Electronic Supplementary Material (ESI) for Integrative Biology

Electronic Supplementary Information

Surface modification of TiO_2 nanoparticle surface enables fluorescence monitoring of aggregation and enhanced photoreactivity

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Portion of Gaussian input file for the geometry optimizations in gas phase.

```
%chk=DJE-003-0A.chk
%nproc=4
%mem=2Gb
#n becke3lyp/gen pseudo=cards scfcon=7 scfcyc=1000 minpop
nosymm int=finegrid vshift=1000 gfinput opt=redundant freq

C1

-1 1
xyz coordinates

C H N O 0
6-31G**
****
Ti 0
LANL2DZ
****
S 0
LANL2DZ
****

Ti 0
LANL2DZ
S 0
LANL2DZ
```

Portion of Gaussian input file for PCM corrections.

```
%chk=DJE-003-0A-pcm.chk
%nproc=4
%mem=2Gb
#n becke3lyp/6-311+G** scfcon=7 scfcyc=1000 minpop
nosymm int=finegrid vshift=1000 gfinput
SCRF=(PCM,Solvent=water)

C1

-1 1
xyz coordinates
```

Table S1. Optimized geometries of the ground state structures of Ti dye complexes in gas phase.

A_{calcd}				B_{calcd}			
65				65			
scf done: -2169.090880				scf done: -2169.067510			
C	-10.596191	3.460860	10.183501	Ti	-8.590691	1.115055	10.054808
H	-11.282740	4.300033	10.204010	O	-6.894763	1.216102	9.219401
C	-10.224098	2.793172	11.344217	H	-6.243873	0.973155	9.892663
H	-10.624834	3.108667	12.303909	O	-8.052595	1.527292	11.781608
C	-9.328225	1.716610	11.277739	H	-8.160558	2.474831	11.941880
H	-9.033381	1.198250	12.186253	O	-10.439075	1.432572	10.272945
C	-8.813144	1.312619	10.051324	H	-10.882937	1.695571	9.458170
H	-8.112703	0.488850	9.968655	O	-8.679083	-0.725316	10.166338
C	-9.188323	1.976669	8.874324	H	-9.540943	-0.964061	10.535983
C	-10.081206	3.059270	8.941320	O	-8.427184	3.512392	9.852279
C	-10.484895	3.795773	7.718281	C	-8.035734	4.179043	8.878672
O	-11.303027	4.741084	7.839672	C	-7.502984	5.545418	9.160054
C	-8.625205	1.527983	7.572818	C	-7.480560	6.018273	10.478439
O	-7.815462	0.577127	7.590959	H	-7.862108	5.369505	11.258520
Ti	-6.204240	-0.086786	6.015398	C	-6.978565	7.284501	10.760676
O	-7.143470	-1.705994	6.294556	H	-6.963592	7.643548	11.786217
H	-7.895430	-1.647116	6.895259	C	-6.492319	8.097170	9.727516
O	-4.975183	-0.418908	7.391376	H	-6.099232	9.085201	9.950681

H	-5.060490	-1.342871	7.659898
O	-5.395302	-0.705597	4.471566
H	-5.678827	-1.621466	4.336762
O	-5.709374	1.716529	6.105249
H	-5.046035	1.829581	6.799478
O	-7.854817	0.710751	4.918337
C	-8.600758	1.727949	5.118656
C	-9.050547	2.220060	6.369843
C	-9.928262	3.366606	6.439128
C	-10.263365	4.053016	5.244589
N	-11.078573	5.179241	5.316832
H	-11.486808	5.272253	6.259890
C	-11.173551	6.270399	4.478896
C	-12.289076	7.126190	4.662044
H	-13.030709	6.864880	5.410727
H	-13.306429	8.921634	4.030676
C	-11.488279	8.566561	2.934999
S	-11.676867	10.078956	1.945902
O	-13.130162	10.566934	1.999699
O	-10.706060	11.179072	2.909392
H	-10.359328	11.813451	2.256262
O	-10.934504	9.960524	0.602676
C	-10.372031	7.762248	2.728817
H	-9.637481	8.032283	1.977678
C	-10.212158	6.618265	3.499361
H	-9.321559	6.016532	3.373497
H	-10.150019	4.072675	3.094303
C	-9.841747	3.551786	3.988086
C	-9.060951	2.417959	3.906113
N	-8.553264	1.821357	2.772777
C	-8.817786	1.957615	1.429085
C	-9.975505	2.575528	0.905160
C	-10.177417	2.639665	-0.468735
C	-9.225620	2.086574	-1.316224
C	-8.076948	1.456614	-0.838771
C	-7.877058	1.396938	0.528794
H	-6.984383	0.925215	0.929034
H	-7.352558	1.042628	-1.531518
S	-9.506888	2.146003	-3.111378
O	-10.548468	3.218301	-3.455298
O	-8.177429	2.069263	-3.882335
O	-10.264452	0.575621	-3.315576
H	-10.154428	0.377583	-4.263064
H	-11.063258	3.110007	-0.881543
H	-10.739200	2.959509	1.567050
H	-7.875163	1.106899	3.057090
C	-12.448393	8.271305	3.900654

