Electronic Supplementary Information
Density functional theory characterization and design of high-performance diarylamine-fluorene dyes with different π spacer for dye-sensitized solar cells

Ji Zhang, Hai-Bin Li, Shi-Ling Sun, Yun Geng, Yong Wu, and Zhong-Min Su*

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024，China

Author for correspondence: Prof. Zhong-Min Su. E-mail: zmsu@nenu.edu.cn

Fig. S1 Optimized molecular structures of (a) **1**, (b) **1-TiO$_2$**, (c) **2**, and (d) **2-TiO$_2$** in gas phase. (Page S2)

Fig. S2 The absorption spectra of **1-6** calculated in THF solution by TD-CAM-B3LYP with the B3LYP/6-31G* geometries. (Page S2)

Fig. S3 Optimized molecular structures of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** in gas phase. (Page S3)

Fig. S4 Optimized molecular structures of dyes **3-6** before and after adsorption in gas phase. (Page S3)

Table S1 Computed maximum absorption wavelengths λ_{max}/nm (eV), oscillator strengths (*f*) and transition natures of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** corresponding to $S_0 \rightarrow S_1$ at the C-PCM/CAM-B3LYP/6-31+G* level. (Page S4)

Table S2 Atomic charge distribution (in e) of the donor (diarylamine), π spacer (fluorene and heteroaromatic ring), acceptor (cyanoacrylic acid) and $(TiO_2)_6$ of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** at C-PCM/B3LYP/6-31G* level. (Page S4)

Cartesian coordinate of final optimized geometries of dyes **1-6** before and after adsorption. (Page S5-S12)

Cartesian coordinate of final optimized geometries of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** . (Page S12-S13)

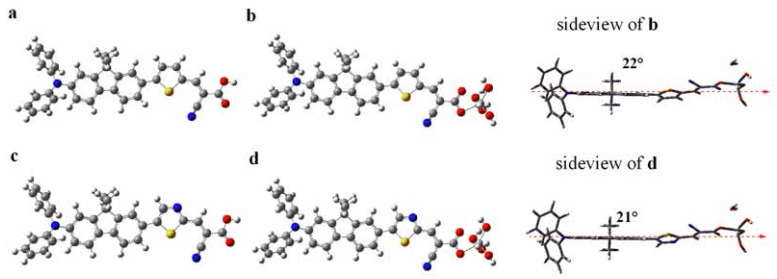

Fig. S1 Optimized molecular structures of (a) **1**, (b) **1-TiO$_2$**, (c) **2**, and (d) **2-TiO$_2$** in gas phase.

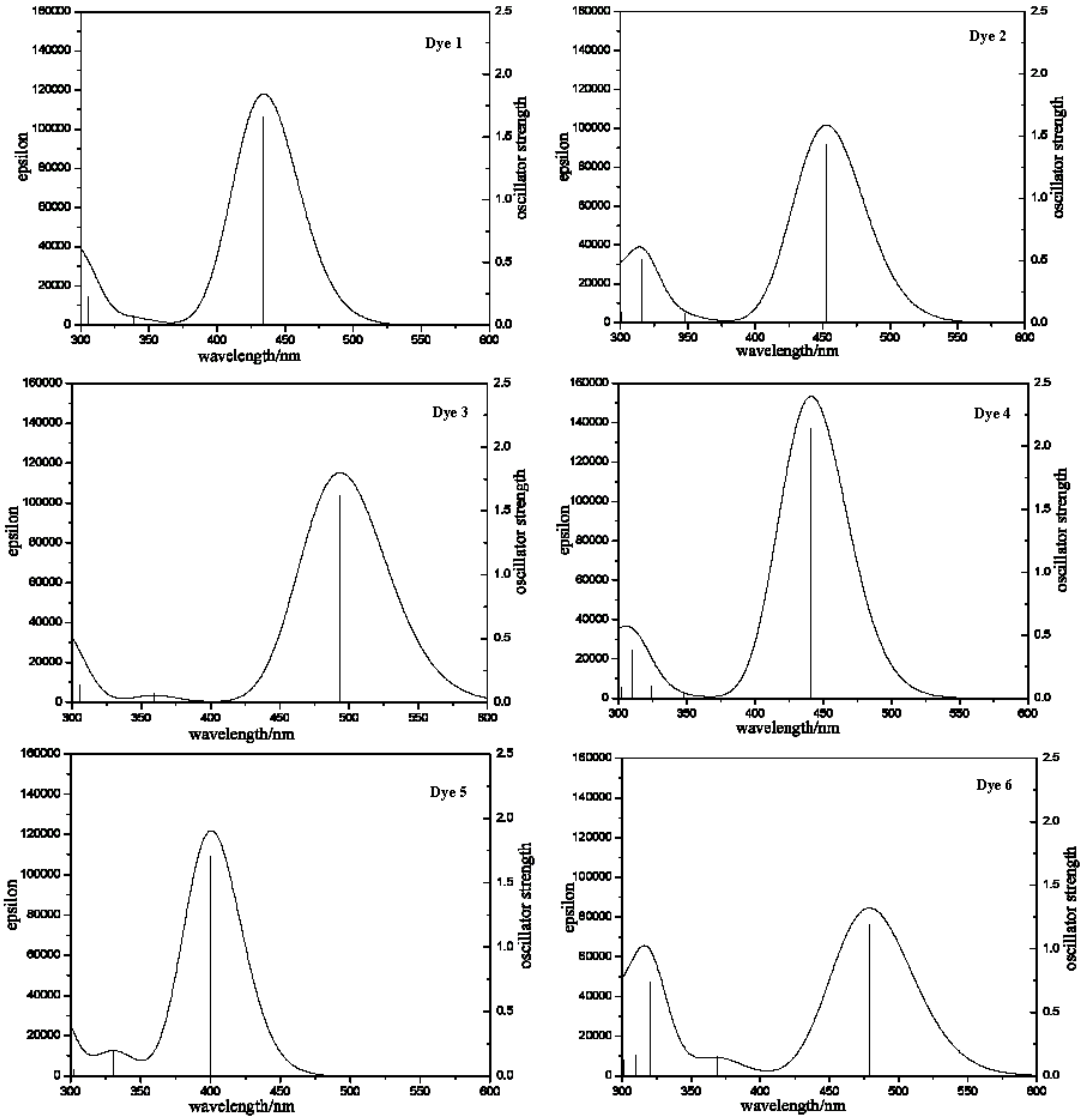

Fig. S2 The absorption spectra of **1-6** calculated in THF solution by TD-CAM-B3LYP with the B3LYP/6-31G* geometries.

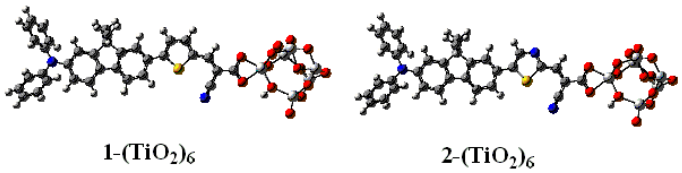

Fig. S3 Optimized molecular structures of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** in gas phase.

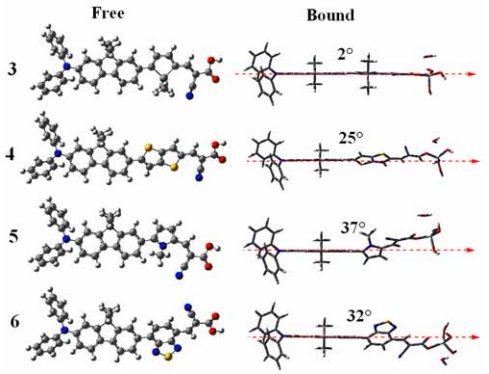

Fig. S4 Optimized molecular structures of dyes **3-6** before and after absorption in gas phase

Table S1 Computed maximum absorption wavelengths λ_{max}/nm (eV), oscillator strengths (*f*) and transition natures of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** corresponding to $S_0 \rightarrow S_1$ at the C-PCM/CAM-B3LYP/6-31+G* level

Dye-(TiO$_2$)$_6$	State	Main configurations[a]	λ_{max}	*f*
1	$S_0 \rightarrow S_1$	H-1→L（0.28）H→L（0.62）	479 (2.59)	1.90
2	$S_0 \rightarrow S_1$	H-1→L（0.24） H→L（0.68）	507 (2.44)	1.64

[a] Data in parentheses are main configuration contributions.

Table S2 Atomic charge distribution (in e) of the donor (diarylamine), π spacer (fluorene and heteroaromatic ring), acceptor (cyanoacrylic acid) and (TiO$_2$)$_6$ of **1-(TiO$_2$)$_6$** and **2-(TiO$_2$)$_6$** at the C-PCM/B3LYP/6-31G* level[a]

	S_0						S_1				
Dyes	D	π	A	(TiO$_2$)$_6$	μ_{total}[b]	μ_{normal}[b]	D	π	A	(TiO$_2$)$_6$	Δq[c]
1	-0.101	0.390	-0.618	0.329	13.11	8.57	0.334	0.367	-0.872	0.170	0.159
2	-0.095	0.326	-0.578	0.347	11.95	9.55	0.334	0.273	-0.852	0..244	0.103

[a] Atomic charge from natural population analysis with NBO 3.1; [b] μ_{total} and μ_{normal} are the total and the vertical dipole moment (Debye) of the free dyes at the geometry of the dyes binded to (TiO$_2$)$_6$. [c] Δq is the charge difference on (TiO$_2$)$_6$ between S_0 and S_1.

