

Supplementary Information for:

Ultrafast Charge Regeneration from LUMO+1 in Ruthenium(II) Polypyridyl Quinoxaline-Sensitized Solar cell

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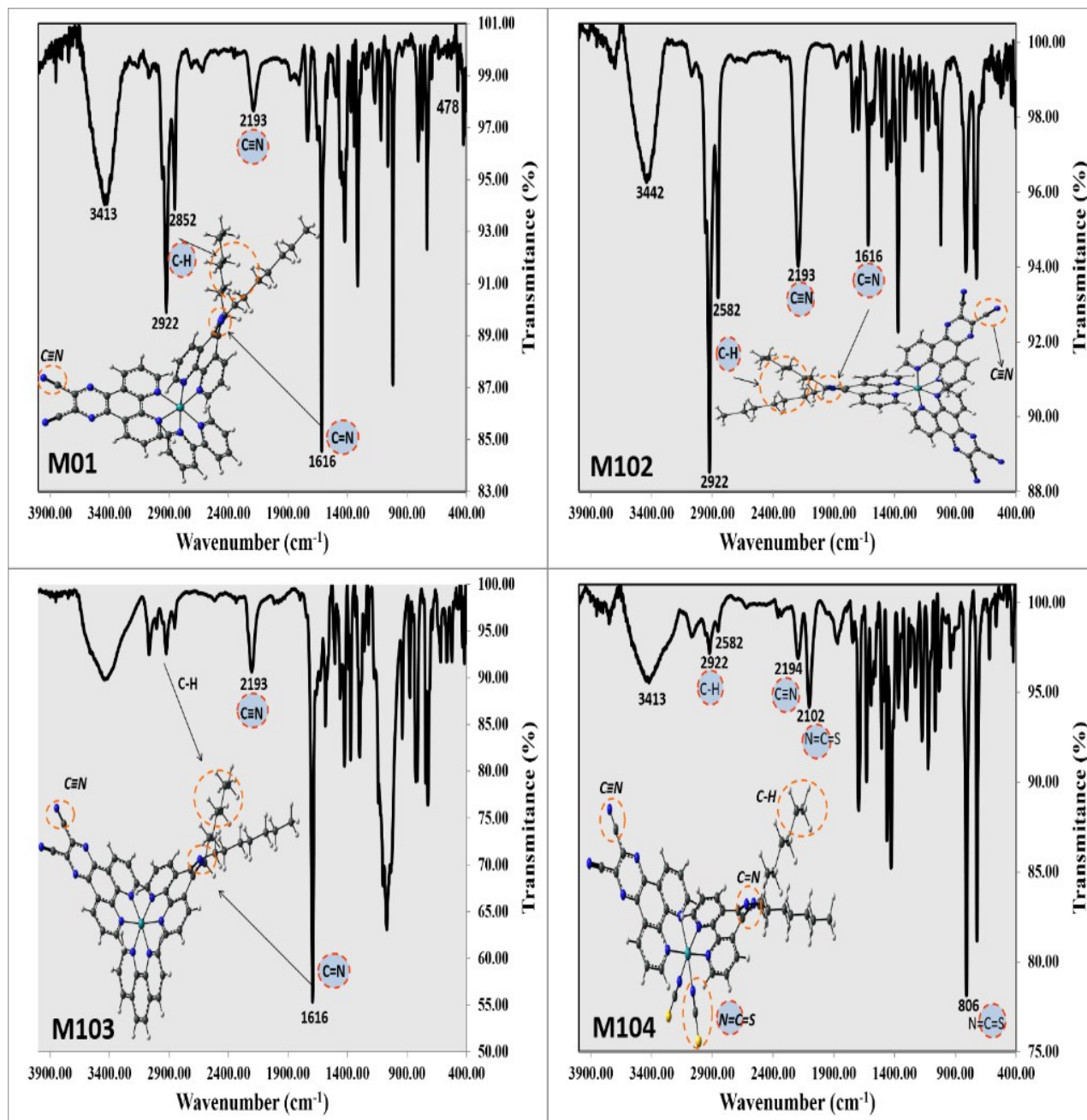


Fig. S1 FT-IR spectra of M101-104. The major stretching bands are assigned to corresponding groups.

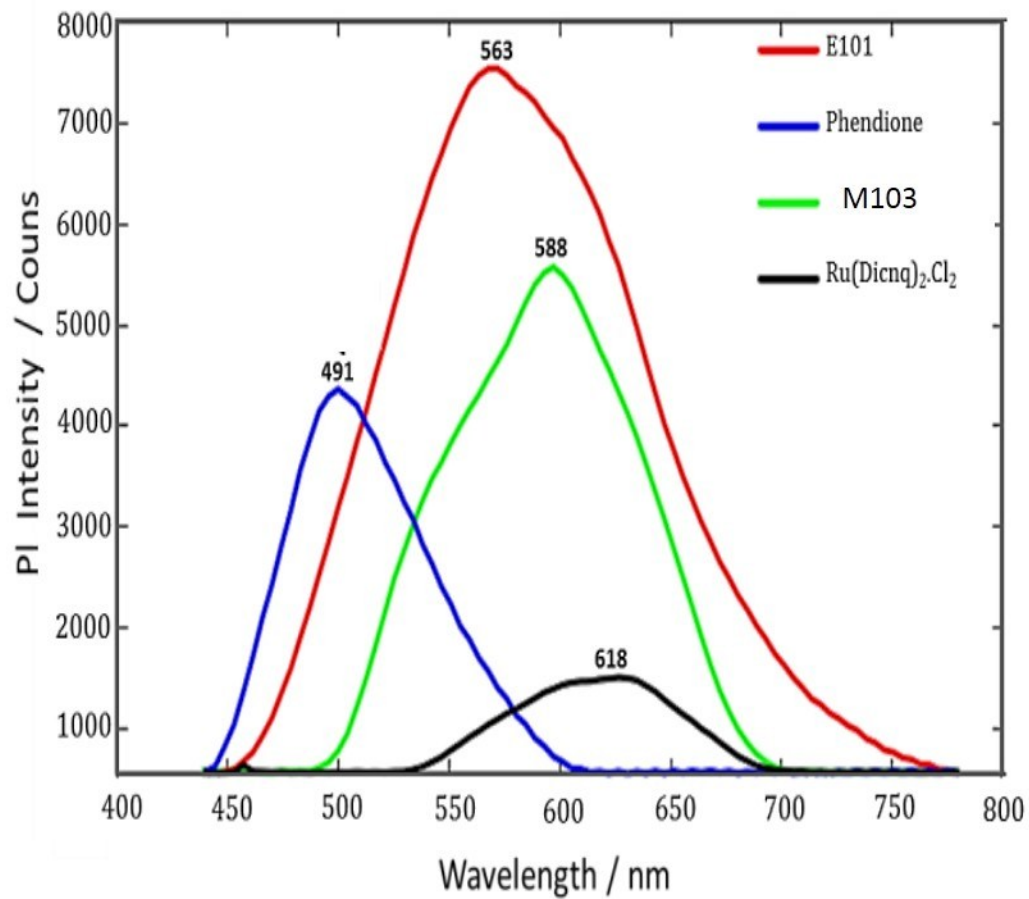


Fig. S2. The PL spectra of Ligands including phendion, E101 as well as complex precursor [Ru(Dicnq)₂ Cl₂]. The PL of M103 is also Shown. PL spectra are recorded in acetonitrile (10^{-5} M) at room temperature , $\lambda_{exc} = 405$ nm .