C	-6.513748	7.637260	8.416110
H	-6.148980	8.244202	7.594823
C	-7.015969	6.359182	8.127424
C	-7.044343	5.892643	6.721946
O	-6.705951	6.690850	5.828372
C	-7.523018	4.513716	6.440459
C	-7.509124	4.042109	5.110739
N	-6.954095	4.811848	4.065475
C	-5.929837	4.412522	3.229029
C	-5.495960	5.318960	2.228575
C	-4.483407	4.978874	1.349361
C	-3.900606	3.715731	1.456142
C	-4.286744	2.800557	2.428190
C	-5.297720	3.148154	3.317463
H	-5.568083	2.463409	4.114122
H	-3.799781	1.833268	2.491786
S	-2.567697	3.265082	0.306067
O	-2.599663	4.184669	-0.921333
O	-2.473515	1.737534	0.142693
O	-1.182121	3.714975	1.281392
H	-0.472172	3.125691	0.968197
H	-4.153719	5.663285	0.575359
H	-5.978466	6.288790	2.154458
H	-6.923040	5.801648	4.323412
O	-9.131639	1.614342	8.054543
C	-8.059336	3.711885	7.501942
C	-8.631031	2.418695	7.205186
C	-8.678003	2.033383	5.824270
C	-8.171306	2.808520	4.806580
N	-8.300501	2.412150	3.456763
C	-9.403442	1.880363	2.820636
C	-9.239308	1.421275	1.491137
C	-10.310382	0.920346	0.769976
C	-11.558727	0.868127	1.383877
C	-11.761240	1.305691	2.689157
C	-10.686880	1.808402	3.409337
S	-12.974932	0.240383	0.435202
O	-14.076957	-0.294200	1.366296
H	-10.187248	0.560571	-0.245603
O	-13.585946	1.764336	-0.187516
H	-14.522631	1.581609	-0.383262
O	-12.488363	-0.591257	-0.758829
H	-8.254707	1.460510	1.033248
H	-7.511752	2.598041	2.854251
H	-10.838561	2.156967	4.422561
H	-12.747643	1.245677	3.136216
H	-9.126465	1.069126	5.614378

C_{calcd}

65
scf done: -2169.063337

C	-7.641570	-2.720516	4.554878
C	-6.888528	-1.551693	4.589885
C	-7.556148	-0.338128	4.497173
C	-8.968927	-0.277073	4.368996
C	-9.687572	-1.497196	4.312907
C	-9.028767	-2.712931	4.408499
N	-9.625258	0.938947	4.220872
Ti	-11.448401	1.097902	2.695040
O	-12.359852	-0.297868	3.533647
S	-6.773933	-4.316122	4.639765
O	-6.588685	-4.710035	2.937276
O	-10.218092	2.852699	2.359634
C	-9.680403	3.669029	3.154409
C	-9.293516	3.355385	4.495444
C	-8.816871	4.415724	5.352636
C	-8.689093	5.791055	4.894341
C	-8.995839	6.081882	3.489663
C	-9.455765	5.049002	2.647483