Cartesian coordinate of final optimized geometries of dyes **1-6** before and after adsorption

Dye 1 B3LYP/6-31G*
E = -2007.5322856 a.u.
C,-3.5790440112,0.3261648125,0.2891225736
C,-4.439101639,1.3019208071,0.8011797606
C,-4.1096684712,-0.7933033669,-0.3838305158
C,-5.813703711,1.1521678141,0.6457616826
H,-4.0500209684,2.1673712052,1.3314429141
C,-5.4775130872,-0.9378197095,-0.5543841183
C,-6.3498669133,0.039839981,-0.0344153545
H,-6.4889462027,1.8967723723,1.0538757277
H,-5.8899021247,-1.7903976632,-1.0853408862
N,-7.7508837399,-0.0945223859,-0.1928779639
C,-8.361887533,-1.3768676796,-0.0978041074
C,-9.3438829457,-1.7671987446,-1.0217981512
C,-7.9945528957,-2.2668732902,0.9241816326
C,-9.9473085167,-3.0193145995,-0.918226424
H,-9.6287013731,-1.0848818444,-1.8163846238
C,-8.5902631205,-3.5238578448,1.0086612122
H,-7.2438643092,-1.9659901287,1.6481801424
C,-9.5721369951,-3.9071452498,0.0923457309
H,-10.7060487893,-3.3059034843,-1.6417117244
H,-8.2952100059,-4.200397821,1.8065253927
C,-8.5565357689,1.0484147813,-0.4606160883
C,-9.7870547414,1.2186218994,0.1932825755
C,-8.1358631671,2.0170162504,-1.3858617741
C,-10.5799638553,2.331326671,-0.0814698985
H,-10.1150166746,0.4759000706,0.9136477761
C,-8.9270965005,3.1356456629,-1.6400855987
H,-7.1898403026,1.8869105841,-1.9018402085
C,-10.154684821,3.2986431737,-0.9944606936
H,-11.5299159848,2.4479237442,0.4335488212
H,-8.5866532991,3.875985155,-2.3592865531
C,1.9924384377,-0.8513750482,-0.1191666722
C,2.5251571835,-2.1145609614,-0.3423712538
S,3.2601621825,0.3478794938,-0.0309106331
C,3.9259012276,-2.1202941702,-0.4303123599
H,1.9167789042,-3.0090395963,-0.4065735183
C,4.509488626,-0.865243814,-0.2774056569
H,4.5195983635,-3.0151262434,-0.5884505265
C,5.9155393685,-0.637422293,-0.3237682107
H,6.4990366693,-1.536281136,-0.5049286802
C,6.6442571443,0.5141518038,-0.1793371302
C,8.1230849563,0.5170296713,-0.2678566758
O,8.8207452208,1.5019293959,-0.1460120749
O,8.642759699,-0.7190870862,-0.5049983003
H,9.6079982833,-0.5891637974,-0.5408497559
C,6.0475379976,1.7869548483,0.0670424307
N,5.5361533781,2.8136723555,0.2683715609
H,-10.0401021644,-4.884649172,0.1659276317
H,-10.7721651853,4.1681986047,-1.2004959911
C,-2.1223686339,0.2159357789,0.3015629644
C,-1.7550674648,-0.9744449173,-0.3637322271
C,-1.1362374723,1.0562351215,0.8261754593
C,-0.4229395544,-1.3196104506,-0.5052508082
C,0.2022683829,0.7030522311,0.6874215502
H,-1.4013494153,1.9740434611,1.3439102746
C,0.5855783109,-0.4819750248,0.0248766718
H,-0.1428813689,-2.2194908448,-1.0459609833
H,0.9653106172,1.3460511154,1.117148205
C,-2.9926343713,-1.7212175531,-0.8637471929
C,-2.9886912979,-1.8506967047,-2.4034860069
H,-2.9092383718,-0.8694727427,-2.8820110993
H,-2.1447760628,-2.4645301682,-2.7390662301
H,-3.9110633794,-2.3287184075,-2.7527048994
C,-3.1090150895,-3.1194674951,-0.2165502162
H,-3.1042951454,-3.0505962236,0.8759638092
H,-4.0390257913,-3.6104146132,-0.5249041029
H,-2.2731962861,-3.7592310701,-0.5230036298

Dye 1-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2369.1045789 a.u.
C,0.0624217092,2.1773127955,0.1744897167
C,-0.9434419786,3.0623762915,-0.2251808306
C,1.2165394311,2.6706901447,0.8173947118
C,-0.7891121768,4.4251991964,0.0103868149
H,-1.836005884,2.7024925256,-0.7304854522
C,1.366786467,4.0258595066,1.0677813413
C,0.3586857615,4.9238722225,0.6606832301
H,-1.5570640012,5.1205072481,-0.3112536908
H,2.2462773863,4.408513681,1.5765935151
N,0.498395737,6.3123533091,0.9005067342
C,1.7744216048,6.9341040673,0.7868817533
C,2.2069107782,7.851250884,1.7579610945
C,2.6148649009,6.6433323492,-0.2999323329
C,3.451769586,8.4671168632,1.6371166622
H,1.5628211067,8.0761179312,2.6021899318
C,3.8652776527,7.2507004647,-0.4030368303
H,2.280981174,5.9427074036,-1.0587840281
C,4.2904376714,8.1682842387,0.5607741624
H,3.7715967255,9.1749130146,2.3973521586
H,4.5032203284,7.0158845017,-1.2510904161
C,-0.6321613176,7.0976665522,1.2648051042
C,-0.8324463527,8.3626153829,0.6892923972
C,-1.5578143948,6.6223939145,2.2078374981
C,-1.9332811834,9.1349072079,1.0567302659
H,-0.1227442508,8.7331421142,-0.0436193372
C,-2.6652026674,7.3943185311,2.5555141945
H,-1.4033834026,5.6493517349,2.6634037308
C,-2.8586009129,8.6554322424,1.9867079772
H,-2.0738972828,10.11175739,0.6015326452
H,-3.372363137,7.0117530656,3.2868067676
C,1.2792697693,-3.4008327278,0.1441578808
C,2.5557050092,-3.93828097,0.2639146752
S,0.0829727036,-4.6676023637,0.031531856
H,3.4496935171,-3.3287751309,0.3231000194
C,1.3113632205,-5.9218975001,0.1275263802
C,1.0850916748,-7.325987575,0.0892746517
H,1.9841558532,-7.9323057377,0.1813692669
C,-0.0717205182,-8.0498386863,-0.0426438591
C,0.0080631362,-9.5211107966,-0.0436633316
O,-1.0545306949,-10.2291109911,-0.1690631206
O,1.1149780218,-10.1365417483,0.0769247506
C,-1.3625703804,-7.4594283557,-0.1783948357
N,-2.4072945664,-6.9560078187,-0.287502787
H,5.2623167924,8.645468197,0.4733205175
H,-3.719101934,9.2569886833,2.2651470524
C,0.176267156,0.725438182,0.0602740145
C,1.4033256843,0.3232159461,0.6332076513
C,-0.6891438277,-0.229627938,-0.4817301218
C,1.7605228621,-1.0131319891,0.6658659315
C,-0.324264794,-1.5720791019,-0.4522434629

H,-1.6349845242,0.0631926604,-0.929284198
C,0.8976151139,-1.9901789048,0.1165344769
H,2.6903792704,-1.3226766716,1.135079051
H,-0.9876305623,-2.3093995235,-0.8956093575
C,2.1727013253,1.5305940128,1.1715066988
C,2.3863516927,1.4271354526,2.6984963959
H,1.4329308857,1.3101770111,3.2234000944
H,3.0201801345,0.5670537921,2.9438282715
H,2.8798742006,2.3279997856,3.0808426436
C,3.533099073,1.6973732541,0.4576436246
H,3.4040336196,1.7656074062,-0.6273376075
H,4.0391557799,2.6070779797,0.8004034722
H,4.1899816543,0.8461281843,0.671686711
Ti,-0.0318735708,-11.993376835,-0.0725553576
O,0.0263047386,-12.2944355261,-1.8583995873
H,0.7767577148,-12.7590724115,-2.2608592495
O,-1.4076733036,-13.1048766247,0.4377748417
O,1.516319278,-12.7907712243,0.5039166812
O,-0.30961392,-11.5870178624,2.2352121559
H,-1.9358359919,-13.5112329572,-0.2680230732
H,2.289760875,-12.2030289106,0.5427219432
H,-1.1514078085,-12.0759847388,2.2970786206
H,0.3630349616,-12.2033287412,2.5726862819
C,2.5717506599,-5.3413649557,0.2545540296
H,3.4752602906,-5.938687054,0.3244434679