S3. The full set data of the optimized molecular structure

M101

2 1

Ru	-0.10168875	0.22757303	0.11195729
C	-0.14951053	-0.19928639	4.52976606
C	1.19830114	-0.29240912	4.83111925
C	2.13055307	-0.24190214	3.78027342
C	1.65275394	-0.09565243	2.46478285
C	-0.54921402	-0.05938838	3.19531819
C	3.56655364	-0.33899585	3.99420101
C	2.56558411	-0.03805383	1.34341380
C	3.95584636	-0.13770434	1.53485467
C	4.46360362	-0.29285178	2.88941759
C	4.79479827	-0.08015958	0.40857261
H	5.86792031	-0.15564327	0.53607544
C	4.22073537	0.07367038	-0.84162252
C	2.82859528	0.17011425	-0.95319396
H	-0.90313333	-0.23464721	5.30735380
H	1.54626585	-0.40376316	5.85099134
H	-1.59796290	0.00891458	2.93423960
H	4.82867364	0.12303526	-1.73701572
H	2.35497964	0.29743302	-1.91869267
N	2.01258384	0.11860356	0.10828442
N	0.32309691	-0.00884592	2.17971849
N	5.78872994	-0.38929820	3.07296835
N	4.02342047	-0.47334368	5.24817848
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C	5.33698270	-0.56452356	5.42049560
C	0.52852080	4.58492234	0.54822348
C	-0.77145413	5.04819294	0.70501258
C	-1.82400205	4.12651479	0.75412026
C	-1.51598073	2.76536070	0.63465702
C	0.75286697	3.21514914	0.40888424
C	-3.24475340	4.55766304	0.87753897
C	-2.57279744	1.75714728	0.62468301
C	-3.91168665	2.10262427	0.88938881
C	-4.20717157	3.49267396	1.34874120
C	-4.88258676	1.10848884	0.70877662
H	-5.93431125	1.33612830	0.81919807
C	-4.48835721	-0.17920165	0.35503028
C	-3.13516618	-0.45954923	0.20061768
H	1.36983742	5.26750449	0.52103576
H	-0.99499556	6.10494345	0.79027065
H	1.75097624	2.82288329	0.25942722

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H	-2.78960334	-1.45793273	-0.03550154
N	-0.24685609	2.31840711	0.43573115
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H	-6.96414611	2.91966864	2.20730774
H	-5.67749693	1.97119643	2.96035610
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H	-6.83474106	4.59439758	4.04620794
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C	-6.43816478	9.20255551	-1.57187906
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H	-6.29637523	8.72351082	-2.55114052
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H	-7.92512353	10.41934260	-0.57985209
C	-7.49180653	2.72202978	4.92617922
C	-7.88576275	3.28508479	6.29764086
H	-7.10382880	1.70129749	5.05199288
H	-8.39043009	2.63118291	4.29943024
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H	-6.98768344	3.37028079	6.92583569
H	-8.26859391	4.30798071	6.17319134
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H	-8.43133147	3.07320124	9.02796072
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H	-7.78999712	10.49924583	-3.64229413
H	-7.11064714	11.71622692	-2.57531216
H	-10.10523796	11.01391711	-2.76565242
H	-9.42055383	12.23950951	-1.69066963
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H	-9.34003247	12.45738152	-3.44465597
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C	-0.08059520	-2.83994635	0.49095680
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C	-0.25445908	-4.46799124	-1.25715177
C	-0.35218411	-3.42080685	-2.16840881
C	-0.40967001	-0.92583932	-2.60062148
C	-0.41586925	1.40629134	-2.72524424
C	-0.57616034	1.38041803	-4.10594861
C	-0.65525266	0.14585507	-4.74741927
C	-0.57146983	-1.01598408	-3.98608695
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H	-0.63649160	2.31237565	-4.65554523
H	-0.78051484	0.08478986	-5.82286795
H	-0.63259944	-1.98241724	-4.46939093
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N	-0.33200241	0.28642166	-1.98302482

M101/TiO2

2 1

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C	7.00023913	0.04119374	2.84542226
C	8.22118915	0.10219932	4.81753261
C	4.53886653	0.03531165	2.79467233
C	7.02286966	0.00551401	1.39895765
C	5.82844194	-0.00597912	0.65557396
C	4.56182737	0.01086409	1.37120844
C	5.91065032	-0.03612453	-0.74727885
H	5.00174609	-0.04489163	-1.33665301
C	7.16131548	-0.05495906	-1.34030639
C	8.30597536	-0.04618243	-0.53440296
H	7.12846488	0.14139597	6.66715047
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H	9.19582815	0.12651872	5.28890183
H	7.27214401	-0.07844007	-2.41776659
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H	16.39327344	-6.58427805	6.02849029
C	17.79307778	-8.97936306	5.67629165
H	16.08863087	-9.13747291	4.35591431
H	17.16505506	-7.80272546	3.97468345
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H	11.97044173	-1.10629342	12.96252381

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O	-6.34704378	3.56075537	-1.92311671
O	-4.57737049	4.62736330	-3.79677490
O	-2.74375696	4.17682448	9.46424711
O	-2.69906877	4.16404978	5.68252197
O	-2.65438087	4.15127516	1.90082064
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O	-0.84720562	5.25396479	-3.75481266
O	-4.93038620	6.22305910	5.64953758
O	-4.88569830	6.21028449	1.86783625
O	-4.84101011	6.19750980	-1.91388889
O	-4.97507039	6.23583266	9.43092461
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O	-3.38972023	-3.15730365	1.91749652
O	-3.33383675	-3.14007542	-1.85962948
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O	-5.49143572	-2.66755027	7.56393129
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O	-0.32052918	3.04912246	-1.74486118
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H	-0.26700930	2.79816278	10.29649001
H	-0.06575110	2.74716879	4.69101461
H	0.37811924	2.43225165	1.93349461
H	0.08958969	2.71957897	-0.92189876
H	-8.44913946	-0.89116764	7.52762053
H	-8.40874299	-0.90995553	3.67714719
H	-8.37888972	-0.95116437	0.09900727
H	-8.32213252	-0.94437319	-3.74889406
H	-7.31868556	4.11811138	9.37683488
H	-7.28218964	4.09350571	5.59995926
H	-7.24010997	4.08066839	1.86195283
H	-7.19958131	4.05299644	-1.91360788

M102

2 1

Ru	0.00504855	0.01314141	0.00079083
C	0.00615469	-0.01129402	4.43544772

C	1.35878206	-0.01940829	4.72978091
C	2.28092480	-0.02531847	3.66876533
C	1.78851888	-0.01948933	2.35076396
C	-0.40817310	-0.00967322	3.09817859
C	3.72151690	-0.03990373	3.87477295
C	2.69036663	-0.02673730	1.21915673
C	4.08503953	-0.04488457	1.40324018
C	4.60835827	-0.05031034	2.76068560
C	4.91224120	-0.05499626	0.26668715
H	5.98864670	-0.06913016	0.38810485
C	4.32259227	-0.04667167	-0.98583436
C	2.92667288	-0.02465250	-1.08994419
H	-0.74012341	-0.00789402	5.22088623
H	1.71808225	-0.02258220	5.75180442
H	-1.46049593	-0.00972353	2.84270780
H	4.92133028	-0.05486884	-1.88871876
H	2.43978759	-0.01142509	-2.05720472
N	2.12228379	-0.01176257	-0.01881045
N	0.45447367	-0.01386361	2.07320377
N	5.93784452	-0.06413611	2.93805455
N	4.19264128	-0.04518505	5.13060636
C	6.39488464	-0.06825818	4.18477972
C	5.51025501	-0.05941026	5.29644819
C	0.46672523	4.40763179	-0.06591797
C	-0.84708749	4.83647884	0.07128190
C	-1.86118601	3.88728445	0.24576742
C	-1.50148157	2.53386508	0.26885083
C	0.74318035	3.04024794	-0.05728337
C	-3.29499968	4.27688306	0.35670101
C	-2.51734841	1.49144103	0.38610955
C	-3.86495087	1.81248931	0.63569988
C	-4.20823592	3.23110029	0.95230035
C	-4.79848022	0.76906456	0.57614478
H	-5.85675879	0.96736867	0.68033732
C	-4.35872085	-0.53273824	0.35084897
C	-2.99767262	-0.77671272	0.20388576
H	1.27916965	5.11412630	-0.18964560
H	-1.11093170	5.88705112	0.04563896
H	1.75247172	2.67066896	-0.18701071
H	-5.05936535	-1.35754504	0.29896811
H	-2.61573325	-1.78028510	0.06716343
N	-0.21903331	2.11549063	0.09416775
N	-2.08863001	0.21498406	0.21362384
C	-6.01670812	2.81631706	2.51664617
C	-6.41613328	3.52875280	3.81452363
H	-6.92141987	2.63294982	1.91905559
H	-5.58110523	1.83407601	2.74798817
H	-5.50903986	3.74743177	4.39262171
H	-6.86747887	4.49596160	3.56108260
C	-4.95639303	5.98719866	-0.04225724
C	-5.10860653	6.99838764	-1.18424860
H	-5.72237238	5.20409216	-0.10545226