D_{calcd}

65
scf done: -2169.061708

Ti	-5.638346	1.577395	8.192757
O	-4.233644	2.785829	7.880396
H	-3.649889	2.418522	7.204232
O	-6.206264	2.704796	9.552567
H	-5.697307	3.524524	9.593116
O	-4.902111	0.173235	9.153174
H	-4.614276	-0.511438	8.532714
O	-5.345162	0.687585	6.539958
H	-5.496070	1.105291	5.685851
O	-6.988911	2.887783	6.873824
C	-7.909132	2.601513	6.087400
C	-8.352343	3.646452	5.125749
C	-7.885519	4.960422	5.275680
H	-7.229757	5.178664	6.111549
C	-8.263258	5.943273	4.367060
H	-7.908559	6.962250	4.495181
C	-9.095340	5.622231	3.285064
H	-9.383339	6.392095	2.574330

C	-9.229339	1.992951	4.960977	C	-9.549455	4.318711	3.118600
C	-8.743041	1.781485	6.306457	H	-10.187626	4.037906	2.287715
C	-8.408470	2.804524	7.158636	C	-9.186038	3.325016	4.038435
C	-8.403797	4.152364	6.659831	C	-9.674984	1.940892	3.860947
C	-9.750367	5.341327	1.306053	O	-10.397486	1.660217	2.865967
C	-9.574569	6.629443	0.814764	C	-9.342903	0.962391	4.872074
C	-9.116153	7.655803	1.655844	C	-8.537634	1.284114	6.022156
C	-8.832746	7.383430	2.987235	C	-8.380169	0.368577	7.085446
N	-8.002711	2.681780	8.490186	N	-7.727028	0.657820	8.261459
C	-8.311896	1.746903	9.458895	C	-9.835743	0.559997	9.520652
C	-7.645237	1.863010	10.702362	C	-10.507064	0.407686	10.724402
C	-7.924882	0.999653	11.747865	C	-9.762554	0.197798	11.881900
C	-8.874232	0.001485	11.547121	C	-8.365411	0.154231	11.866982
C	-9.549404	-0.148765	10.341123	C	-7.698164	0.307389	10.665169
C	-9.269228	0.721066	9.294536	C	-8.413165	0.510204	9.448245
S	-9.271490	-1.111108	12.931126	H	-10.405409	0.745304	8.616270
O	-8.161715	-1.045214	13.987532	H	-11.590031	0.445184	10.774793
O	-7.973830	5.105948	7.495208	H	-6.616811	0.255667	10.624678
O	-8.287502	6.711763	5.663221	H	-7.818260	-0.021028	12.787241
O	-10.673838	-0.273882	13.572615	S	-10.629944	0.021717	13.461166
O	-9.806304	-2.462552	12.427313	O	-12.105891	-0.327628	13.226185
O	-12.528066	1.523405	1.233037	O	-9.785347	-0.782304	14.473388
O	-12.334273	2.257177	3.933529	O	-10.580209	1.664608	14.087779
O	-10.303062	0.137603	1.587721	H	-10.313603	1.526764	15.014328
O	-5.364387	-4.125711	5.214270	H	-10.744908	0.147710	3.160630
O	-7.701518	-5.426502	5.176232	O	-10.693628	-0.673925	3.739702
H	-11.223428	-0.990782	13.937769	C	-9.916438	-0.324490	4.769183
H	-7.414152	1.079663	12.701044	C	-9.666112	-1.290371	5.758439
H	-6.900258	2.643234	10.832086	C	-8.888830	-0.987981	6.865139
H	-10.283097	-0.938502	10.220581	N	-8.531831	-1.924723	7.818549
H	-9.817238	0.623691	8.367538	C	-8.549886	-3.311603	7.804144
H	-8.687126	0.758194	6.650399	C	-8.481361	-3.962516	9.058759
H	-7.563866	3.528659	8.829936	C	-8.450356	-5.344599	9.144420
H	-8.017316	5.964015	6.936921	C	-8.494725	-6.081843	7.963603
H	-8.481657	8.154631	3.664535	C	-8.549002	-5.481945	6.712154
H	-8.985915	8.661641	1.266077	C	-8.574966	-4.094226	6.630265
H	-9.798181	6.843401	-0.227002	S	-8.440010	-7.899793	8.061773
H	-10.117593	4.535204	0.680362	O	-8.941887	-8.514679	6.749621
H	-13.353988	1.909421	1.552930	O	-8.971622	-8.396306	9.417950
H	-12.150388	3.201336	3.968241	O	-6.702663	-8.121471	8.133120
H	-10.657723	0.055884	0.692468	H	-6.591558	-8.953806	8.627255
H	-12.899525	0.106866	4.228314	H	-8.415880	-5.847030	10.104797
H	-6.985611	0.584545	4.489374	H	-8.465775	-3.362822	9.964055
H	-5.809370	-1.600754	4.685921	H	-8.094550	-1.512939	8.633691
H	-10.764401	-1.449871	4.183766	H	-8.570263	-3.622743	5.657401
H	-9.578715	-3.647742	4.386539	H	-8.565694	-6.094363	5.817302
H	-6.901265	-5.631824	2.901567	H	-10.109897	-2.267294	5.622536