Dye 2 B3LYP/6-31G*
E = -2023.5744215 a.u.
C,-3.6021279121,0.3763637938,0.2860206031
C,-4.4752658824,1.3487883178,0.782464641
C,-4.1175779806,-0.7596875778,-0.3708766774
C,-5.8473097966,1.17990302,0.626755255
H,-4.0980317827,2.2265600076,1.3009044921
C,-5.4830786262,-0.9239475422,-0.5413535114
C,-6.3687225357,0.0508128727,-0.0380552628
H,-6.532308307,1.9219623474,1.0228465759
H,-5.8835183406,-1.7894837791,-1.0602218252
N,-7.7667199942,-0.1027300382,-0.1973890891
C,-8.3612071342,-1.3932004111,-0.0997625247
C,-9.3279418085,-1.8025535559,-1.031299391
C,-7.9931851204,-2.2704986376,0.9327205367
C,-9.9163069525,-3.0616272144,-0.9249080452
H,-9.6128794423,-1.1295042043,-1.8337424549
C,-8.5735435467,-3.5344787288,1.0202712
H,-7.2543866283,-1.9544298436,1.662519981
C,-9.5404589014,-3.9369220172,0.0962887132
H,-10.6635159638,-3.3634125295,-1.6541517175
H,-8.2785540752,-4.2013784875,1.8261984844
C,-8.589033733,1.0275247233,-0.4697770572
C,-9.821485997,1.1820790545,0.1841539934
C,-8.1836172978,1.9976597113,-1.4001197057
C,-10.6312875962,2.2814058552,-0.0951951733
H,-10.1376465292,0.4377317968,0.9080913358
C,-8.9917885745,3.1030522727,-1.6589950856
H,-7.2363036378,1.8791515793,-1.9165339539
C,-10.2211825375,3.2506392987,-1.0130783405
H,-11.5826005052,2.386021334,0.419839793
H,-8.6632100158,3.8448669376,-2.3821670634
C,1.9807468201,-0.7364024867,-0.0961575452
C,2.5372935259,-1.9920034966,-0.3133574452
S,3.2693061281,0.4308567029,-0.004029606
H,1.960019584,-2.9064687571,-0.3885982926
C,4.4409575282,-0.8674857755,-0.2541670851
C,5.8668410656,-0.7320255252,-0.3088884134
H,6.3682150837,-1.6782587188,-0.4862458054
C,6.6565186028,0.3743210817,-0.1753048312
C,8.1376767947,0.2952561142,-0.2675095218
O,8.8816389158,1.2456475242,-0.1532635907
O,8.5841456922,-0.966043157,-0.4961574563
H,9.555647179,-0.8972629618,-0.536607448
C,6.1331321451,1.6812339543,0.0627830702
N,5.6760936045,2.734392343,0.2567420253
H,-9.996537358,-4.9198419981,0.1721800128
H,-10.8518417143,4.1097671905,-1.2228462652
C,-2.144685577,0.2849372227,0.3018837385
C,-1.7612700827,-0.9105089169,-0.3455749427
C,-1.1702676023,1.1462530587,0.8148139092
C,-0.4249435801,-1.2403177374,-0.4815664127
C,0.172723022,0.8088091903,0.6820693932
H,-1.4481775913,2.0685866198,1.317497792
C,0.5714723265,-0.3812058429,0.0380307002
H,-0.1331638188,-2.1444521252,-1.0087045471
H,0.9276558086,1.4691435001,1.0999028012
C,-2.9884015035,-1.6807608143,-0.8350488606
N,3.8816516241,-2.0602705235,-0.4001788875
C,-2.9807217667,-1.8348793839,-2.3724955268
H,-2.9127898095,-0.8606299917,-2.8668301786
H,-2.1291273183,-2.4438152568,-2.6972471606
H,-3.8967609789,-2.3296366023,-2.7148327382
C,-3.0868269806,-3.0698868743,-0.1652742128
H,-3.0851838544,-2.9833638444,0.9259900525
H,-4.009353016,-3.578535331,-0.4672043377
H,-2.2417924127,-3.7029726563,-0.4599001293

Dye 2-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2385.1458266 a.u.
C,-0.0018525415,2.2004988366,0.1706525056
C,-0.9864633142,3.1105288195,-0.2262430504
C,1.1650064555,2.664634609,0.8125110929
C,-0.7988713573,4.468483891,0.0117135491
H,-1.888130776,2.7735027799,-0.7311715373
C,1.3486014148,4.0151937375,1.0651153046
C,0.3616715009,4.9383078897,0.6616348599
H,-1.5501999734,5.182631858,-0.3077263682
H,2.2378574311,4.3750574474,1.5735161298
N,0.5339328044,6.3217981284,0.9046809834
C,1.8254902888,6.9132957024,0.801538484
C,2.2732132696,7.8156646584,1.7793839349
C,2.6649145214,6.6082669947,-0.2820754031
C,3.5324661555,8.4034870401,1.6683134675
H,1.6295146119,8.0515763465,2.620899765
C,3.9294707843,7.1873196095,-0.3753990667
H,2.3193046684,5.9192052412,-1.0462804647
C,4.3699972626,8.0904234606,0.5951476471
H,3.8641368328,9.1003182437,2.4335567635
H,4.5666740576,6.9419464796,-1.22099158
C,-0.579593255,7.1350437081,1.261322263
C,-0.7459499399,8.4031683761,0.6822370454
C,-1.5211333494,6.6843965124,2.2006056076
C,-1.8296097301,9.2027728611,1.0423335552
H,-0.0234111727,8.7547120832,-0.0474596635
C,-2.6112720366,7.4836859516,2.5409439427
H,-1.3926203413,5.7089958273,2.6591857036
C,-2.7710679301,8.7478302332,1.9684253638
H,-1.9440282631,10.1818125637,0.5845495858
H,-3.3311844264,7.1200978741,3.2694546988

C,1.0782404163,-3.4020683787,0.1301252866
C,2.3384724894,-3.9789283082,0.2539010246
S,-0.1014808462,-4.67446231,0.0033217366
H,3.2598556143,-3.4124398868,0.3271823285
C,1.1960418695,-5.8676254831,0.1167952631
C,1.0433886646,-7.2906281384,0.0833554935
H,1.9827933131,-7.8277645641,0.1827859703
C,-0.077128585,-8.0604525412,-0.0489061652
C,0.0618261244,-9.5334449289,-0.0437301344
O,-0.9734965157,-10.2774445507,-0.1656314852
O,1.1918995961,-10.0982218101,0.0794819934
C,-1.3919806438,-7.5254987579,-0.1904552467
N,-2.4546606096,-7.0627669398,-0.3040285565
H,5.3530191121,8.5455777133,0.5152844529
H,-3.6181023444,9.3707235147,2.2411486233
C,0.0762132727,0.7468266166,0.0543035855
C,1.2939249488,0.3137981331,0.6252666956
C,-0.8138832863,-0.1857897024,-0.4873829482
C,1.6179441987,-1.0307960293,0.6567107742
C,-0.4827181234,-1.5368566965,-0.4592740824
H,-1.7532067499,0.1310976248,-0.9321551429
C,0.7295585703,-1.9848950835,0.106830459
H,2.540569537,-1.3635313963,1.1241240441
H,-1.1656821338,-2.2582678587,-0.8992705214
C,2.0938974716,1.5011750111,1.1630837066
C,2.309110972,1.3906830403,2.6893658869
H,1.3546301636,1.2962914359,3.2169213003
H,2.9228805446,0.5155258057,2.9321441045
H,2.8251986338,2.2790402,3.0710622896
C,3.4560623251,1.6342864816,0.4453203764
H,3.3255770982,1.7086629877,-0.6390828929
H,3.9869910085,2.5293951337,0.7887600499
H,4.0908375512,0.7654914736,0.6552269289
Ti,0.1238282857,-12.0069674003,-0.0606761163
O,0.1888137193,-12.300047349,-1.8462151671
H,0.9581270235,-12.7195019212,-2.2624569615
O,-1.2046781931,-13.1702081179,0.4538649764
O,1.7037149575,-12.735900991,0.5125033222
O,-0.1689820094,-11.5918796397,2.2373820463
H,-1.7158824022,-13.6036531534,-0.2484241258
H,2.4582741705,-12.1232085563,0.5402423126
H,-0.983061132,-12.1235984663,2.3144335835
H,0.5372699019,-12.1605613609,2.5894327042
N,2.3991183654,-5.3258226141,0.2469531091

