951	0.221605
C	7.813569	-0.240734	1.090156
O	8.068457	3.096413	-0.302433
O	9.547349	1.749117	0.716014
N	8.188585	-1.152599	1.706722
H	10.090548	2.539168	0.556438
H	5.961270	2.161715	-0.426004
O	3.137529	-2.818264	-0.025707
O	5.849794	-1.924681	-0.002910
C	4.237418	-3.681966	-0.314588
C	5.480653	-3.233460	0.421280
H	3.928803	-4.680345	0.002475
H	4.419971	-3.686420	-1.396833
H	5.313634	-3.229989	1.505161
H	6.332304	-3.876839	0.194015
C	-0.628522	3.879907	-1.072044
H	0.145194	4.387403	-0.496043
H	-0.471829	4.061513	-2.138838
H	-1.620035	4.221914	-0.778782
N	-0.548179	2.462897	-0.797742

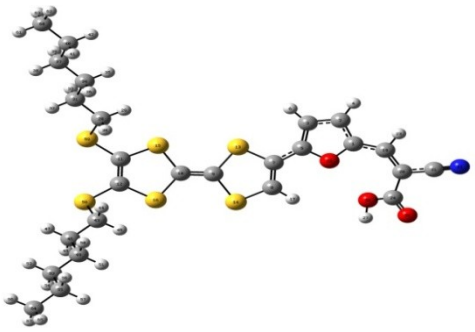

Fig. S1: Optimized geometry of the molecule (dye-2a) adopted for validation of methology.

Table S2: $\Delta_{H-L}$and λ_{max} values of the reference compound dye-2a for validation of functional.

Functional	**Basis set**	**Δ_{H-L}(eV)**	**λ_{max} (nm)**
B3LYP	6-31G(d)	2.32	653.13
B3LYP-D3	6-31G(d)	2.29	646.16
CAM-B3LYP	6-31G(d)	6.26	416.56
B3PW91	6-31G(d)	2.16	694.19
HSEH1PBE	6-31G(d)	1.81	684.95
ωB97XD	6-31G(d)	2.30	412.48
Experimental		**1.94**	**503**