E_{calcd}				F_{calcd}			
64				64			
scf done: -2168.466016				scf done: -2168.455706			
O	-12.778691	-4.280353	6.096444	C	-9.453314	2.214482	9.541503
O	-11.142651	-5.047128	4.219581	C	-8.468193	1.180980	9.588390
H	-10.991000	-5.514675	5.060018	C	-8.676384	0.133432	10.533548
S	-12.392986	-3.883079	4.654584	C	-9.766914	0.132350	11.381919
O	-13.414511	-3.948037	3.510842	C	-10.707486	1.164902	11.290075
C	-11.532890	-2.295742	4.643116	C	-10.553553	2.212856	10.377449
C	-10.899234	-1.854027	5.806073	N	-7.423381	1.084760	8.710256
H	-10.993745	-2.425082	6.723705	C	-6.968932	2.152061	7.988878
C	-10.186714	-0.666574	5.786645	C	-6.611206	1.835380	6.585237
H	-9.737343	-0.302338	6.700212	C	-6.476973	2.907641	5.681280
C	-11.466062	-1.568292	3.450818	C	-6.450586	4.230310	6.110584
H	-11.978021	-1.930002	2.565668	C	-6.525303	4.552181	7.500055
C	-10.753748	-0.386364	3.432974	C	-6.767074	3.480851	8.451334
H	-10.694439	0.197094	2.518957	C	-6.668673	3.777523	9.885070
C	-10.076557	0.097788	4.591371	C	-6.442449	5.207402	10.275117
N	-9.419445	1.284877	4.469505	C	-6.308251	6.232458	9.320596