Dye 3 B3LYP/6-31G*
E = -1978.6796197 a.u.
C,1.4975910439,0.7468744513,-0.427143006
C,2.3580315362,1.7488129155,-0.8867764239
C,2.0308408202,-0.4275687779,0.1435200841
C,3.7335133897,1.5727311392,-0.7788897611
H,1.9669550658,2.6561398423,-1.3399877109
C,3.4003846144,-0.5997663035,0.2666502959
C,4.2724499647,0.4060614763,-0.1979838561
H,4.4078556856,2.3384232403,-1.1471928043
H,3.8144372523,-1.4947615442,0.7206810065
N,5.6741102053,0.2480233069,-0.0824109121
C,6.2698176747,-1.0330846857,-0.2606934555
C,7.2573103349,-1.4869051068,0.6275340741
C,5.8836783033,-1.8561633287,-1.3305250876
C,7.8481712017,-2.7356119675,0.4422308596
H,7.5567228706,-0.8563205205,1.4587733889
C,6.4672563267,-3.1106840114,-1.4973770828
H,5.1283356816,-1.5059211851,-2.0271062402
C,7.4547676596,-3.5570785166,-0.6163306827
H,8.6114849636,-3.0719788261,1.1389666603
H,6.1579502576,-3.7352055788,-2.3314178209
C,6.5013030454,1.3645344817,0.2294580809
C,7.7112683097,1.5629742954,-0.4538412333
C,6.1233515298,2.2764509836,1.2276543308
C,8.5261355712,2.6484985076,-0.1374683315
H,8.0056853647,0.8635217671,-1.2298984788
C,6.9360346927,3.3689596217,1.5244529993
H,5.1935177493,2.1230704314,1.7662229206
C,8.1430175664,3.5603339634,0.8484048964
H,9.4597277458,2.7879745489,-0.6761355343
H,6.6289824674,4.0657900024,2.2999404906
C,-4.0964740175,-0.3538990401,0.0379722707
C,-4.5946916363,-1.5549594809,0.4770982844
C,-6.0291834921,-1.6743998515,0.5747772076
H,-3.9773307846,-2.4095577878,0.7477456763
C,-6.8198522008,-0.5965700928,0.2317191916
H,-6.4656889013,-2.6139111057,0.9188823351
C,-8.2364494351,-0.7363770323,0.3411140515
H,-8.5883454525,-1.7045827949,0.6948400514
C,-9.2358791927,0.1678856171,0.0712399427
C,-10.6674693714,-0.1573230996,0.2484630166
O,-11.5853023604,0.6057441795,0.0237540259
O,-10.875109994,-1.4260790071,0.6996018245
H,-11.8429480911,-1.5136283506,0.7733426376
C,-8.9703131099,1.4883060985,-0.3986190973
N,-8.7227409616,2.5603418817,-0.7817404144
H,7.9128699339,-4.5323390056,-0.753880581
H,8.7772888157,4.4091909437,1.0871856824
C,0.0413686905,0.6568698107,-0.4068068589
C,-0.3268195693,-0.5773404912,0.1786420745
C,-0.9472168037,1.5458349727,-0.8358576826
C,-1.6566802946,-0.9167808684,0.3291359722
C,-2.2848567603,1.1965411473,-0.6784344579
H,-0.6843386079,2.500210956,-1.2845079916
C,-2.6805912912,-0.0335144279,-0.1028479838
H,-1.9232399188,-1.8626322648,0.7923095532
H,-3.0470231258,1.8918387953,-1.016026758
C,0.914224728,-1.3770595945,0.580384302
C,0.952200918,-1.6306382097,2.1038796012
H,0.8981816181,-0.6902241025,2.6615036462
H,0.1099159392,-2.2603183488,2.41285956
H,1.8776374985,-2.1446423828,2.3878730209
C,0.990023415,-2.7191365432,-0.1814923444
H,0.9604676926,-2.5602595918,-1.2642095031
H,1.9173341175,-3.2506261903,0.0613673603
H,0.1491586687,-3.3671321371,0.091851354
Si,-5.610271902,0.7731550979,-0.3096786973
C,-5.5972933153,2.286430665,0.8168129625
H,-4.7080319559,2.8999178567,0.6302801237
H,-6.4831675399,2.9041976565,0.642881613
H,-5.5814560237,1.9893682816,1.8711881405
C,-5.7513087359,1.2054252658,-2.1426428064
H,-4.9058642386,1.8203920366,-2.4717131627
H,-5.7641942127,0.2990683255,-2.7578993312
H,-6.671597494,1.7664785918,-2.3300568982

Dye 3-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2340.2508697 a.u.
C,-0.9193559543,3.1497871335,-0.0845297907
C,0.0075499709,4.1706272476,0.1513213897

C,-2.2533024007,3.4749511328,-0.4089601999
C,-0.3999940745,5.4980316626,0.0680572757
H,1.0371724439,3.9406094632,0.4131271952
C,-2.6596266103,4.7964125097,-0.5062608846
C,-1.7302573832,5.8296012845,-0.2652355928
H,0.3086967471,6.2951704515,0.2652028757
H,-3.681361547,5.0513274032,-0.7701488773
N,-2.1293661509,7.1841109481,-0.3536917736
C,-3.4253564897,7.5792613129,0.0868961733
C,-4.2075773906,8.4442305129,-0.6944414197
C,-3.9334851385,7.1163163547,1.3112791761
C,-5.4689900394,8.8413842722,-0.2531388972
H,-3.8204232025,8.801330824,-1.643559901
C,-5.2028896184,7.5050362132,1.7363164097
H,-3.3281883827,6.4556448191,1.9240365095
C,-5.9765154515,8.3717933351,0.9605384856
H,-6.0622455841,9.5118149562,-0.8693407574
H,-5.5814740178,7.1396127511,2.6873104627
C,-1.2433909539,8.1658352098,-0.8820915643
C,-1.1206114547,9.4183445008,-0.2596574355
C,-0.4875185228,7.8996438274,-2.03537409
C,-0.2634470258,10.3832587933,-0.7863589449
H,-1.6988554451,9.627997189,0.6345583844
C,0.380364527,8.8644880218,-2.5441716549
H,-0.5849955688,6.9370527017,-2.5274010866
C,0.4955108439,10.1124595118,-1.9272547875
H,-0.1798366089,11.3475587832,-0.2920883906
H,0.958185081,8.6424560109,-3.4375027701
H,-6.962210623,8.6784769526,1.2985201103
H,1.1674298811,10.8643884738,-2.330907845
C,-0.7834118067,1.6975110961,-0.0678766868
C,-2.0365184312,1.1221733461,-0.388139559
C,0.3144093668,0.8740186776,0.1960837806
C,-2.1876005088,-0.2490711335,-0.4463677452
C,0.1521728569,-0.5066641197,0.1385603908
H,1.2840760237,1.2975936697,0.4438469983
C,-1.0878279847,-1.1082628607,-0.1826997211
H,-3.1562130847,-0.6756170757,-0.6912494646
H,1.008841045,-1.1405165191,0.3449424534
C,-3.0842885766,2.2104069271,-0.6314409737
C,-3.6403187908,2.1457824465,-2.0716508037
H,-2.8340984274,2.2095979705,-2.8094319732
H,-4.1809707462,1.2064428138,-2.2358146783
H,-4.3381487572,2.9710300831,-2.2542704121
C,-4.2424911929,2.1146601457,0.387078034
H,-3.8683049289,2.152008945,1.4152267686
H,-4.9481716178,2.9418799089,0.2490560696
H,-4.7942739902,1.176362337,0.2577658085
C,-1.0619301127,-5.296107788,-0.1964281511
C,-2.2562106437,-4.6948750029,-0.5457967572
C,-2.3388636699,-3.2560684611,-0.5659034247
H,-3.1360260655,-5.2865176323,-0.8048379513
C,-1.2022835095,-2.5604702227,-0.2306063425
H,-3.2818174966,-2.7880759523,-0.8417783958
Si,0.1470776601,-3.8683708022,0.1578334972
C,0.7031051415,-3.7691524579,1.9589885175
H,1.4314562504,-4.5560820695,2.1768444702
H,1.1704588767,-2.8005442956,2.1713753194
H,-0.1477350295,-3.8853834785,2.6393702414
C,1.5808648413,-3.776258114,-1.0687599277
H,2.2983536817,-4.5788131886,-0.8727940864
H,1.2220073641,-3.8736147166,-2.0994000173
H,2.1098378401,-2.8194584858,-0.988436788
C,-1.0008893757,-6.718814992,-0.1777152686
H,-1.9166729834,-7.2471472122,-0.4452641026
C,0.0445908933,-7.5586824836,0.1328480961
C,-0.1575648252,-9.0138986247,0.0787243415
O,0.8044041601,-9.8164829062,0.3837275627
O,-1.2648979493,-9.532542874,-0.2641607111
C,1.3378058706,-7.0907468248,0.5062710129
N,2.3896525779,-6.6838367148,0.8003059924
Ti,-0.3815454667,-11.4956231665,0.1863605854
O,-0.893267414,-11.61543198,1.9227925534
H,-1.8013956386,-11.8870299835,2.1307534215
O,0.9132036643,-12.8051039425,0.1299870015
O,-1.8149256009,-12.1765526767,-0.6982348101
O,0.6266516443,-11.2333719118,-1.9388459555
H,1.1106183534,-13.2714756302,0.9575441256
H,-2.37321828,-11.5279020692,-1.159403347
H,1.3883580932,-10.682737477,-1.6847897444
H,0.985936912,-12.1390323722,-1.9684565286