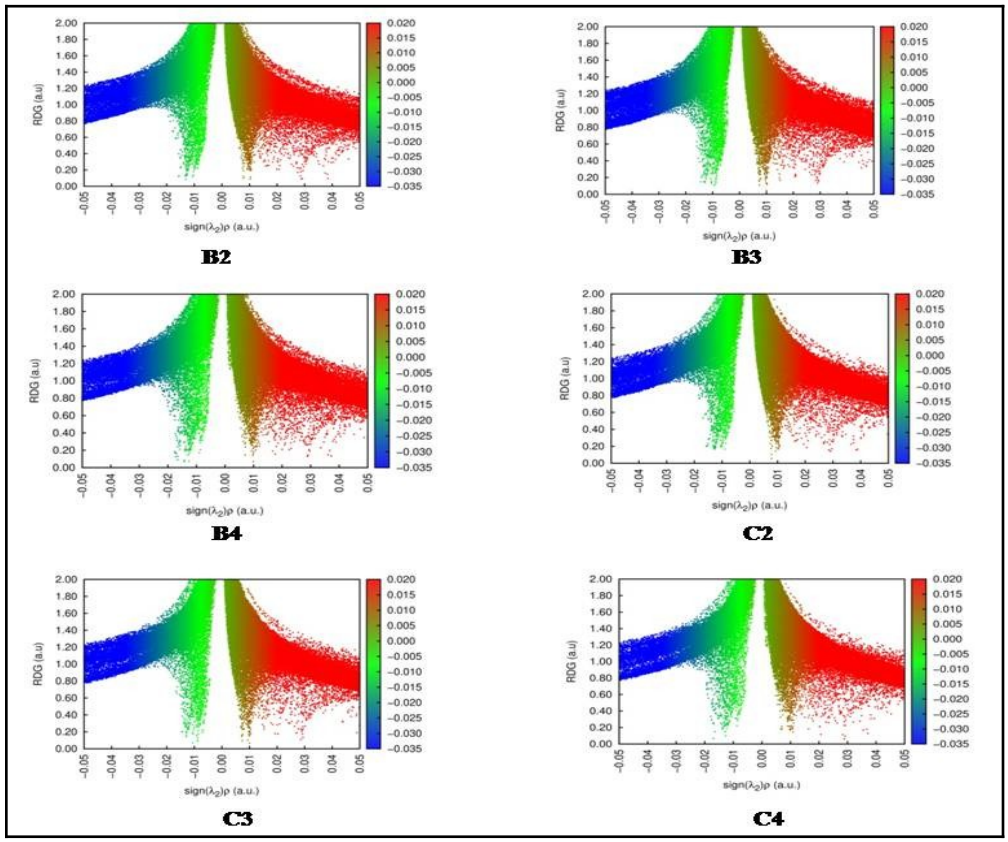

Fig. S2: RDG plots of B2, B3, B4, C2, C3 and C4

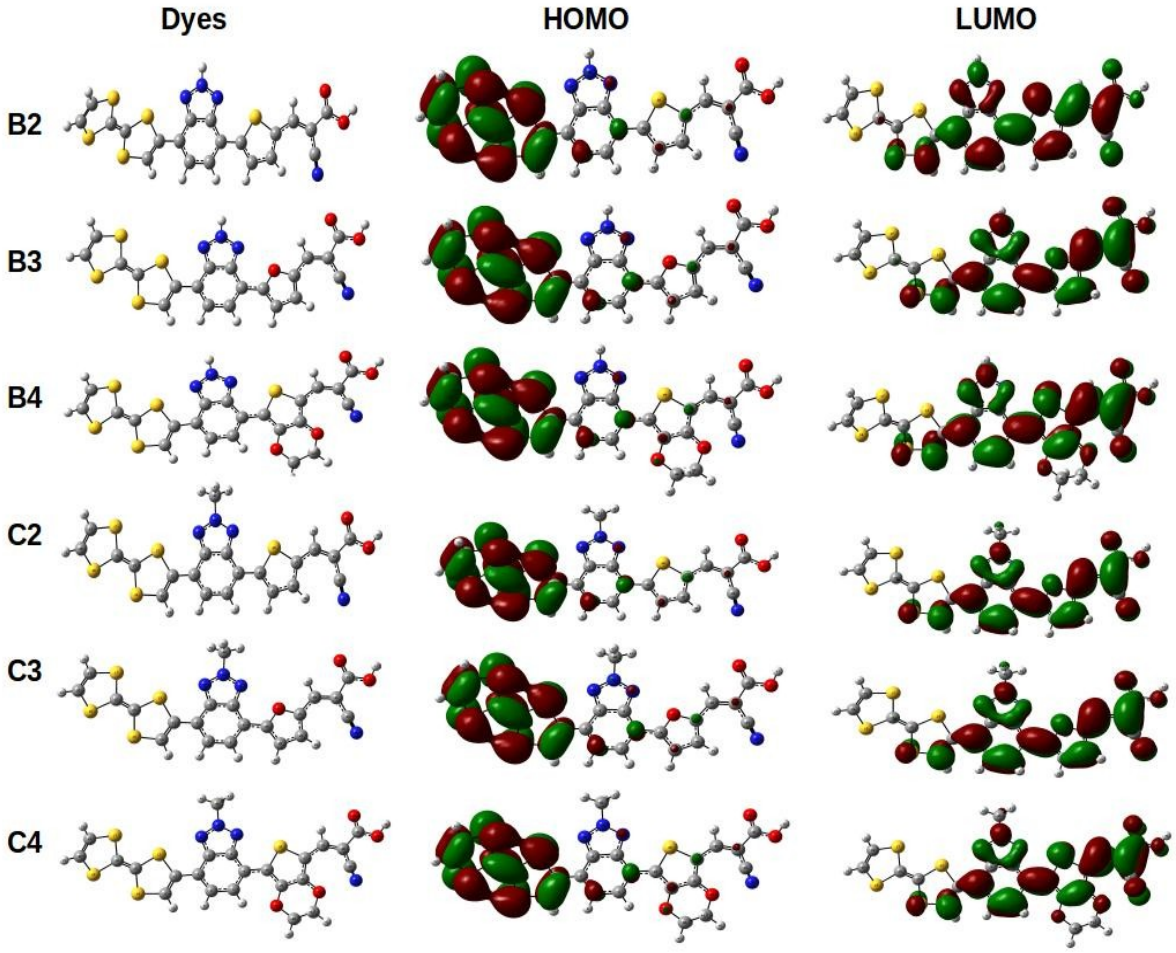

Fig. S3: FMO plots along with optimized structures of B2, B3, B4, C2, C3 and C4.