H	-5.12072064	6.49297198	0.91955508
H	-4.31903193	7.75515365	-1.09359181
H	-4.93966693	6.48543179	-2.14043319
C	-6.48381198	7.67612616	-1.19567992
C	-6.64805394	8.68993066	-2.33521977
H	-6.64586203	8.18238586	-0.23327754
H	-7.26983292	6.91172873	-1.27371246
C	-8.01199808	9.39164821	-2.34000766
H	-5.85248997	9.44526519	-2.26407865
H	-6.49837488	8.18042293	-3.29780196
H	-8.80942899	8.63790899	-2.41079650
H	-8.16085639	9.90170211	-1.37730336
C	-7.38673987	2.69834569	4.66191432
C	-7.81156897	3.39729564	5.95986321
H	-6.92341603	1.73195028	4.90621201
H	-8.28120971	2.46535709	4.06674582
C	-8.77478947	2.56252152	6.81281634
H	-6.91715951	3.63803716	6.55186687
H	-8.28305516	4.35966380	5.71504470
H	-9.66538848	2.31437959	6.21755798
H	-8.29980590	1.60279850	7.06267638
C	-9.21225162	3.26063794	8.10697630
C	-10.17048012	2.41722326	8.95431481
H	-9.69019530	4.21773663	7.85696069
H	-8.32255702	3.51150669	8.70071852
H	-11.08368045	2.17669122	8.39761912
H	-9.70619551	1.46971493	9.25158404
C	-8.17410836	10.40666341	-3.47884638
C	-9.53524607	11.11025002	-3.47306039
H	-8.03002133	9.89615157	-4.44093582
H	-7.37412349	11.15651625	-3.41017909
H	-10.35422729	10.38840658	-3.57252238
H	-9.69213357	11.66018282	-2.53782996
H	-10.46667677	2.94352794	9.86787646
H	-9.62038407	11.82561648	-4.29791320
N	-5.12412250	3.66126517	1.73761754
N	-3.60329924	5.45638868	-0.02878042
C	6.01198860	-0.06584019	6.64575858
C	7.82244642	-0.08183951	4.37024163
N	8.97244622	-0.09264788	4.53323007
N	6.42980235	-0.07126707	7.72954486
C	-0.11984306	-2.46837605	-1.57686629
C	0.16049637	-3.04393098	0.65495926
C	0.16947674	-4.41206173	0.33525946
C	0.02683821	-4.80587022	-0.98104422
C	-0.26911823	-1.42774047	-2.54903794
C	-0.38683728	0.84966987	-2.98560896
C	-0.54966807	0.61128940	-4.36049805
C	-0.56857085	-0.68757045	-4.83024818
C	-0.42499199	-1.75508458	-3.91652214
H	0.26700194	-2.71403306	1.68126445
H	0.28742961	-5.13804270	1.13111053

H	0.02910821	-5.85672043	-1.25239901
H	-0.36348452	1.86062242	-2.59768575
H	-0.65662457	1.45514048	-5.03190142
H	-0.69117506	-0.89682369	-5.88803264
N	0.01872230	-2.09117814	-0.26942218
N	-0.24725105	-0.13683017	-2.09670867
C	-0.12449519	-3.82303461	-1.98425740
C	-0.28167000	-4.12851740	-3.37832492
C	-0.42707782	-3.13759872	-4.30407791
H	-0.54659260	-3.37808810	-5.35555735
H	-0.28336717	-5.17063469	-3.68100943

M102/TiO2

2 1

N	-4.73052739	20.15538290	-8.61818398
Ru	-2.16683910	18.14561825	-18.12380159
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C	-3.20185530	15.27703939	-14.26413868
C	-3.21959222	16.68129280	-14.20173700
C	-2.90333785	17.40937870	-15.36341652
C	-2.56477257	15.46025400	-16.57604470
C	-3.54805556	17.41361026	-12.98774341
C	-2.90384998	18.85640647	-15.35820328
C	-3.21544503	19.57744278	-14.19100848
C	-3.54518667	18.83760148	-12.98251549
C	-3.19639269	20.98204777	-14.24429515
H	-3.43336695	21.55474292	-13.35578275
C	-2.87245263	21.59843691	-15.44082871
C	-2.57744659	20.81389212	-16.56215630
H	-2.84380483	13.58958555	-15.55681830
H	-3.44355866	14.69847307	-13.38069129
H	-2.29729581	15.00769218	-17.52277202
H	-2.84464598	22.67803249	-15.52716978
H	-2.32707410	21.27030745	-17.51180036
N	-2.59332353	19.47473310	-16.53155344
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N	-3.84587240	19.52343970	-11.86968190
N	-3.85007213	16.72107220	-11.87946517
C	-4.14449205	18.82930103	-10.77779174
C	-4.14593698	17.40858588	-10.78237777
C	-6.48618322	18.46514395	-19.00147510
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C	-5.53749012	16.77863961	-20.43072818
C	-4.31517658	16.98963890	-19.78027217
C	-5.23021306	18.63588379	-18.41869945
C	-5.62359902	15.80032971	-21.55117896
C	-3.11301568	16.27195114	-20.19514130
C	-3.17435317	15.23869130	-21.14908653
C	-4.51871698	14.77120184	-21.60149912
C	-1.95984743	14.71075771	-21.60736704

H	-1.94112587	13.97157163	-22.39691601
C	-0.76361636	15.16598878	-21.05906699
C	-0.79621944	16.12676981	-20.05437257
H	-7.32023302	19.06316234	-18.65327418
H	-7.59093813	17.39232751	-20.52420597
H	-5.06932888	19.36545089	-17.63515941
H	0.18922418	14.77557272	-21.39606964
H	0.11070161	16.47535867	-19.57718474
N	-4.15846070	17.92415506	-18.80439073
N	-1.94749269	16.67880536	-19.63041215
C	-3.98860330	12.42413932	-21.91784025
C	-4.80205532	11.15535668	-21.63486069
H	-3.52008438	12.33226740	-22.90844157
H	-3.17413978	12.51728108	-21.18569255
H	-5.30188578	11.26383844	-20.66365650
H	-5.59504362	11.06984404	-22.38805072
C	-6.84893350	15.07491265	-23.50486791
C	-7.60250904	15.87163611	-24.57592908
H	-5.92038812	14.65265015	-23.90918415
H	-7.45860499	14.21645460	-23.18983836
H	-8.51525563	16.28711702	-24.13027140
H	-6.98783371	16.72857363	-24.88217341
C	-7.95853404	15.02439117	-25.80315050
C	-8.71245297	15.81171759	-26.88252505
H	-8.56925874	14.16688136	-25.48618095
H	-7.04127310	14.60124813	-26.23651382
C	-9.09507052	14.96614473	-28.10374756
H	-9.62190106	16.24622575	-26.44363990
H	-8.09592042	16.66170708	-27.20805832
H	-8.18681630	14.53019499	-28.54426092
H	-9.71232486	14.11656632	-27.77766946
C	-3.93359322	9.89222702	-21.63592962
C	-4.72862822	8.60768555	-21.36843246
H	-3.14245392	9.99233850	-20.87939362
H	-3.41988713	9.80502738	-22.60396257
C	-3.85845700	7.34479543	-21.35942233
H	-5.24926698	8.69729576	-20.40443123
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H	-3.33097476	7.26013425	-22.32049907
H	-3.07715393	7.44774977	-20.59256274
C	-4.64936042	6.05539089	-21.10349778
C	-3.77101741	4.80003905	-21.09174915
H	-5.42747675	5.95073345	-21.87197529
H	-5.17902559	6.14066800	-20.14474648
H	-3.25234976	4.67107940	-22.04885618
H	-3.00696542	4.85912180	-20.30789009
C	-9.85072707	15.75423860	-29.18142120
C	-10.23748140	14.90210639	-30.39470403
H	-9.23211031	16.60037650	-29.51060728
H	-10.75543818	16.19345376	-28.73920164
H	-9.35061439	14.47513269	-30.87724030
H	-10.88690391	14.06891771	-30.10188543