Dye 4 B3LYP/6-31G*
E = -2481.9323457 a.u.
C,7.3652973966,1.5199568554,0.1258166928
C,8.2202066052,2.5065013372,-0.3735804126
C,7.9040256737,0.3694004825,0.7370654625
C,9.5971907123,2.3379909972,-0.2655573505
H,7.8249640855,3.3955492708,-0.8584417885
C,9.2746466821,0.2062108021,0.8620777309
C,10.1418608225,1.1955422645,0.3553613531
H,10.2674432481,3.0914456788,-0.6654231637
H,9.6933224585,-0.6707467511,1.3461033475
N,11.5452325455,1.0427668402,0.4671867785
C,12.140924284,-0.2425274599,0.321998668
C,13.1436688945,-0.6643894662,1.2091146307
C,11.7390311326,-1.1026952487,-0.7122598142
C,13.7343167826,-1.91755243,1.0568761265
H,13.4552624328,-0.0051406106,2.0130837774
C,12.3227148786,-2.3611785703,-0.8456675741
H,10.9706232604,-0.7780507917,-1.4067490685
C,13.3255996221,-2.7755205804,0.0337054993
H,14.5097153044,-2.2285470912,1.7520684292
H,12.0010299451,-3.0144571499,-1.6525466662
C,12.3727166659,2.1695761177,0.7376387432
C,13.5804051129,2.3447797825,0.0438945924
C,11.9984678603,3.115196847,1.7054817045
C,14.3969054145,3.4397266496,0.3209186374
H,13.8719809529,1.6191840597,-0.7088093952
C,12.8125997594,4.2167614954,1.9624475465
H,11.0704896258,2.980511182,2.2521583823
C,14.0176205127,4.3845088716,1.2767804365
H,15.3287529369,3.5604121226,-0.225275942
H,12.5083171045,4.9394596272,2.7150440333
C,-4.0504989964,-1.0291031455,1.2839544013
H,-4.1642433668,-1.7142360557,2.1198430176
C,-5.2139620986,-0.6958980545,0.6404490511
C,-6.5233280868,-1.2411639828,1.0689539064
O,-7.5848517999,-0.9838020964,0.541396682
O,-6.4246640339,-2.0797356769,2.1372326882
H,-7.3368713983,-2.3686994234,2.3222461024
C,-5.2618673898,0.1896116227,-0.4775759942
N,-5.2765580428,0.9149436511,-1.3885772577
H,13.7836484053,-3.7540979758,-0.0779741545
H,14.6531977907,5.2403974724,1.4850397002
C,5.9076012415,1.4228063249,0.1524372216

C,5.5481954991,0.2126984884,0.7837579179
C,4.9143151432,2.2892550628,-0.3141091014
C,4.2164243914,-0.1303596392,0.942298784
C,3.5770713517,1.944449799,-0.1468864547
H,5.173719099,3.230517838,-0.791376458
C,3.2018772509,0.7343045322,0.4746686842
H,3.944866422,-1.0763766687,1.4046972442
H,2.8057852443,2.6329486949,-0.4782342202
C,6.7920638096,-0.5700919353,1.2065122582
C,6.833662585,-0.7789792578,2.736887446
H,6.7810238517,0.1768512275,3.2677817044
H,5.9930335398,-1.4005729159,3.0662675154
H,7.7602063396,-1.2844292714,3.0322899243
C,6.8722224202,-1.9343129717,0.4850296199
H,6.8378093593,-1.8082676649,-0.6017941276
H,7.8045954542,-2.4502918388,0.7408770383
H,6.0373733394,-2.5797773823,0.7815937179
C,1.7867551336,0.3973815074,0.6236834088
C,0.7234317,0.8457138369,-0.1359450412
C,-0.5118991176,0.3133104886,0.301573449
C,-0.406601839,-0.5520068122,1.3978494854
C,-2.7031236575,-0.6309321545,1.0474778932
C,-1.6338722409,-1.0838359702,1.8195581866
H,0.8419941526,1.5024603582,-0.9890693551
H,-1.7686971375,-1.7705856156,2.6479600691
S,1.2553203596,-0.6999414858,1.9115822563
S,-2.158596311,0.4782086965,-0.2299284462

Dye 4-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2843.5002901 a.u.
C,-1.9482706562,-3.3553545544,-0.6067325238
C,-1.2151814514,-4.5441974258,-0.5457825308
C,-3.3525632709,-3.4027263172,-0.7266840792
C,-1.882263673,-5.7640107442,-0.6101613117
H,-0.1312805826,-4.5290671483,-0.4645726787
C,-4.0219472948,-4.6157030448,-0.7743245133
C,-3.2872295754,-5.8180564095,-0.7187950465
H,-1.3193407439,-6.6908177153,-0.5796335699
H,-5.1041863171,-4.6565492026,-0.8503193981
N,-3.9533281702,-7.0666089538,-0.7728172822
C,-5.0946980457,-7.2341375596,-1.6078288934
C,-6.2325730505,-7.9033049211,-1.1297049159
C,-5.0956539934,-6.7396024733,-2.9221421649
C,-7.3426849784,-8.0786465601,-1.9545440163
H,-6.2386802207,-8.2839398535,-0.1132355993
C,-6.2171016225,-6.9037833101,-3.7336203029
H,-4.2147593217,-6.2302751687,-3.3001721883
C,-7.3451359618,-7.576937796,-3.2581575323
H,-8.2152881196,-8.5994685991,-1.569162197
H,-6.201092869,-6.5162383753,-4.7489221849
C,-3.4950556339,-8.1623198502,0.0125451907
C,-3.4319795036,-9.4524793318,-0.537979385
C,-3.1069893517,-7.9714521791,1.3486797483
C,-2.9970421866,-10.5265496948,0.23685317
H,-3.7251706496,-9.6060549733,-1.5716512864
C,-2.656017224,-9.0485132553,2.110018492
H,-3.1612738575,-6.9783865726,1.7834167219
C,-2.6020216415,-10.3324997243,1.5624512605
H,-2.9545762132,-11.5185688917,-0.2051043229
H,-2.3595719417,-8.8830698424,3.142491341
H,-8.2143677507,-7.7098551731,-3.8958408809
H,-2.2571350278,-11.1706798939,2.161055874
C,-1.5307101773,-1.9555097191,-0.56663016
C,-2.6790980052,-1.1401608831,-0.6642285251
C,-0.2655220652,-1.3700698902,-0.4535830356
C,-2.5670993974,0.2396320267,-0.6433995833
C,-0.1561053819,0.0170068852,-0.4402700498
H,0.6294007901,-1.983121539,-0.3881104949
C,-1.2956665082,0.8452606663,-0.5285875932
H,-3.456456246,0.8634467901,-0.6904036363
H,0.8282364574,0.4718546669,-0.3859050128
C,-3.9437816995,-1.9930094734,-0.7727970085
C,-4.8984634233,-1.7396454685,0.4157272208
H,-4.3944258464,-1.9144078821,1.3716395945
H,-5.2644661771,-0.7063911303,0.4055650558
H,-5.7682839609,-2.4041144933,0.3603031751
C,-4.6817595357,-1.73875957,-2.1066115302
H,-4.0203437242,-1.9085878989,-2.9622662151
H,-5.5448682581,-2.4074479434,-2.2026785793
H,-5.0478026694,-0.7066912157,-2.1561414954
C,-0.6441333493,6.8945694706,-0.348733644
C,-1.6808138293,6.1543300999,-0.918356405
C,-1.4903214608,4.7725004099,-0.7760964068
C,-0.3111347432,4.4302351658,-0.099963302
C,-1.1479218401,2.2999368691,-0.4973420121
C,-0.1196939011,3.0375261146,0.0585916816
H,-2.5258460407,6.6252750913,-1.408217873
H,0.7127228011,2.5879067031,0.585749006
S,0.5867520421,5.8388590743,0.3767939497
S,-2.3743001339,3.3415564325,-1.2406447694
C,-0.6089405989,8.3164126768,-0.3615874542
H,-1.4570527324,8.7851246712,-0.8569080812
C,0.306341035,9.2037284288,0.1432835704
C,0.0588714173,10.6467611962,-0.0258290437
O,0.891585349,11.5074915096,0.433594159
O,-0.9734342168,11.0868218447,-0.6251681105
C,1.492278326,8.8144752733,0.8323335817
N,2.4554815267,8.4762430226,1.3932954635
Ti,-0.2029805621,13.0967880128,-0.2369820486
O,0.7617115134,13.3879538947,-1.7425391699
H,0.3417946202,13.7339963768,-2.5456272402
O,0.4611563291,14.4007262411,0.8791829504
O,-1.8792658543,13.6488295181,-0.7370668637
O,-1.2868081138,12.7262739795,1.824685997
H,1.2486815345,14.8833502438,0.5805762245
H,-2.4495962829,12.9504296802,-1.1005195743
H,-0.7095215048,13.3306567102,2.3275143578
H,-2.0970547949,13.2372793614,1.6554734654

Dye 5 B3LYP/6-31G*
E = -1704.0063719 a.u.
C,1.2955079046,0.5853939242,-0.5972525918
C,2.1183288777,1.587938512,-1.1175667257
C,1.8664109489,-0.5020933988,0.0942483345
C,3.4973218499,1.4959338165,-0.9525757561
H,1.6979738564,2.4297697873,-1.6619164683
C,3.2381494597,-0.5883944085,0.2750126313
C,4.0733305025,0.416033116,-0.2540896452
H,4.1445697533,2.2615975008,-1.367216366
H,3.6815698048,-1.4164047441,0.8197708556
N,5.4786778198,0.3400591049,-0.0865636883
C,6.1420753241,-0.9161187588,-0.1747579387
C,7.1409364726,-1.2598769551,0.7498794586
C,5.8097279595,-1.8277386032,-1.1897367183
C,7.7948406466,-2.4869345711,0.6536457208
H,7.3991091324,-0.5611765154,1.5392889583