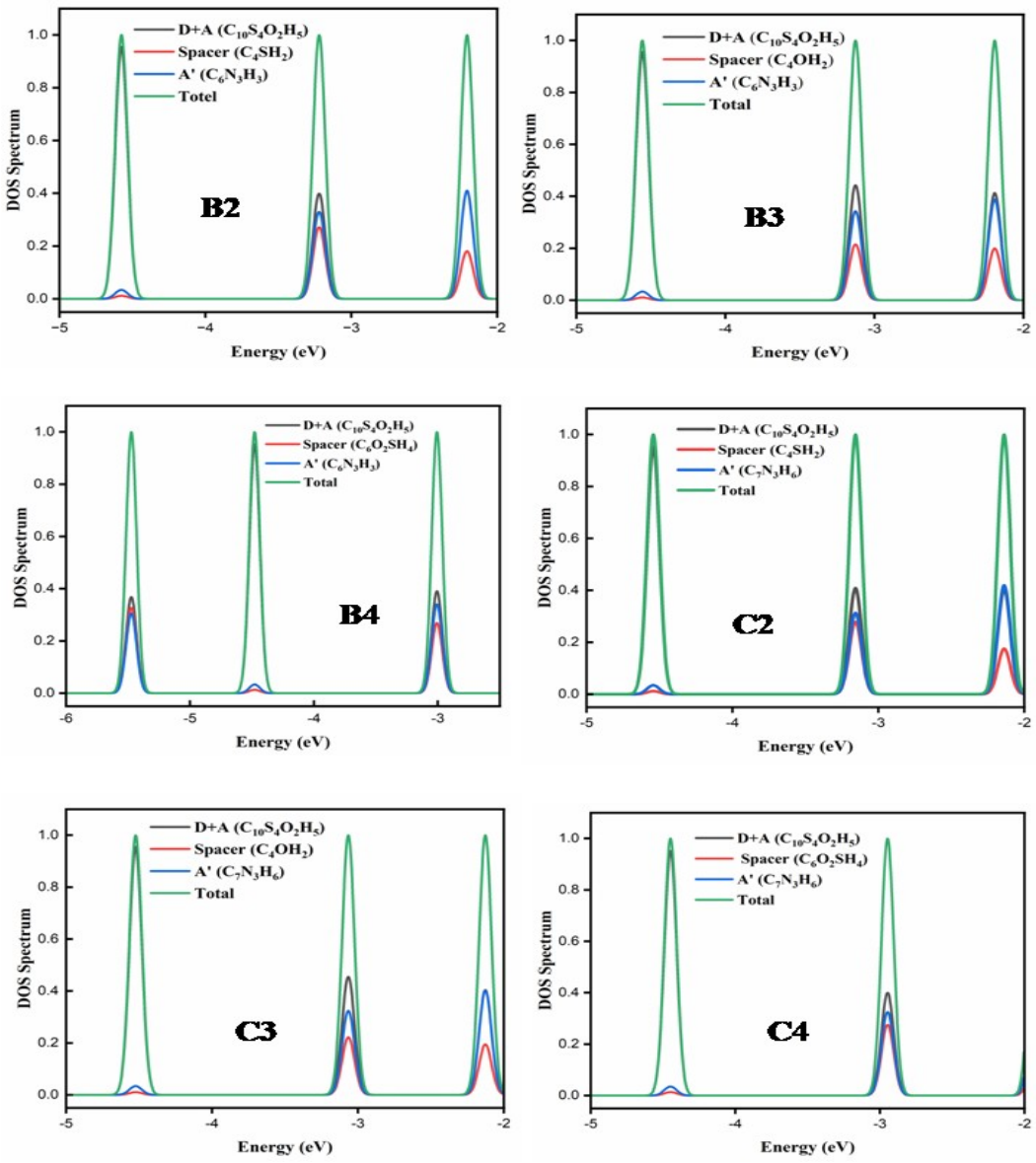

Fig. S4: PDOS of B2, B3, B4, C2, C3 and C4.