H	-4.36428069	3.89751317	-20.91061472
H	-10.77264767	15.49303027	-31.14556079
N	-4.86557014	13.58518544	-21.93865061
N	-6.62998072	15.90619115	-22.33275897
C	-4.46875107	16.66173629	-9.59476537
C	-4.46775728	19.56964214	-9.58619287
N	-4.73096195	16.07104789	-8.62961090
C	0.50830361	19.31624668	-18.49227059
C	0.63606114	17.74242503	-16.79001844
C	2.00396219	18.00470554	-16.60528620
C	2.62979269	18.95022177	-17.39422315
C	-0.30213156	19.98148567	-19.46745014
C	-2.39811474	20.24085279	-20.43214339
C	-1.90799897	21.21910519	-21.31331755
C	-0.57619142	21.58145724	-21.25809969
C	0.27093922	20.95863678	-20.31493430
H	0.12711563	17.00219707	-16.18461323
H	2.54707812	17.45693224	-15.84416224
H	3.68569259	19.16903614	-17.27125813
H	-3.44022354	19.94669354	-20.45526103
H	-2.58739446	21.67558889	-22.02349444
H	-0.17479520	22.33585590	-21.92704694
N	-0.09920576	18.37522396	-17.70722452
N	-1.62406018	19.63466971	-19.52870994
C	1.88054856	19.63878061	-18.37392937
C	2.43721203	20.63587638	-19.24420156
C	1.66619980	21.26732931	-20.17527040
H	2.09597567	22.01883691	-20.82968386
H	3.49069616	20.87676098	-19.14533265
N	-1.64088858	28.02891884	-9.61614270
N	-2.91509820	28.82069153	-8.65571999
C	-2.66651190	28.20104349	-9.63027080
C	-1.39882280	28.64443401	-10.59856820
Ti	-6.72330355	12.39169198	-3.17304567
Ti	-6.72330355	16.17370273	-3.17304567
Ti	-6.72330355	19.95571348	-3.17304567
Ti	-6.72330355	23.73770041	-3.17304567
Ti	-5.31961380	12.37457997	-6.51672462
Ti	-5.28731335	16.21126161	-6.71352458
Ti	-5.28673337	19.92646902	-6.71076863
Ti	-5.31441622	23.75701115	-6.50975324
Ti	-1.61031147	10.50086758	-3.17327693
Ti	-4.51684239	10.50086758	-2.29493741
Ti	-1.61031147	14.28287833	-3.17327693
Ti	-4.51684239	14.28287833	-2.29493741
Ti	-1.61031147	18.06486527	-3.17327693
Ti	-4.51684239	18.06486527	-2.29493741
Ti	-1.61031147	21.84687602	-3.17327693
Ti	-4.51684239	21.84687602	-2.29493741
Ti	-3.16712554	10.51800340	-5.80032764
Ti	-3.14840007	14.28657622	-5.79518615
Ti	-3.14979234	18.06503460	-5.75069345

Ti	-3.14784285	21.84704535	-5.78890958
Ti	-0.18743217	21.84286379	-6.47387661
Ti	-0.20696992	18.06247233	-6.49972427
Ti	-0.19643559	14.28747053	-6.47741998
Ti	-0.19065751	10.52498854	-6.46595535
Ti	0.59626558	12.39169198	-2.29544701
Ti	0.59626558	16.17370273	-2.29544701
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Ti	0.59626558	23.73770041	-2.29544701
Ti	-8.24788649	12.38016332	-5.73932144
Ti	-8.21233795	16.17544266	-5.72838916
Ti	-8.21038899	19.94996132	-5.72913054
Ti	-8.25888543	23.75295077	-5.74506565
O	-6.39275986	12.39169198	-5.07661213
O	-6.35468185	10.50086758	-3.02636621
O	-4.88455866	12.39169198	-2.44131578
O	-6.39275986	16.17370273	-5.07661213
O	-6.35468185	14.28287833	-3.02636621
O	-4.88455866	16.17370273	-2.44131578
O	-6.39275986	19.95571348	-5.07661213
O	-6.35468185	18.06486527	-3.02636621
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O	-6.39275986	23.73770041	-5.07661213
O	-6.35468185	21.84687602	-3.02636621
O	-4.88455866	23.73770041	-2.44131578
O	-7.16355626	12.39169198	-7.41878133
O	-4.93092094	10.50654724	-6.76183899
O	-3.37879379	12.40899713	-6.08785027
O	-7.16355626	16.17370273	-7.41878133
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O	-3.38642823	16.20570261	-6.09313093
O	-7.16355626	19.95571348	-7.41878133
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O	-3.39533852	19.95409419	-6.05456767
O	-7.16355626	23.73770041	-7.41878133
O	-4.91405130	21.85219319	-6.72471139
O	-3.36078748	23.72675173	-6.12768726
O	-3.44905636	10.50086758	-3.90505286
O	-2.67812078	10.50086758	-1.56316201
O	-1.24171359	12.39169198	-3.02655142
O	-3.44905636	14.28287833	-3.90505286
O	-2.67812078	14.28287833	-1.56316201
O	-1.24171359	16.17370273	-3.02655142
O	-3.44905636	18.06486527	-3.90505286
O	-2.67812078	18.06486527	-1.56316201
O	-1.24171359	19.95571348	-3.02655142
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O	-1.24171359	23.73770041	-3.02655142
O	-1.27962914	10.50086758	-5.07707516
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O	-1.27962914	18.06486527	-5.07707516