H	-9.732110	1.934312	3.712094	C	-6.343862	5.913997	7.879875
C	-8.580877	1.977209	5.356078	C	-6.125174	7.560003	9.742392
C	-8.510686	3.401472	5.210419	C	-6.074650	7.865990	11.096649
C	-9.212328	4.051552	4.133456	C	-6.207120	6.844995	12.050860
O	-9.906301	3.451818	3.247815	C	-6.390195	5.529664	11.639941
C	-9.114690	5.524827	4.028052	N	-6.581514	0.530390	6.269744
C	-9.794665	6.189816	2.991246	C	-6.171461	0.052537	5.049005
H	-10.370657	5.585608	2.298331	C	-6.857924	-1.076551	4.522316
C	-9.720582	7.571443	2.873598	C	-6.476973	-1.666713	3.330891
H	-10.250038	8.078755	2.069451	C	-5.384765	-1.132936	2.637760
C	-8.961643	8.313007	3.793508	C	-4.661850	-0.041742	3.123679
H	-8.902210	9.395812	3.702553	C	-5.061761	0.550335	4.311408
C	-8.287215	7.661589	4.818890	O	-6.307796	5.200681	5.194826
H	-7.688773	8.195010	5.550634	O	-6.732448	2.930431	10.790021
C	-8.356190	6.266015	4.948081	O	-6.196445	6.865266	7.037522
C	-7.607286	5.608736	6.072000	S	-4.797199	-1.978894	1.146974
O	-6.963827	6.340039	6.837738	O	-3.457589	-2.954924	1.762228
C	-7.697960	4.150782	6.159686	S	-12.094799	1.193675	12.434692
C	-6.978353	3.475990	7.190760	O	-13.232360	2.086112	11.911794
O	-6.315945	4.064318	8.109981	Ti	-6.361306	-0.969767	8.130941
C	-6.958793	1.991979	7.196590	O	-4.862785	0.054721	8.589157
C	-7.792060	1.305472	6.288382	O	-6.397082	-1.855651	9.791405
H	-7.797093	0.224260	6.302869	O	-5.487865	-2.207579	7.055295
N	-6.196154	1.450731	8.155077	O	-8.112802	-1.490329	7.689847
C	-5.846266	0.129823	8.191689	O	-5.869031	-2.962770	0.643387
C	-5.505383	-0.641175	7.041225	O	-4.094161	-1.021875	0.174878
H	-5.525325	-0.166881	6.066420	O	-12.402960	-0.222008	12.983676
C	-5.116498	-1.967162	7.144661	O	-11.469463	2.020638	13.876339
H	-4.844686	-2.545817	6.268079	H	-6.250342	6.056592	5.740806
C	-5.052325	-2.548628	8.412054	H	-6.024317	8.322483	8.976858
S	-4.632970	-4.297469	8.551034	H	-5.933265	8.896055	11.417591
O	-3.903482	-4.795856	7.293791	H	-6.169997	7.083228	13.111640
O	-4.084311	-4.641218	9.956918	H	-6.501807	4.715477	12.348487
O	-6.214508	-5.097460	8.553964	H	-7.688220	-1.465560	5.102403
H	-6.159317	-5.620561	9.372998	H	-7.012694	-2.517370	2.922315
C	-5.357510	-1.830503	9.574623	H	-3.803768	0.330146	2.573020
H	-5.275543	-2.309572	10.544574	H	-4.497191	1.385010	4.709238
C	-5.727885	-0.503383	9.463381	H	-7.951345	-0.674026	10.568710
H	-5.918535	0.097757	10.342857	H	-9.914051	-0.672901	12.094235
O	-6.788246	3.147832	10.579313	H	-11.302404	2.995913	10.319997
H	-7.573762	3.335714	10.053778	H	-9.341384	3.018345	8.823204
H	-3.435118	1.654361	10.062400	H	-6.375931	2.724403	4.618641
O	-4.253056	1.843632	10.542297	H	-3.804847	-3.366101	2.573220
Ti	-5.139413	3.221867	9.657429	H	-11.552599	1.314474	14.540691
O	-3.799695	3.311819	8.331974	H	-5.551338	-1.669639	10.221636
H	-4.030921	3.927830	7.625605	H	-6.101975	-2.912944	6.810736
O	-4.620425	4.775888	10.548367	H	-8.749785	-0.777257	7.568547
H	-5.364533	5.000119	11.123937	H	-4.990410	0.907933	9.020652

G_{calcd}

65
scf done: -2169.106705

C	-1.553192	5.255319	2.503674
C	-2.858658	5.557260	2.063250
C	-3.353759	6.868558	2.247171
C	-2.577284	7.850780	2.839369
C	-1.286901	7.521174	3.239533
C	-0.763280	6.244644	3.083460
N	-3.735363	4.650608	1.480238
C	-3.583503	3.393936	0.919767
C	-4.825488	2.788848	0.514663
C	-4.837380	1.517114	-0.058658
C	-3.616169	0.788320	-0.261653
C	-2.385671	1.409279	0.109390
C	-2.404758	2.710604	0.691969
C	-6.135901	0.964646	-0.436340

C	-6.175458	-0.382425	-1.029522
C	-4.981635	-1.107709	-1.210514
C	-3.653464	-0.548579	-0.818382
C	-7.404748	-0.941713	-1.410297
C	-7.447002	-2.213529	-1.969006
C	-6.260152	-2.937384	-2.149900
C	-5.037984	-2.389463	-1.773017
N	-1.210225	0.745984	-0.069284
C	0.099627	1.179870	0.263312
C	0.905354	0.329754	1.035179
C	2.206677	0.696928	1.375735
C	2.679006	1.926828	0.930393
C	1.914547	2.774896	0.140125
C	0.618365	2.395706	-0.207580
S	4.366310	2.513734	1.446625
O	4.798384	3.542610	0.375378
O	-5.939367	3.509529	0.717403
O	-2.636280	-1.256869	-0.987676
O	-7.199808	1.612610	-0.265159
S	-0.263020	8.826150	4.009447
O	-0.989716	10.169171	3.877716
O	-0.353364	8.317595	5.679465
O	1.215651	8.674029	3.621135
O	4.190231	3.069404	2.901602
O	5.253242	1.182515	1.431194
Ti	6.013024	-0.071911	3.115816
O	6.815820	-1.304222	4.231891
O	5.958782	1.398157	4.164419
O	7.305914	-0.325131	1.801291
O	4.344074	-0.924246	2.969674
H	-8.306028	-0.358152	-1.256751
H	-8.398572	-2.646088	-2.264333
H	-6.294056	-3.931802	-2.586246
H	-4.106570	-2.929730	-1.901323
H	0.498603	-0.617328	1.379261
H	2.845659	0.042474	1.971620
H	2.353712	3.701407	-0.215737
H	0.020773	3.022476	-0.862364
H	-1.456693	3.154389	0.944869
H	-4.695158	4.968452	1.418935
H	-4.358491	7.108863	1.909961
H	-2.946032	8.860522	2.981105
H	0.247152	6.016588	3.406443
H	-1.153407	4.254473	2.435225
H	0.560307	8.428896	6.001271
H	-1.343937	-0.218604	-0.386731
H	-6.691774	2.925230	0.371266
H	7.476340	-1.832250	3.763891
H	5.375068	2.135518	3.868427
H	7.153652	0.294699	1.073185
H	4.239926	-1.610572	3.641393