C,6.4561672918,-3.0598834978,-1.2667343392
H,5.0456667795,-1.5629841969,-1.9137720488
C,7.4545974019,-3.396465563,-0.3499621979
H,8.5659066275,-2.737199149,1.3776118216
H,6.1873111724,-3.7534879612,-2.0591967687
C,6.2337023466,1.5167373364,0.1805410507
C,7.460730438,1.7355305204,-0.4656637487
C,5.7660942763,2.4719524315,1.0972837304
C,8.2040890223,2.8820323874,-0.1914772817
H,7.8250705074,1.0036953148,-1.1796566479
C,6.5077563776,3.6241759201,1.35096993
H,4.8224803968,2.304871565,1.6070011995
C,7.7320907529,3.8353773343,0.7132230027
H,9.1519217987,3.0359127833,-0.7006211912
H,6.1311841413,4.3533280092,2.0636072979
C,-4.2209917064,-0.8476379458,-0.2337849222
C,-4.6847177936,-2.1673084532,-0.3089201276
C,-6.0642004627,-2.1428520607,-0.1101201066
H,-4.0676778826,-3.0276551611,-0.5273785267
C,-6.459576741,-0.8044339368,0.0487145825
H,-6.7468177385,-2.9819428493,-0.1451790535
C,-7.8175081543,-0.3989206307,0.1717020894
H,-8.4614900708,-1.207019874,0.507352939
C,-8.4866469164,0.7723133263,-0.101874482
C,-9.9384018367,0.9014624242,0.1613036631
O,-10.6063641552,1.8803952228,-0.1022784775
O,-10.4768607278,-0.205067904,0.747440238
H,-11.4241125079,-0.0014179327,0.8518114072
C,-7.9052245076,1.8974656769,-0.7579123413
N,-7.4231963779,2.794007631,-1.3238912528
H,7.9619609897,-4.3545414637,-0.4177610334
H,8.31098089,4.7312148918,0.9187646204
C,-0.1568257581,0.4149753122,-0.6176580319
C,-0.4790633489,-0.7792123177,0.0629004849
C,-1.1711517469,1.2033595874,-1.1668731558
C,-1.7987055198,-1.175697827,0.2003379673
C,-2.4972914775,0.7991113804,-1.0308747796
H,-0.9382273782,2.1179028105,-1.7057555346
C,-2.8348313365,-0.3853697951,-0.3449679515
H,-2.0546276308,-2.0825524645,0.7422342178
H,-3.2817460724,1.3924832858,-1.4898803967
C,0.7847764801,-1.4687107561,0.5790851588
C,0.7765959406,-1.5808098734,2.1201725184
H,0.6556663283,-0.5979575952,2.5867286077
H,-0.0444428662,-2.2238024531,2.4578633501
H,1.7149936518,-2.0177070278,2.4804175757
C,0.9614099963,-2.868519998,-0.0507952042
H,0.9608382204,-2.8121055353,-1.1440197232
H,1.9086395674,-3.317848553,0.2685574296
H,0.1500570059,-3.5378016497,0.2581749751
N,-5.3020616908,-0.0202524933,-0.0187964924
C,-5.1902705863,1.3459782637,0.504451996
H,-5.2489260147,2.0931482866,-0.2875551051
H,-6.0076571889,1.5231933833,1.2050224492
H,-4.2413598489,1.4430477972,1.0344296987

Dye 5-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2065.5764186 a.u.

C,-0.3860139424,2.6435526852,1.3368327874
C,-1.4600759904,3.4883862324,1.0422160656
C,0.7239217801,3.1428240589,2.0485074822
C,-1.4170795615,4.8183418393,1.4502971844
H,-2.3202786167,3.1256410061,0.4853292933
C,0.762787102,4.4622876134,2.472118608
C,-0.3145423067,5.3210984916,2.1717326405
H,-2.2387182472,5.484663448,1.210322278
H,1.608434562,4.8458690841,3.0347450592
N,-0.2886022623,6.6740193825,2.5883447675
C,0.9341537529,7.4041504579,2.5778739906
C,1.2825085167,8.2218484759,3.6647289627
C,1.8047603775,7.3221821472,1.4790187229
C,2.4738180148,8.945567999,3.645952428
H,0.6152446012,8.2866284244,4.5183545924
C,3.0023500485,8.035533192,1.4769588207
H,1.5357346656,6.6998835798,0.6312385728
C,3.3432435121,8.8539612964,2.5565582688
H,2.7282208355,9.5742506211,4.4952134934
H,3.6644270297,7.9620117734,0.6181524104
C,-1.4804887559,7.3158687354,3.0301598061
C,-1.7732652105,8.6264775047,2.6202447295
C,-2.3741716811,6.6533922342,3.8871960154
C,-2.9323801711,9.2595733571,3.0659799115
H,-1.0881698012,9.1420698421,1.9547611504
C,-3.5399218531,7.2881297106,4.3129751668
H,-2.1491963891,5.6435518947,4.2154348876
C,-3.8250693367,8.5948758701,3.9099850051
H,-3.1437927842,10.2742846365,2.7391014134
H,-4.2209585728,6.7611795648,4.9761200841
C,1.3316968521,-2.7467108719,0.5625536404
C,2.6638819178,-3.0970725677,0.2937803418
C,2.7291764375,-4.4853304911,0.226509875
H,3.4664635528,-2.3921584363,0.1287098792
C,1.4313923642,-4.9967370698,0.4175308261
H,3.5952763354,-5.0922869899,-0.002653041
H,4.2736824109,9.4143885126,2.5480730411
H,-4.7308651882,9.0888030966,4.2496703558
C,-0.1521543912,1.231423962,1.0381209048
C,1.1049781635,0.8626753596,1.5659371136
C,-0.9328919956,0.2885000144,0.3634596468
C,1.5740168217,-0.4325621142,1.4249845925
C,-0.4573004341,-1.0135884165,0.2220216814
H,-1.8960915241,0.5607692545,-0.0596753789
C,0.7928424346,-1.3970977326,0.7495774931
H,2.5322882588,-0.7276741161,1.8444747151
H,-1.0466319481,-1.7357468987,-0.3343395334
C,1.7724253266,2.0501057894,2.26089326
C,1.9999818409,1.7687431631,3.7632308331
H,1.0615454505,1.5060757416,4.2620671082
H,2.7043555041,0.9400437621,3.9001614432
H,2.4175081264,2.65066991,4.2623226093
C,3.1117036124,2.4181135522,1.5832328315
H,2.9726008708,2.6155842094,0.5154118478
H,3.5441952943,3.3139233706,2.0433695015
H,3.8363255352,1.6023102348,1.6891479326
N,0.5854203018,-3.9008298692,0.6344547985
C,-0.7396172773,-3.9794039322,1.25756894
H,-1.5404769606,-3.9868247716,0.5172914125
H,-0.8016066842,-4.8991264292,1.8413692292
H,-0.8646907352,-3.1265506429,1.926379696
C,1.1246141861,-6.3756816575,0.3145937848
H,2.0076490728,-7.0063763417,0.3944744866
C,-0.023526433,-7.1058658703,0.0804128392
C,0.0903236739,-8.5706482712,0.0569657456
O,-0.9020463637,-9.3181504652,-0.2430256887
O,1.1952437883,-9.1603723304,0.3368554415
C,-1.2983779273,-6.57235977,-0.2654423747

N,-2.3363413499,-6.1394830038,-0.5700852125
Ti,0.4490902839,-11.0080772337,-0.2199116254
O,1.1197969471,-10.9835401617,-1.8977515314
H,0.6813503901,-11.4258432298,-2.6407994894
O,-1.0766207705,-12.0391885296,-0.4447706385
O,1.5996653519,-12.0497065937,0.7108043502
O,-0.6163564557,-11.0220910196,2.0118360826
H,-1.8295550031,-11.5791428184,-0.8530869065
H,1.4955007136,-12.0645493221,1.677463678
H,-1.1297064167,-10.1968944976,2.010998151
H,-1.2204506141,-11.6747684035,1.6045712964