O	-1.27962914	21.84687602	-5.07707516
O	0.20279213	19.95602781	-6.52253816
O	0.20279213	16.17404087	-6.52253816
O	0.20279213	12.39203012	-6.52253816
O	0.20279213	23.73770041	-6.52253816
O	0.22854877	14.28254019	-2.44177934
O	0.22854877	18.06452712	-2.44177934
O	0.22854877	21.84653787	-2.44177934
O	0.22854877	10.50086758	-2.44177934
O	-8.54090886	14.28720489	-6.00094931
O	-8.56766353	18.06418845	-5.99407054
O	-8.53592031	21.84163134	-5.99833253
O	-8.50587045	10.50458982	-5.97628277
O	-8.56376509	12.39169198	-3.90551589
O	-8.56376509	16.17370273	-3.90551589
O	-8.56376509	19.95571348	-3.90551589
O	-8.56376509	23.73770041	-3.90551589
O	-1.87959602	10.60034814	-7.46790591
O	-1.85142633	14.46260016	-7.51293095
O	-1.86722809	18.06249667	-7.52733728
O	-1.82984648	21.74157133	-7.55330083
O	-7.79359575	12.39169198	-1.56434313
O	-7.79359575	16.17370273	-1.56434313
O	-7.79359575	19.95571348	-1.56434313
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H	-7.30640078	13.21136425	-7.93198536
H	-7.29848852	16.53249337	-8.30939563
H	-7.28484422	19.55177502	-8.29186293
H	-7.30254890	22.91014922	-7.92003442
H	-2.07033425	9.70260952	-7.80932419
H	-2.07140160	15.31021193	-7.94808240
H	-2.27733887	18.07383218	-8.41723402
H	-2.05991581	20.92463014	-8.03676616
H	-7.49342631	12.38705162	-0.62539113
H	-7.50020190	16.23777498	-0.62170859
H	-7.53136514	19.81613663	-0.61610354
H	-7.50955352	23.66439507	-0.62268121
H	-2.35941161	10.53441425	-0.63027808
H	-2.37277757	14.31151899	-0.62499742
H	-2.37345016	18.04978372	-0.62300560
H	-2.38890425	21.82563167	-0.62235683

M103

2 1

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C	-3.79153840	-0.74667314	-2.06367963
C	-4.25413237	0.54947316	-2.24912706

C	-3.46436930	1.62488427	-1.82489437
C	-2.23329954	1.34122108	-1.22013384
C	-2.56458725	-0.95012369	-1.43179652
C	-3.91894279	3.03707578	-1.96146818
C	-1.38892437	2.41454621	-0.70295675
C	-1.70792721	3.76626063	-0.93196875
C	-2.83326245	4.08269872	-1.86106255
C	-0.93724841	4.73236744	-0.27117837
H	-1.18496404	5.78263757	-0.34586686
C	0.14092886	4.33138287	0.51292710
C	0.44331012	2.97790762	0.61439454
H	-4.36930263	-1.60290063	-2.39153652
H	-5.21160907	0.75359153	-2.71332421
H	-2.18581957	-1.94786746	-1.24993227
H	0.75246104	5.05715548	1.03551235
H	1.29778184	2.63415633	1.18284487
N	-1.80174087	0.06941565	-1.00392662
N	-0.30861812	2.03115435	0.02429630
C	-1.94873995	6.13804254	-2.80683192
C	-2.01791014	6.71087268	-4.22732231
H	-2.17762177	6.93928187	-2.08922209
H	-0.92740025	5.79502651	-2.58879293
H	-1.81649969	5.90525836	-4.94515449
H	-3.04296242	7.05170373	-4.41848346
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H	-5.24094184	5.31112482	-1.75193191
H	-5.73807338	4.82504625	-3.35902952
H	-7.76186791	3.68203351	-2.42162323
H	-7.29009824	4.16713822	-0.79765633
C	-7.97304027	5.80746170	-2.03912188
C	-9.44346059	5.77725573	-1.60287237
H	-7.91547377	6.10445259	-3.09619514
H	-7.44462784	6.58927949	-1.47520829
C	-10.16347773	7.11648153	-1.80423448
H	-9.97207188	4.99289751	-2.16313054
H	-9.50299636	5.48786928	-0.54396795
H	-9.63455062	7.90074217	-1.24357689
H	-10.10005748	7.40582507	-2.86323018
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C	-1.09712188	8.45807101	-5.85765453
H	-0.00777333	7.51095867	-4.24793768
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C	-0.11381285	9.61424620	-6.07940366
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H	-2.12010981	8.80918191	-6.05420504
H	-0.30787920	10.40306548	-5.33833749
H	0.91001881	9.26238730	-5.88688258
C	-0.18393250	10.21770893	-7.48793570
C	0.80108087	11.37196839	-7.70039264
H	-1.20689011	10.56972880	-7.67938447
H	0.00960088	9.42974326	-8.22863304

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C	1.41405582	-0.00170623	2.67331516
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C	3.75576175	0.10893260	3.26299375
C	0.01228098	-0.05949612	3.02791599
C	-2.18619844	-0.18062939	2.29360570
C	-2.66581925	-0.18652397	3.60875417
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H	-3.73377813	-0.23910576	3.78281352
H	-2.10153273	-0.12396127	5.69210709
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C	2.40992509	0.05938175	3.66536741
C	2.00320637	0.07553851	5.06234176
C	0.62439686	0.01397592	5.41103661
C	2.14645607	0.66017438	-3.73662400
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C	1.36317853	-1.43733122	-2.15124747
C	1.45559972	0.85014245	-2.53398520
C	2.33220830	-3.09164418	-3.69515489
C	0.93556217	-2.51065699	-1.28015313
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C	1.90808826	-4.14792278	-2.84022216
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H	-0.65959023	-2.80598143	1.57840509
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M103/TiO2

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C	8.88044198	12.53757748	4.94413426
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C	9.85798847	10.04202044	7.57001496
C	11.24737561	10.22424686	7.70308028
C	11.95225453	11.07092305	6.69513627
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H	12.93182935	9.75494760	8.97793336
C	11.14377488	8.75640495	9.61622802
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H	9.32510168	13.34094686	4.36900273
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H	13.73435152	17.77735619	6.90123969
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H	15.19646455	19.89167383	7.04135524
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H	17.18159945	21.21479158	6.27515263
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C	6.63416976	11.68073791	9.37876290
C	6.31215746	12.46615443	10.49193646
C	5.96059326	11.85088057	11.68086968
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H	6.24750311	4.45725362	10.36247325
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H	6.91117182	12.13812645	8.43732536
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C	7.48046388	5.64099931	4.27507430
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C	6.27133197	7.22579362	5.64302659
C	8.54320579	6.92301110	6.00972155
C	5.02045644	5.99772616	3.91483318
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C	3.83863377	7.64589474	5.37264506
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Ti	3.79439191	14.69123205	19.40919436
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Ti	7.49848554	8.99909252	22.74565639
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Ti	5.94167571	1.45221901	20.11860938
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Ti	5.96095628	12.78125778	20.13003961
Ti	8.92137437	12.77707146	19.44506570
Ti	8.90183715	8.99669746	19.41922492
Ti	8.91236354	5.22169619	19.44151492
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O	2.75411305	5.21710029	22.89256234
O	4.22423306	7.10791304	23.47762071
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O	4.22423306	10.88992697	23.47762071
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O	1.94524922	7.10791304	18.50015516
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O	7.82916682	5.21710029	20.84186503
O	7.82916682	8.99909252	20.84186503
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O	0.54112872	8.99840194	19.92486859
O	0.57287935	12.77584165	19.92061824
O	0.60292180	1.43879749	19.94264895
O	0.54503616	3.32589912	22.01343277
O	0.54503616	7.10791304	22.01343277
O	0.54503616	10.88992697	22.01343277
O	0.54503616	14.67191972	22.01343277
O	7.22921264	1.53456058	18.45103957
O	7.25737651	5.39682317	18.40601929
O	7.24157581	8.99671916	18.39160821
O	7.27894207	12.67578482	18.36563830
O	1.31520973	3.32589912	24.35459864
O	1.31520973	7.10791304	24.35459864
O	1.31520973	10.88992697	24.35459864
O	1.31520973	14.67191972	24.35459864
H	1.80240311	4.14558145	17.98694319
H	1.81030320	7.46671162	17.60954403
H	1.82394750	10.48598745	17.62706456
H	1.80624652	13.84436112	17.99891741
H	7.03847387	0.63683042	18.10961547
H	7.03740599	6.24442754	17.97084773
H	6.83146397	9.00804725	17.50169718
H	7.04889337	11.85884257	17.88218038
H	1.61537917	3.32125982	25.29354800
H	1.60858877	7.17199958	25.29722843
H	1.57743610	10.75036070	25.30282712
H	1.59923662	14.59861915	25.29626956
H	6.74938646	1.46863991	25.28864941
H	6.73601997	5.24573407	25.29393695
H	6.73535797	8.98400938	25.29593247
H	6.71989912	12.75985256	25.29658072