Table S2. Sum of electronic and thermal energies, enthalpies, Gibbs free energies and solvation energies (Hartree/particle and kcal/mol), as well as the entropy (cal/molKelvin) and dipole (Debye). of the ground state structures of Ti dye complexes in gas phase. Relative total Gibbs free energies in solution (**ΔG_{PCM}**) where calculated using complex A_{calcd} as the reference structure for C_{calcd}, E_{calcd} and G_{calcd}; complex B_{calcd} for D_{calcd} and F_{calcd}.

	Energies	Enthalpy	Free energy	PCM	Entropy	
Complex	**E (Hartree /particle)**	**H (Hartree /particle)**	**G (Hartree /particle)**	**E_{PCM}(Hartree /particle)**	**S (cal/ /molKelvin)**	**Dipole (Debye)**
A_{calcd}	-2168.600713	-2168.599769	-2168.725551	-3737.637904	264.73	44.1504
B_{calcd}	**-2168.577697**	**-2168.576753**	**-2168.702763**	**-3737.622447**	**265.21**	**50.8715**
C_{calcd}	-2168.574764	-2168.57382	-2168.697416	-3737.610608	260.13	51.5101
D_{calcd}	**-2168.572869**	**-2168.571925**	**-2168.696884**	**-3737.606677**	**262.998**	**60.5772**
E_{calcd}	-2167.992001	-2167.991057	-2168.113385	-3737.148356	257.46	98.5545
F_{calcd}	**-2167.981164**	**-2167.98022**	**-2168.102566**	**-3737.129546**	**257.499**	**100.2309**
G_{calcd}	-2168.615454	-2168.61451	-2168.737457	-3737.668445	258.765	31.1253

	Gas Phase			PCM (water)		
Complex	**E (kcal/mol)**	**H (kcal/mol)**	**G(kcal/mol)**	**E_{PCM} (kcal/mol)**	**G_{PCM} (kcal/mol)**	**ΔG_{PCM} (kcal/mol)**
A_{calcd}	-1360817.549	-1360816.957	-1360895.886	-2345403.292	-2345481.629	0
B_{calcd}	**-1360803.106**	**-1360802.514**	**-1360881.586**	**-2345393.593**	**-2345472.073**	**0**
C_{calcd}	-1360801.266	-1360800.674	-1360878.231	-2345386.164	-2345463.129	18.50032293
D_{calcd}	**-1360800.077**	**-1360799.484**	**-1360877.897**	**-2345383.697**	**-2345461.517**	**10.5553122**
E_{calcd}	-1360435.577	-1360434.984	-1360511.746	-2345096.096	-2345172.266	49.36328164*
F_{calcd}	**-1360428.776**	**-1360428.184**	**-1360504.957**	**-2345084.293**	**-2345160.474**	**51.59908544***
G_{calcd}	-1360826.799	-1360826.207	-1360903.357	-2345422.457	-2345499.015	-17.38562133

* The solvation free energy of H^+ in water ($\Delta G_{sol}(H+)$ = -260 kcal/mol) was added to the total free energies of complexes E_{calcd} and F_{calcd} in water.