Dye 6 B3LYP/6-31G*
E = -2193.23953 a.u.
C,2.1799254433,-0.9843726852,0.0161580092
C,3.1191654539,-1.9872366732,0.2733822514
C,2.6106736732,0.3386015249,-0.2131087552
C,4.4723039702,-1.6657428039,0.305978264
H,2.8056479932,-3.0107012505,0.4627337798
C,3.9588866649,0.6596480814,-0.1967634569
C,4.9100388752,-0.3467169608,0.0680259384
H,5.2068242576,-2.4347489204,0.5203042557
H,4.2965199371,1.6737850413,-0.3877124934
N,6.2914373162,-0.0367114895,0.0961717234
C,6.7384270803,1.1978692982,0.6471897847
C,7.7236795205,1.953264601,-0.0079689253
C,6.2057068428,1.6735029687,1.8560252683
C,8.1682082907,3.1546379988,0.5411791073
H,8.1366395209,1.5925350227,-0.9446900098
C,6.6434558701,2.8848399463,2.388093573
H,5.4510803695,1.0887952275,2.3726118055
C,7.6290037891,3.6309656332,1.7380308185
H,8.9317418821,3.7271836331,0.021132797
H,6.2212191015,3.2383222444,3.3251421488
C,7.2446100601,-0.9533004774,-0.431697148
C,8.4397307436,-1.2106781474,0.2583001127
C,7.0066176391,-1.6062685679,-1.6516513407
C,9.376974307,-2.0976613388,-0.2680599081
H,8.6269828991,-0.7119790306,1.2039052352
C,7.9417509028,-2.5052352306,-2.161003651
H,6.0885265478,-1.4041157081,-2.1941656195
C,9.1333820571,-2.7538812983,-1.4764850893
H,10.2972122424,-2.285991317,0.2786856219
H,7.7422210408,-3.0021518615,-3.1067868597
H,7.9732374898,4.57105393,2.1594805834
H,9.8633347645,-3.4497075259,-1.8800883982
C,0.7225147564,-1.0235043536,-0.0760248495
C,0.2558123447,0.2758540377,-0.371255262
C,-0.1870652041,-2.0727881425,0.0816207418
C,-1.0983737857,0.5185827746,-0.5156215079
C,-1.5497802623,-1.8228840553,-0.0530590238
H,0.1562115739,-3.0791285164,0.3065570719
C,-2.0318998959,-0.53283014,-0.3605078266
H,-1.4550131417,1.5258314485,-0.7130895692
H,-2.2540724918,-2.6358393661,0.0711730958
C,1.4202505863,1.2618605083,-0.4768452989
C,1.4974787887,1.897172564,-1.883083425
H,1.5663010691,1.1293008309,-2.6602137525
H,0.6088745804,2.5074479393,-2.0818485089
H,2.3756962088,2.5476563065,-1.9653167614
C,1.3214531756,2.3681652745,0.5975459094
H,1.2628822625,1.9380185768,1.6024412743
H,2.197773076,3.025119702,0.5562625981
H,0.4301897197,2.9856886966,0.4369901939
C,-3.4679201741,-0.267123282,-0.5532325256
C,-4.5056627693,-0.9530133135,0.1775278883
C,-3.9162957734,0.6872850734,-1.4582882274
C,-5.9072102052,-0.6352631562,-0.0411683393
C,-5.2777452198,0.9985214356,-1.674913446
H,-3.1850369976,1.2126628829,-2.063774557
C,-6.3141797855,0.3673532863,-0.9956214392
H,-5.5037872417,1.7560636707,-2.4149450081
N,-4.3204225541,-1.8924632657,1.1125912135
N,-6.7406592374,-1.3440434574,0.723941799
S,-5.8072821355,-2.330970281,1.649140296
C,-7.7307893406,0.6121235568,-1.1516828475
H,-8.3567428162,-0.0127217976,-0.5223429269
C,-8.4070998864,1.4916808196,-1.9488208605
C,-7.782536722,2.4095526084,-2.8492679539
N,-7.2497985563,3.1478574184,-3.5747743207
C,-9.8931866522,1.5661877742,-1.9392622011
O,-10.4644975485,0.6867214415,-1.078154135
O,-10.5422098958,2.3284407555,-2.6238879326
H,-11.425453605,0.8284331898,-1.1595625689

Dye 6-TiO_2 B3LYP/6-31G* with LANL2DZ for Ti
E = -2554.8074889 a.u.
C,-1.3692940975,3.9131623805,-0.1269764641
C,-2.2034284423,4.9558749558,-0.5416093169
C,-0.1332232551,4.2051159782,0.4861814602
C,-1.7992237686,6.2734266835,-0.3497050928
H,-3.1550730082,4.7515054012,-1.0255565433
C,0.2654566951,5.5164336031,0.6940792212
C,-0.568897829,6.5721314397,0.2719554031
H,-2.4327619283,7.0879672626,-0.6843380885
H,1.208790214,5.7449697422,1.1805073983
N,-0.1770135968,7.9183466408,0.4687191102
C,1.1878398274,8.2983767815,0.326858029
C,1.7840911156,9.1651591055,1.2566995153
C,1.9546458363,7.8181935731,-0.7471964907
C,3.1168685896,9.5458163875,1.1080521288
H,1.1977343221,9.5367340639,2.091048958
C,3.291649023,8.1902472929,-0.8775457645
H,1.4964575407,7.1559876067,-1.4750110043
C,3.8805939902,9.0583881979,0.0450396405
H,3.5628519659,10.2174919036,1.8368758093
H,3.8707008498,7.81005314,-1.7150562869
C,-1.1434555887,8.9030398867,0.8220026823
C,-1.1309876468,10.1634663333,0.2035122902
C,-2.1167664332,8.6305145521,1.796751913
C,-2.0698586055,11.1299611871,0.560515366
H,-0.3840352721,10.3781348742,-0.5541892179
C,-3.062709732,9.5971143772,2.1343347277
H,-2.125411634,7.6609151409,2.2845641707
C,-3.0436781234,10.8529809223,1.5229101512
H,-2.0467348529,12.1005664369,0.0720425066
H,-3.8091896495,9.3700581523,2.890920554
C,-0.6339113856,-6.1616841985,0.0747514291
H,-1.5743561714,-6.6884966223,0.2139549176
C,0.4539507917,-6.9816949244,-0.031499982
C,0.2481797287,-8.4462461574,0.0477704138
O,1.2466910064,-9.24264983,-0.0538145727
O,-0.902516081,-8.9551432499,0.2168275023
C,1.7978139652,-6.5373316051,-0.2197968142
N,2.8860726389,-6.1524968009,-0.3734634186
H,4.9206979405,9.3519139911,-0.0638115809

H,-3.7779329369,11.6063446847,1.7934127129
C,-1.5234653325,2.4624643758,-0.1994917931
C,-0.378724871,1.8594618996,0.3664183772
C,-2.5599519543,1.6660901521,-0.6949745444
C,-0.2694874773,0.4814235064,0.4263592853
C,-2.4512404298,0.2799682649,-0.6244783528
H,-3.4470401829,2.1151024038,-1.1337875264
C,-1.3081428257,-0.338913135,-0.0743364675
H,0.5989545576,0.0213290072,0.8900355153
H,-3.2551288053,-0.3365498222,-1.0066605435
C,0.6068389594,2.9198876294,0.8602936343
C,0.8266145369,2.8180378944,2.3864558561
H,-0.1225807798,2.8887142087,2.9272184343
H,1.2987627347,1.8636937896,2.6471611439
H,1.4819204432,3.623638062,2.7369954415
C,1.9613639393,2.8192146051,0.123101632
H,1.826199082,2.8820150832,-0.9615196811
H,2.6304128376,3.6305526609,0.4320879931
H,2.4577582783,1.8689086583,0.3518311244
Ti,0.0744219815,-10.9101962391,0.1722251207
O,0.4254834294,-11.1524125765,1.9323395
H,-0.2453471433,-11.513720109,2.532793051
O,1.1839322034,-12.1574226689,-0.6018808966
O,-1.6299230571,-11.5654481478,0.0200037287
O,-0.1745584472,-10.5715605449,-2.144907583
H,1.8307527599,-12.5977351191,-0.0273450863
H,-2.3381058869,-10.9111545159,0.1464514203
H,0.5702866648,-11.1518274457,-2.3898820416
H,-0.9713982796,-11.1091909684,-2.2936458577
C,-0.7495045746,-4.7231550997,0.0332435095
C,-2.0641797715,-4.1460703833,0.1765634516
C,0.2877869743,-3.8111135665,-0.1356530289
C,-2.2714148815,-2.7079470405,0.1363583161
C,0.0818843246,-2.4135921018,-0.1723129471
H,1.3024711147,-4.1697644774,-0.2580614081
C,-1.160890328,-1.8041002404,-0.042039698
H,0.9514050681,-1.7875894744,-0.3435146033
N,-3.1883922245,-4.8415726295,0.3652690745
N,-3.5525531356,-2.3581549233,0.3046355432
S,-4.4058455034,-3.7459602628,0.4859335336

Dye 1-$(TiO_2)_6$ B3LYP/6-31G* with LANL2DZ for Ti
E = -3259.9421275 a.u.