M104

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C	2.26527249	-0.04751322	3.64448584
C	1.75767779	0.05724686	2.33511575
C	-0.42769897	0.05608851	3.10710703
C	3.70901438	-0.10646004	3.82661496
C	2.64596297	0.11786335	1.19810981
C	4.04364960	0.05822124	1.35622794
C	4.58286991	-0.05757091	2.70199551
C	4.84831469	0.10845950	0.20476088
H	5.92621680	0.05725119	0.30656131
C	4.23275201	0.21137701	-1.03322071
C	2.83518305	0.26773117	-1.11336590
H	-0.73636678	-0.08410947	5.22859703
H	1.73212165	-0.18409276	5.72858719
H	-1.48213619	0.08106231	2.85746285
H	4.81536252	0.23878522	-1.94718579
H	2.30798899	0.32542296	-2.05930604
N	2.05739131	0.23245865	-0.02330196
N	0.41918559	0.10641485	2.06942905
N	5.91461348	-0.11029752	2.86275910
N	4.19580618	-0.20404670	5.07312075
C	6.38858696	-0.21227814	4.10069730
C	5.51591366	-0.25916452	5.22383510
N	0.23055091	-1.95283750	0.12006405
N	-0.19259779	0.09345932	-2.03230525
S	-0.47397530	0.65677282	-4.77590839
S	0.85624233	-4.56295941	0.97031970
C	0.50493944	-3.04884521	0.47920352
C	-0.32282270	0.33111524	-3.18580219
C	-0.22420285	4.46558768	-0.51751112
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C	-2.46405650	3.61295476	-0.33311321
C	-1.90486629	2.35199720	-0.08909964
C	0.25444506	3.17634321	-0.28693504
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C	-4.76231479	2.64846452	0.19416232
C	-4.89082232	0.08987190	0.10983097
H	-5.97195803	0.10913890	0.06708586
C	-4.21884736	-1.13170233	0.10932879
C	-2.82841364	-1.14990549	0.14549988
H	0.47917687	5.27438109	-0.68288700
H	-2.01943061	5.66308706	-0.76337986
H	1.31605283	2.95811211	-0.28400827
H	-4.76467945	-2.06806287	0.08082019
H	-2.24860004	-2.06583745	0.16251384
N	-0.56148847	2.13126743	-0.08262665
N	-2.10956864	-0.01303744	0.13013340
C	-6.71616926	2.11442058	1.53684193
C	-7.42289844	2.90534010	2.64456711
H	-7.47646325	1.70243779	0.85579053

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H	-6.66313649	3.33731270	3.30862837
H	-7.94852555	3.75162141	2.18641264
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C	-5.92744311	6.13913730	-2.31314590
H	-6.40268683	4.28626981	-1.26209150
H	-6.14409484	5.65746477	-0.20942664
H	-5.29302659	7.01705209	-2.13807738
H	-5.53821642	5.65361675	-3.21742193
C	-7.37989126	6.57419566	-2.53975549
C	-7.54797700	7.54033896	-3.71946831
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H	-8.00721607	5.68679812	-2.70691396
C	-8.99890265	7.98265425	-3.94656842
H	-6.91955050	8.42681553	-3.55338163
H	-7.16528755	7.06538418	-4.63380130
H	-9.62754548	7.09615737	-4.11398936
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C	-9.11562814	2.83309022	4.56448276
H	-7.86577519	1.19830495	3.90193536
H	-9.15158669	1.61298506	2.78022124
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H	-9.64792759	3.68493028	4.11832816
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H	-10.07604368	3.20533152	7.15848794
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H	-11.30462328	1.08279598	7.77542892
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C	-10.62038635	9.38785136	-5.34317518
H	-8.78667511	8.47745620	-6.03909396
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M104/TiO2

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C	-2.91471150	1.33094630	-5.13006530
C	-2.63318193	-0.62582462	-6.34280194
C	-3.50829894	1.35482068	-2.74215380
C	-2.90171207	2.77703890	-5.13163471
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H	-2.39824883	-1.08513537	-7.29482855
H	-2.82053383	6.59503360	-5.33790148
H	-2.33874762	5.15381735	-7.32392832
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C	-6.40125569	2.57721964	-9.02024046
C	-6.52177565	1.70285247	-10.09334413
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C	-4.25337224	1.02186499	-9.69377641
C	-5.18798257	2.65827616	-8.33687632
C	-5.47374570	-0.03425265	-11.60389625
C	-3.06232283	0.25304509	-10.04194235
C	-3.10246313	-0.75446683	-11.02367080
C	-4.43083853	-1.12917186	-11.59246405
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Ti	-6.61607294	7.82087004	7.08892152

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Ti	-5.18008274	0.29443125	3.54844262
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Ti	-5.20718561	7.84018078	3.75221396
Ti	-1.50308087	-5.41596278	7.08869027
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Ti	-1.50308087	-1.63395203	7.08869027
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Ti	-1.50308087	2.14803490	7.08869027
Ti	-4.40961178	2.14803490	7.96702978
Ti	-1.50308087	5.93004565	7.08869027
Ti	-4.40961178	5.93004565	7.96702978
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Ti	-3.04116947	-1.63025414	4.46678105
Ti	-3.04256173	2.14820424	4.51127374
Ti	-3.04061224	5.93021499	4.47305762
Ti	-0.08020156	5.92603343	3.78809059
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Ti	-0.08920498	-1.62935983	3.78454722
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Ti	0.70349619	7.82087004	7.96652018
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Ti	-8.15165483	7.83612040	4.51690154
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O	-6.24745124	-1.63395203	7.23560099
O	-4.77732805	0.25687236	7.82065142
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O	0.31002274	7.82087004	3.73942903
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O	0.33577938	5.92970750	7.82018786
O	0.33577938	-5.41596278	7.82018786
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H	-7.42413454	3.89930626	9.64586365
H	-7.40232291	7.74756471	9.63928598

H	-2.25218100	-5.38241612	9.63168911
H	-2.26554696	-1.60531137	9.63696977
H	-2.26621955	2.13295335	9.63896160
H	-2.28167364	5.90880130	9.63961037

TiO2 anatase

0 1			
Ti	2.85235000	1.89083000	9.81532000
Ti	2.85235000	5.67283000	9.81532000
Ti	2.85235000	9.45483000	9.81532000
Ti	2.85235000	13.23683000	9.81532000
Ti	4.25605000	1.87372000	6.47164000
Ti	4.28834000	5.71039000	6.27484000
Ti	4.28893000	9.42562000	6.27760000
Ti	4.26124000	13.25613000	6.47861000
Ti	7.96534000	0.00000000	9.81513000
Ti	5.05881000	0.00000000	10.69345000
Ti	7.96534000	3.78200000	9.81513000
Ti	5.05881000	3.78200000	10.69345000
Ti	7.96534000	7.56400000	9.81513000
Ti	5.05881000	7.56400000	10.69345000
Ti	7.96534000	11.34600000	9.81513000
Ti	5.05881000	11.34600000	10.69345000
Ti	6.40854000	0.01714000	7.18806000
Ti	6.42726000	3.78570000	7.19320000
Ti	6.42585000	7.56417000	7.23768000
Ti	6.42781000	11.34618000	7.19947000
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Ti	9.36868000	7.56160000	6.48867000
Ti	9.37921000	3.78660000	6.51097000
Ti	9.38500000	0.02411000	6.52241000
Ti	10.17193000	1.89083000	10.69295000
Ti	10.17193000	5.67283000	10.69295000
Ti	10.17193000	9.45483000	10.69295000
Ti	10.17193000	13.23683000	10.69295000
Ti	1.32777000	1.87931000	7.24908000
Ti	1.36333000	5.67458000	7.25999000
Ti	1.36526000	9.44909000	7.25924000
Ti	1.31677000	13.25208000	7.24330000
O	3.18291000	1.89083000	7.91180000
O	3.22097000	0.00000000	9.96202000
O	4.69109000	1.89083000	10.54710000
O	3.18291000	5.67283000	7.91180000
O	3.22097000	3.78200000	9.96202000
O	4.69109000	5.67283000	10.54710000
O	3.18291000	9.45483000	7.91180000
O	3.22097000	7.56400000	9.96202000
O	4.69109000	9.45483000	10.54710000
O	3.18291000	13.23683000	7.91180000
O	3.22097000	11.34600000	9.96202000