Table S3: Spectral data of designed compounds obtained from PDOS spectra.

Dyes	**Groups**	**Contribution to HOMO (%)**	**C[illegible]bution to L[illegible]MO (%)**
A1	Donor+anchoring group Auxiliary acceptor Spacer	94 2 4	22 26 53
A2	Donor+anchoring group Auxiliary acceptor Spacer	94 1 4	26 15 59

A3	Donor+anchoring group Auxiliary acceptor Spacer	95 1 4	28 12 60
A4	Donor+anchoring group Auxiliary acceptor Spacer	95 1 4	24 15 61
B1	Donor+anchoring group Auxiliary acceptor Spacer	95 2 3	36 45 19
B2	Donor+anchoring group Auxiliary acceptor Spacer	95 1 3	40 27 33
B3	Donor+anchoring group Auxiliary acceptor Spacer	96 1 3	44 21 34
B4	Donor+anchoring group Auxiliary acceptor Spacer	95 1 3	39 27 34
C1	Donor+anchoring group Auxiliary acceptor Spacer	95 2 4	37 46 17
C2	Donor+anchoring group Auxiliary acceptor Spacer	95 1 3	41 28 31
C3	Donor+anchoring group Auxiliary acceptor Spacer	96 1 3	45 22 32
C4	Donor+anchoring group Auxiliary acceptor Spacer	95 1 3	40 28 33

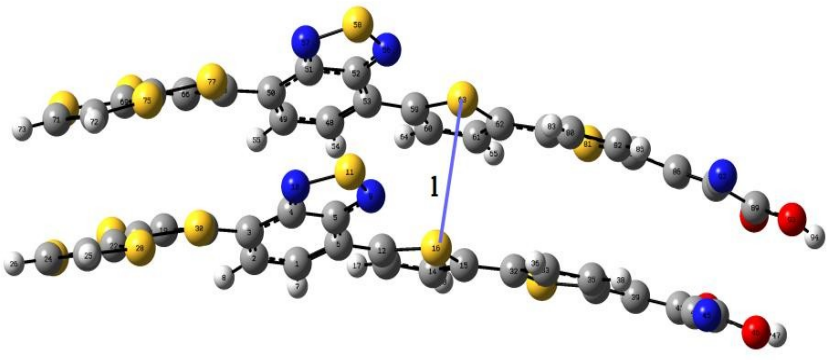

Fig. S5: Representative structure of two stacked A2 monomers along with distance l.

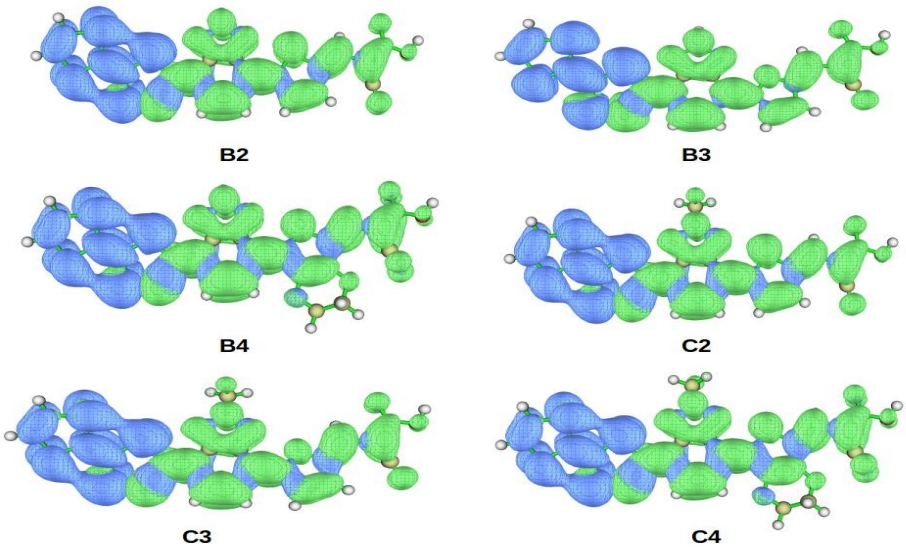

Fig. S6: CDD maps of B2, B3, B4, C2, C3 and C4.