Ti,13.0037114919,14.3266784981,19.1365268778
Ti,14.0733411744,16.0367663814,17.1485119222
Ti,15.5838219202,13.2294050522,18.8620669842
Ti,14.665398119,14.3613814084,14.6062489249
Ti,13.3677313172,11.9518819632,17.1626740605
Ti,17.087313436,15.2901867406,16.9009296238
O,12.821256113,16.0533994898,18.5049277921
O,12.2005504147,12.9751221845,18.3686289702
O,14.3633687504,14.2434301675,17.7278938308
O,15.7097740177,16.6076957273,17.3373521638
O,15.0374334089,11.7381545779,18.1053853394
O,17.0751302611,14.0174128373,18.3310325935
O,16.2122419953,14.4235089511,15.3704747699
O,13.6508935773,15.6381640179,15.4198744291
O,13.7497226492,12.7390576815,15.3580483151
O,12.7077130236,10.5202015944,16.8013520959
O,18.5407983505,15.917587995,16.557124827
O,14.3857267014,13.7932318402,20.187956479
H,13.5402956147,12.1199199727,14.6343190442
C,16.2123269487,14.5896015731,0.6139108613
C,16.3494655084,13.5180868092,-0.2750354525
C,16.1363807913,15.9075742031,0.1166595726
C,16.4151042878,13.766761152,-1.641152049
H,16.4221374738,12.4961218744,0.08796036
C,16.185632358,16.1589662145,-1.2449786564
C,16.3294445306,15.0827472737,-2.1469040967
H,16.540144519,12.9420638754,-2.3341156858
H,16.1110524335,17.1707196134,-1.6306516453
N,16.3888839028,15.3169950582,-3.5374980937
C,16.9981184662,16.4999583816,-4.0492332742
C,16.3693387712,17.2344206289,-5.0665293906
C,18.2375549989,16.937193646,-3.5554451596
C,16.9736275341,18.380795521,-5.580562026
H,15.4103954544,16.9004937774,-5.4500439367
C,18.8260168862,18.094444327,-4.0633031677
H,18.7340903367,16.3651877382,-2.7778226886
C,18.2010687698,18.8208837975,-5.0798565268
H,16.4746232301,18.9384074803,-6.3686315998
H,19.7865109956,18.4194828645,-3.6722134868
C,15.8379498266,14.3745246626,-4.4554311807
C,16.5620926146,13.9937106127,-5.5955857106
C,14.5639991728,13.8267216177,-4.2382015125
C,16.0167396385,13.0850888642,-6.501383655
H,17.5488475386,14.4130178308,-5.7652418271
C,14.0339692241,12.9052235066,-5.1401546087
H,13.9959971934,14.1270303513,-3.3632059075
C,14.7538208461,12.5319186882,-6.2776552904
H,16.5893585624,12.7993347079,-7.3796905883
H,13.0464760256,12.4893617992,-4.9587416704
C,15.8202103983,15.6289841544,6.2060467784
C,16.0743754855,16.8637031431,6.8067453846
S,15.3384214668,14.448295807,7.3964487078
H,16.4103230258,17.7311998501,6.2519169231
C,15.5049663908,15.6126090687,8.7070670669
C,15.2868727005,15.3666595889,10.0793859605
H,15.4432507545,16.2283153372,10.7253975138
C,14.9128953022,14.2131139393,10.742972908
C,14.7802465218,14.2510427352,12.1860625116
O,14.4663952023,13.2198924998,12.8859261204
O,14.9777940641,15.3307403136,12.8705934224
C,14.6562875084,12.9689899373,10.0951443333
N,14.4461046074,11.9613161814,9.5505647461
H,18.6664314329,19.7177218564,-5.4784893007
H,14.3348369351,11.8191334727,-6.9820477049
C,16.1241380891,14.6336167568,2.0681602547
C,15.9983085697,15.9829042345,2.4729533461
C,16.1419183703,13.6133130441,3.0259785184
C,15.8956759206,16.3084692242,3.8122553505
C,16.0402227824,13.9442638877,4.371940675
H,16.2417543846,12.572371912,2.731651592
C,15.9180571352,15.2870395388,4.7934501213
H,15.7718999394,17.3439043088,4.1167683467
H,16.079768119,13.1514617061,5.1137252322
C,15.9876806033,16.9134878155,1.259055064
C,14.6562726993,17.6916685721,1.1581993366
H,13.8009565324,17.0091488224,1.1292175724
H,14.5317462575,18.3607090093,2.0176148811
H,14.6363311787,18.3048421336,0.2501133871
C,17.1766266947,17.900131271,1.2935857077
H,18.1297139376,17.3675961506,1.3742130167
H,17.1995746768,18.5069521606,0.3813384022

H,17.0917701407,18.5818888804,2.1479255801
C,15.9012581311,16.8526371705,8.1923201989
H,16.070269925,17.7120871041,8.8332510753

Dye 2-$(TiO_2)_6$ B3LYP/6-31G* with LANL2DZ for Ti
E = -3275.9812653 a.u.
Ti,13.0234421601,14.5500915677,19.1305673074
Ti,14.112498082,16.1755623838,17.0827804144
Ti,15.5970676682,13.4256654747,18.9091526883
Ti,14.7019088091,14.3969756168,14.6105875118
Ti,13.3786024983,12.0985526518,17.2520797089
Ti,17.1237036917,15.3997580408,16.8762144071
O,12.8569906894,16.2529797695,18.4326150561
O,12.2137897343,13.1748013439,18.4126095917
O,14.3873511933,14.4029322418,17.7309314361
O,15.7519583176,16.7404039648,17.2563858394
O,15.0425934729,11.9099741046,18.2089570509
O,17.0952615137,14.1816420281,18.3518746717
O,16.2466491492,14.4830327168,15.3723393921
O,13.6934254464,15.7076978616,15.3687502929
O,13.7766380022,12.8101388124,15.4174661904
O,12.711011693,10.6586979603,16.9411957443
O,18.5837583927,16.0019557645,16.5188784834
O,14.3981125482,14.0493232976,20.2068099059
H,13.5692706578,12.160930536,14.7200271068
C,16.195426978,14.513572992,0.5731289108
C,16.3399061859,13.4714842966,-0.3494082805
C,16.1234392652,15.8473986428,0.1186043332
C,16.415978587,13.7644255056,-1.7058463675
H,16.4096672938,12.4382040135,-0.0193659362
C,16.1847678604,16.1430965811,-1.2334342474
C,16.3352083468,15.0966709833,-2.1690610102
H,16.5459311671,12.9627727395,-2.4243961273
H,16.1133748216,17.1669150381,-1.5865846572
N,16.405252596,15.3755058503,-3.5501339847
C,17.013769117,16.5769471337,-4.0187225011
C,16.3874372433,17.3444767889,-5.0126894988
C,18.2502434,16.9990122974,-3.5049754506
C,16.991321642,18.5092454919,-5.4841206349
H,15.4308748963,17.0218711072,-5.4115361787
C,18.8384018843,18.1742075796,-3.9700964373
H,18.74456819,16.4013526624,-2.7454395265
C,18.2158175323,18.9341023239,-4.9634146623
H,16.4943906884,19.0928218278,-6.2544707935
H,19.7965850829,18.4874704164,-3.5640892427
C,15.861659183,14.4632451547,-4.5025697349
C,16.5945257117,14.1200282009,-5.6490053799
C,14.5861592221,13.9089173343,-4.3129452076
C,16.056141454,13.2415701024,-6.5881255996
H,17.5825365722,14.5444649329,-5.7974092363
C,14.0630555361,13.0175336702,-5.2485604364
H,14.0113444016,14.1807056192,-3.4330742019
C,14.7915996722,12.6815723779,-6.3921386944
H,16.6353762911,12.9847401478,-7.4709933235
H,13.0741869455,12.5962383876,-5.0884719001
C,15.7539159363,15.37137965,6.188632343
C,15.9717482747,16.5936530356,6.8350229935
S,15.3176984805,14.1875597092,7.3827049812
H,16.2771978369,17.5006511467,6.3264864765
C,15.478290036,15.4188548782,8.6419687793
C,15.2846894397,15.232706464,10.036935521
H,15.4434871285,16.1370305543,10.6185968817
C,14.9368656521,14.1055034971,10.7450705046
C,14.8156382554,14.1953379433,12.1941758708
O,14.5112639648,13.1862020054,12.9249389364
O,15.0122756698,15.2985498543,12.8322999105
C,14.6884487912,12.8342431388,10.1477257133
N,14.4865283184,11.8066452395,9.6387298207
H,18.6808180892,19.8451366881,-5.3288524669
H,14.3780107627,11.9923852497,-7.1226998508
C,16.0940511621,14.5097490163,2.0265371521
C,15.9617685086,15.8451196716,2.4740431116
C,16.1044685855,13.4584831883,2.9510276252
C,15.845216559,16.1272908941,3.8215743977
C,15.989546767,13.7453964297,4.3057298251
H,16.2075460864,12.4277750906,2.6237102778
C,15.8614378517,15.0738616426,4.7693241753
H,15.7176729473,17.1524703061,4.1572259449
H,16.0198420159,12.9292036416,5.0223098653
C,15.9619861147,16.8152226415,1.2915826262
N,15.8219800159,16.6140358659,8.166794068
C,14.6302765667,17.5943523232,1.2027430437
H,13.7762297447,16.9122559074,1.1426110661
H,14.4960834713,18.2348713294,2.0821242311
H,14.61901438,18.2367341037,0.3149949154
C,17.1486535653,17.8020588157,1.3718079609
H,18.1021999406,17.268975397,1.4424862395
H,17.1783540251,18.440799084,0.4818802945
H,17.0542159083,18.4527167999,2.248949373