○	4.69109000	13.23683000	10.54710000
○	2.41210000	1.89083000	5.56960000
○	4.64473000	0.00568000	6.22656000
○	6.19686000	1.90814000	6.90053000
○	2.41210000	5.67283000	5.56960000
○	4.66240000	3.78182000	6.26308000
○	6.16156000	5.67859000	6.97370000
○	2.41210000	9.45483000	5.56960000
○	4.57962000	7.56737000	6.68324000
○	6.16865000	9.45865000	6.96631000
○	2.41210000	13.23683000	5.56960000
○	4.66160000	11.35134000	6.26370000
○	6.21488000	13.22589000	6.86071000
○	6.12661000	0.00000000	9.08335000
○	6.89755000	0.00000000	11.42524000
○	8.33396000	1.89083000	9.96184000
○	6.12661000	3.78200000	9.08335000
○	6.89755000	3.78200000	11.42524000
○	8.33396000	5.67283000	9.96184000
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○	6.89755000	7.56400000	11.42524000
○	8.33396000	9.45483000	9.96184000
○	6.12661000	11.34600000	9.08335000
○	6.89755000	11.34600000	11.42524000
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○	1.00800000	7.56332000	6.99432000
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○	1.06979000	0.00372000	7.01212000
○	1.01189000	1.89083000	9.08285000
○	1.01189000	5.67283000	9.08285000
○	1.01189000	9.45483000	9.08285000
○	1.01189000	13.23683000	9.08285000
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○	7.70842000	7.56164000	5.46104000
○	7.74583000	11.24070000	5.43510000
○	1.78206000	1.89083000	11.42406000
○	1.78206000	5.67283000	11.42406000
○	1.78206000	9.45483000	11.42406000

O	1.78206000	13.23683000	11.42406000
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H	2.27715000	6.03163000	4.67901000
H	2.29082000	9.05091000	4.69651000
H	2.27311000	12.40928000	5.06835000
H	7.57378000	13.99468000	5.09777000
H	7.50425000	4.80935000	5.04031000
H	7.29831000	7.57295000	4.57116000
H	7.51573000	10.42375000	4.95163000
H	2.08223000	1.88621000	12.36300000
H	2.07546000	5.73692000	12.36666000
H	2.04430000	9.31526000	12.37225000
H	2.06611000	13.16352000	12.36570000
H	7.21624000	0.03353000	12.35812000
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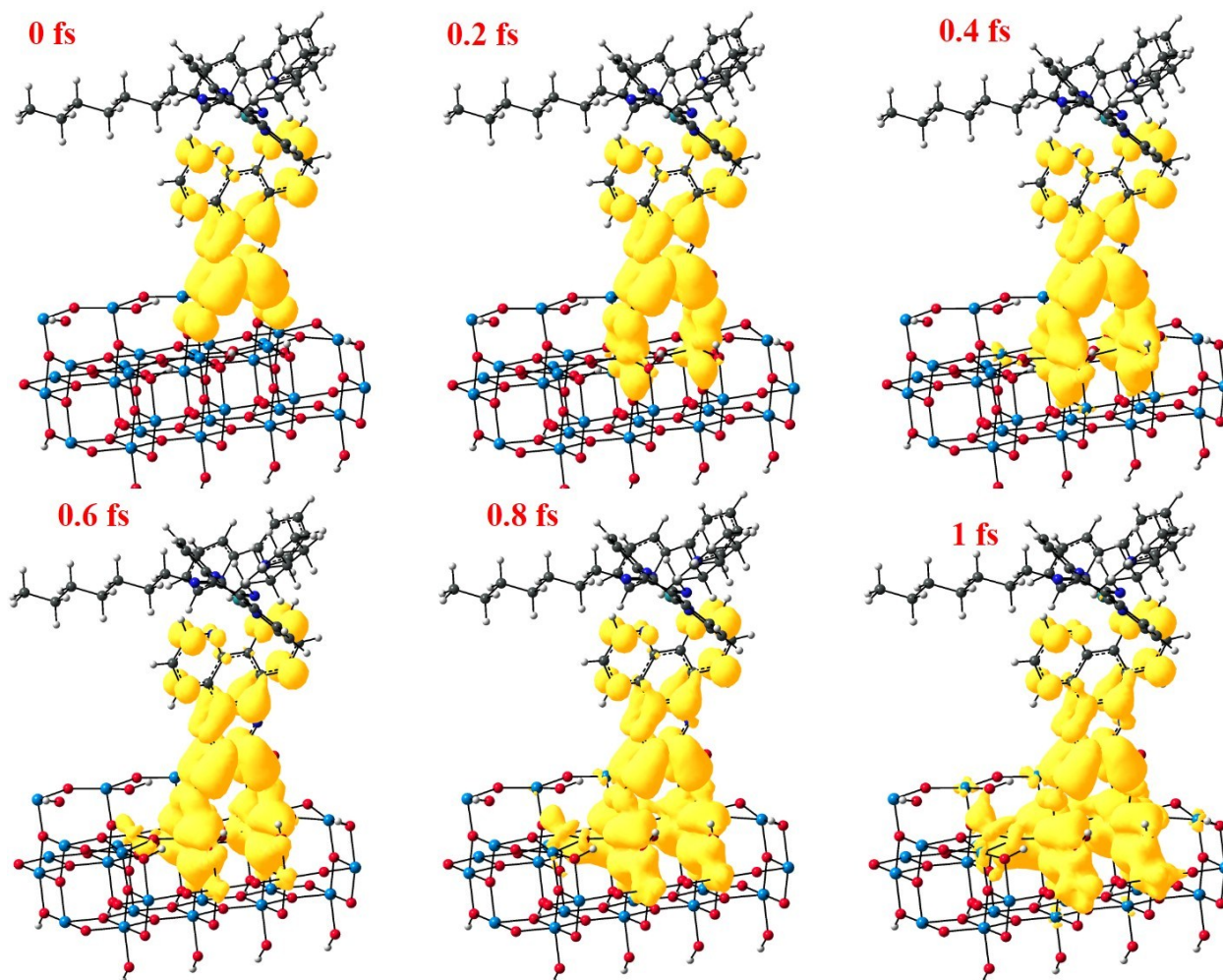


Fig. S4. Snapshots of the electronic charge distribution at 1 fs after initiating the IET from M101 attached to a pristine (101) surface. Only the local TiO₂ structure, next to photoexcited adsorbate is shown for detailed view of the time dependent charge distribution.