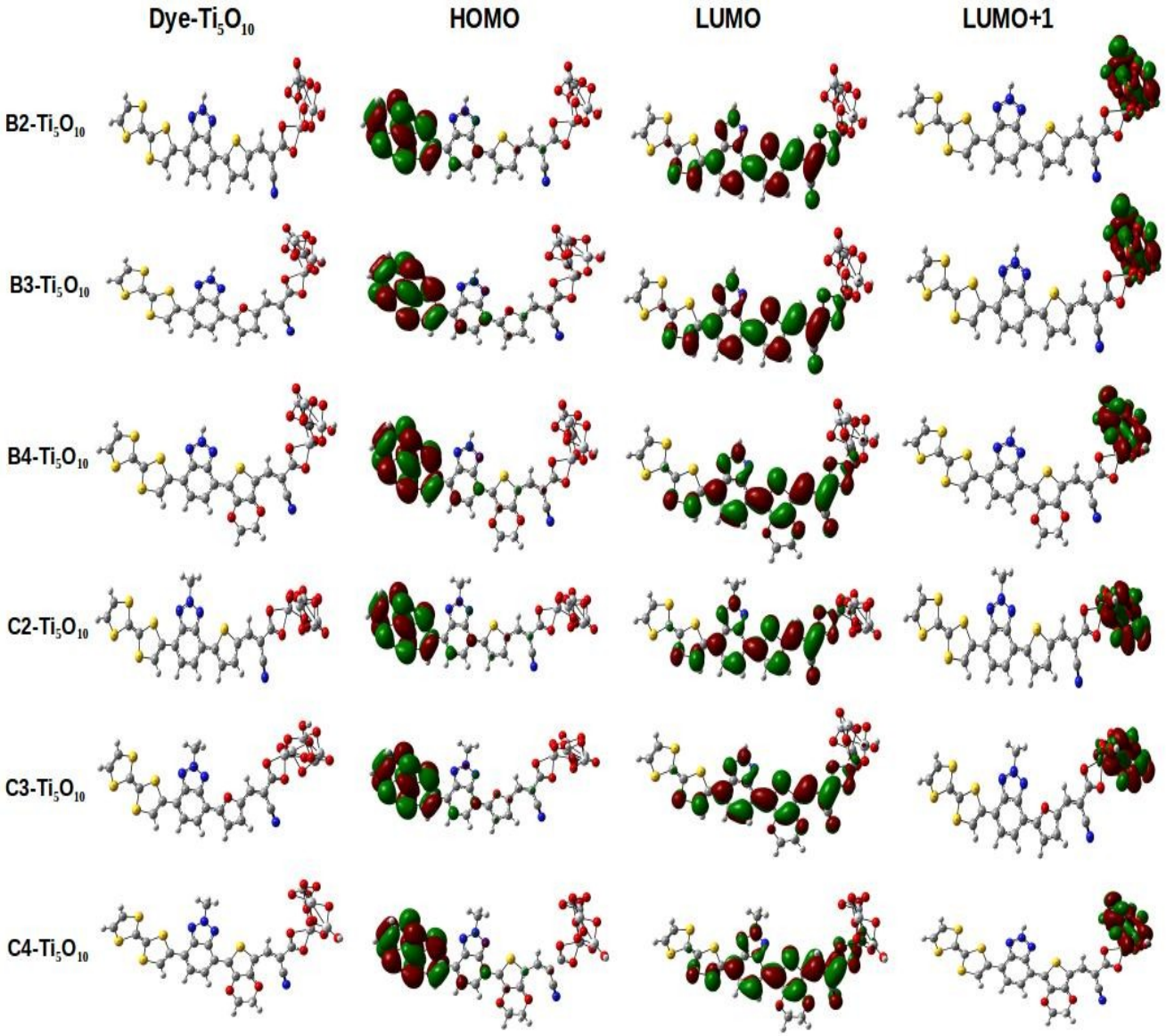

Fig. S7: FMO plots along with optimized structures of B2-Ti_5O_{10}, B3-Ti_5O_{10}, B4-Ti_5O_{10}, C2-Ti_5O_{10}, C3-Ti_5O_{10} and C4-Ti_5O_{10} dye-clusters.

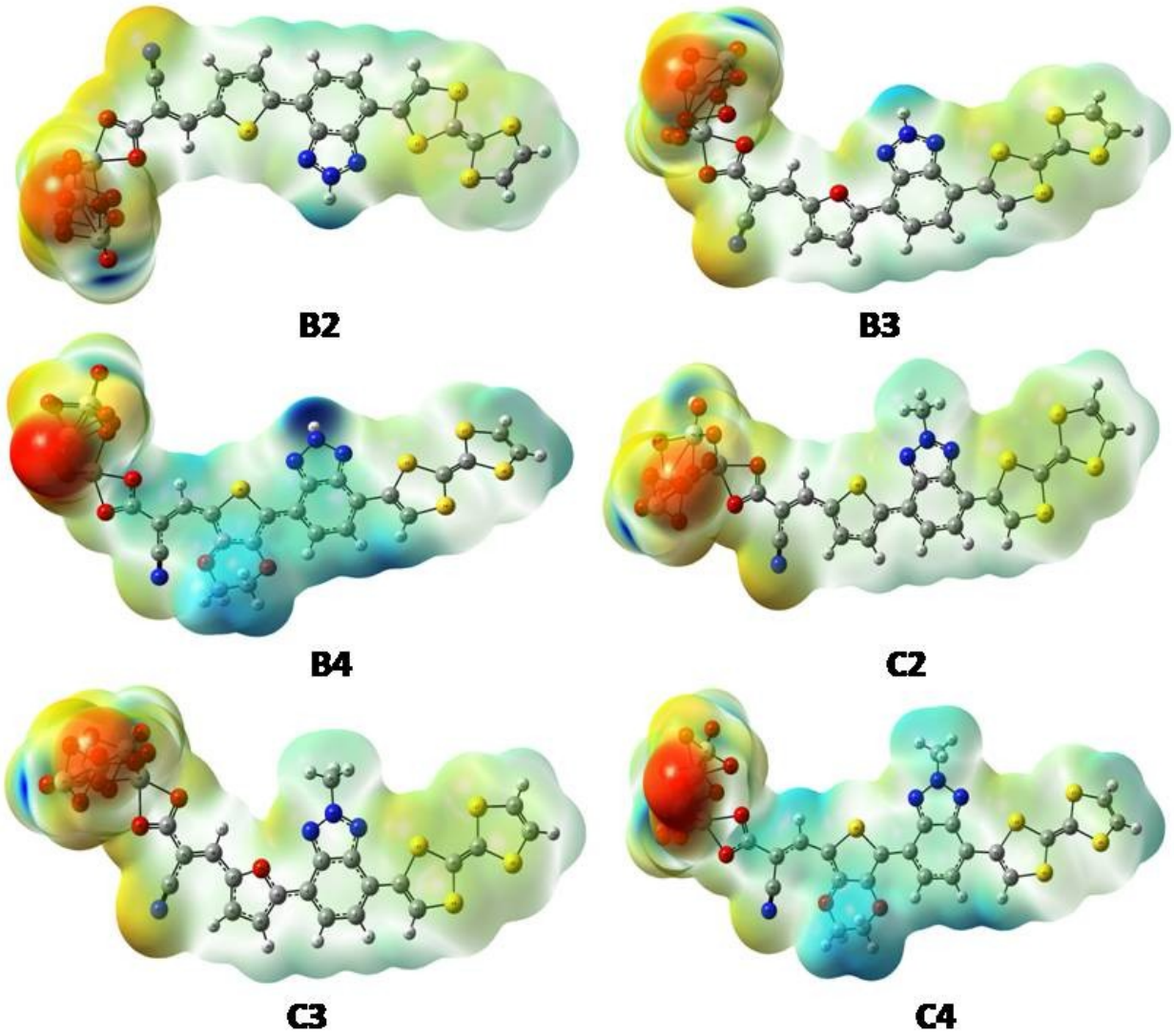

Fig. S8: MEPS contour plots of B2-Ti_5O_{10}, B3-Ti_5O_{10}, B4-Ti_5O_{10}, C2-Ti_5O_{10}, C3-Ti_5O_{10} and C4-Ti_5O_{10} dye-clusters.