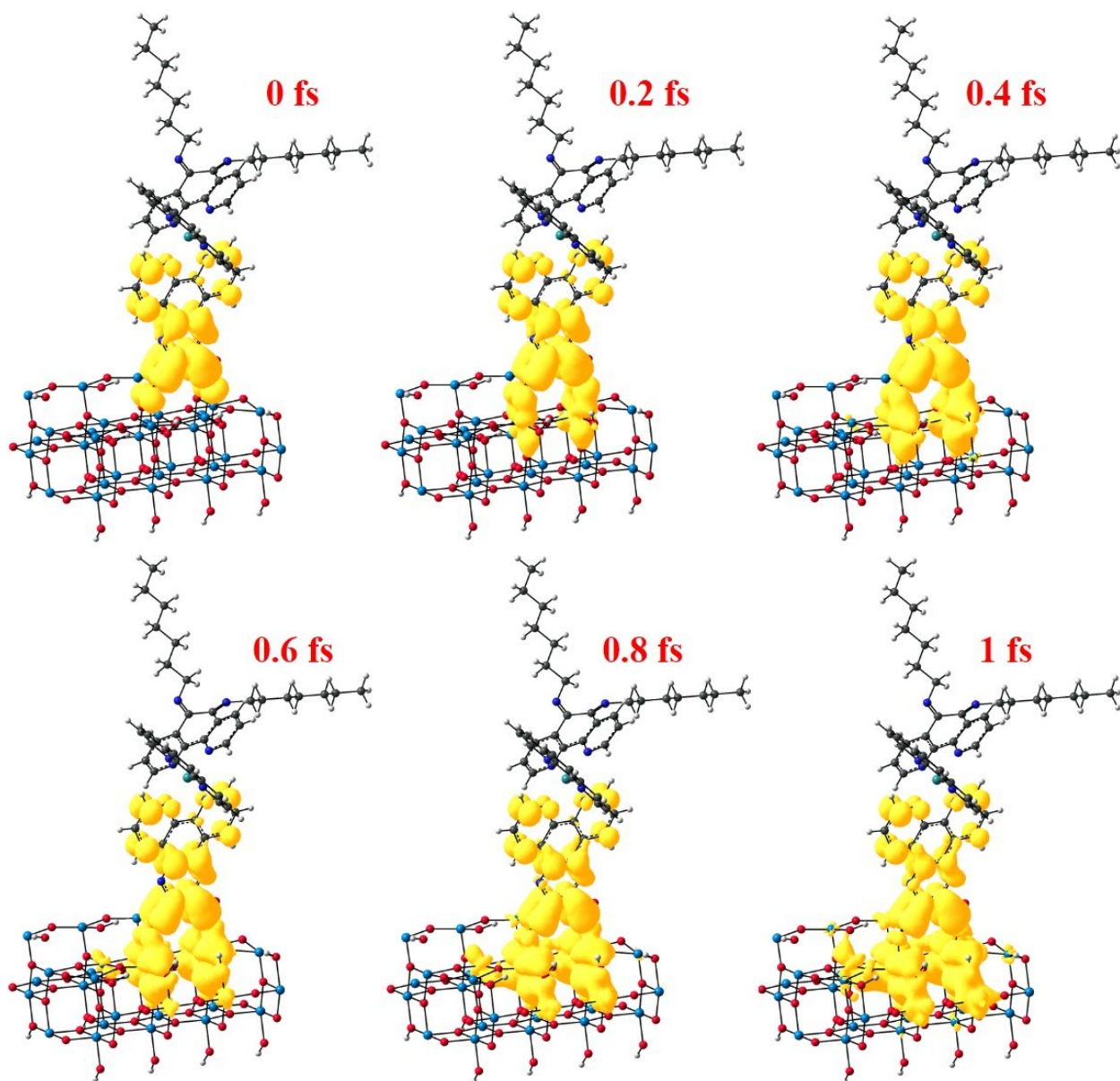


Fig. S5. Snapshots of the electronic charge distribution at 1 fs after initiating the IET from M103 attached to apristine (101) surface. Only the local TiO₂ structure, next to photoexcited adsorbate is shown for detailed view of the time dependent charge distribution.

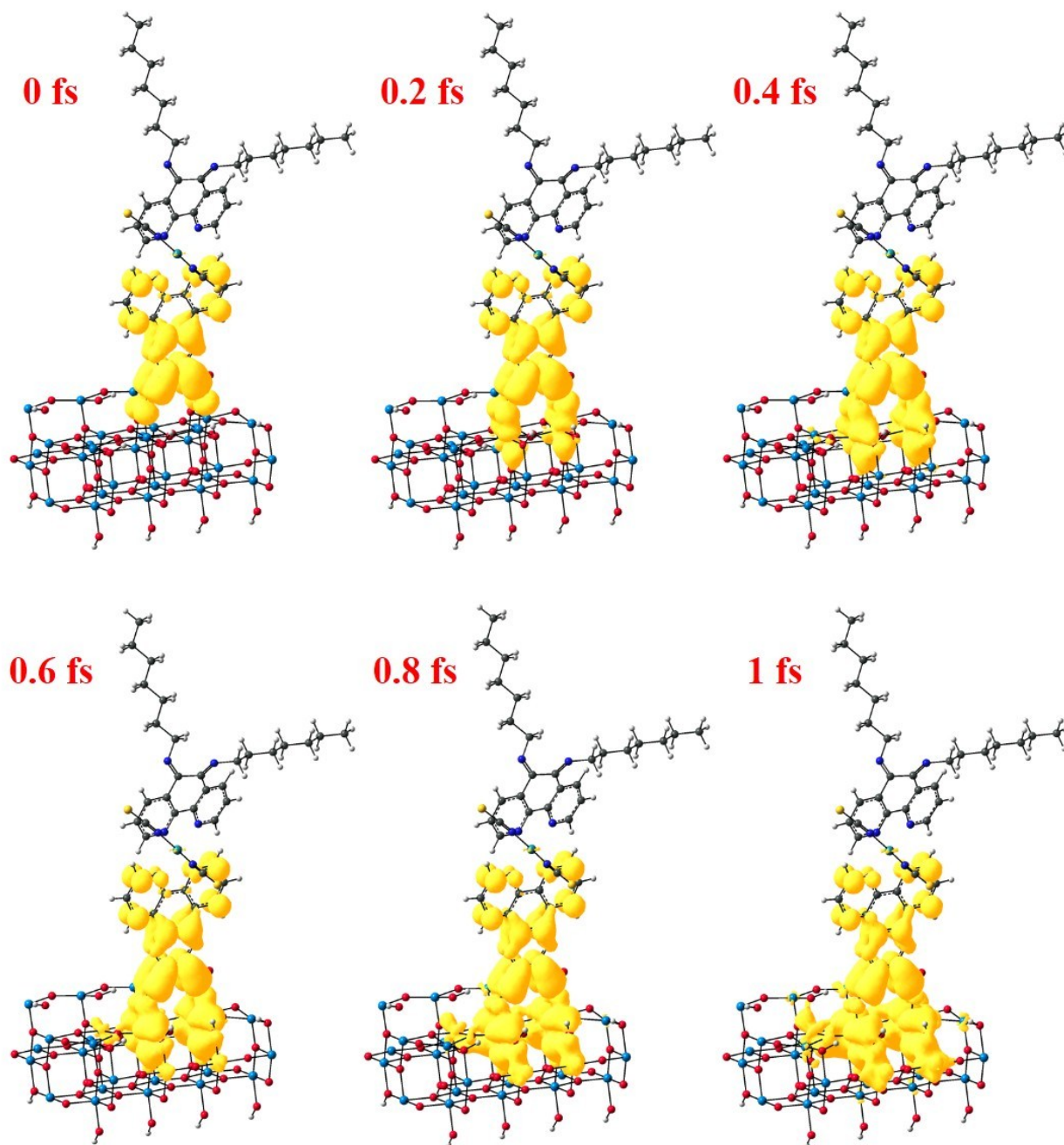


Fig. S6. Snapshots of the electronic charge distribution at 1 fs after initiating the IET from M104 attached to apristine (101) surface. Only the local TiO₂ structure, next to photoexcited adsorbate is shown for detailed view of the time dependent charge distribution.

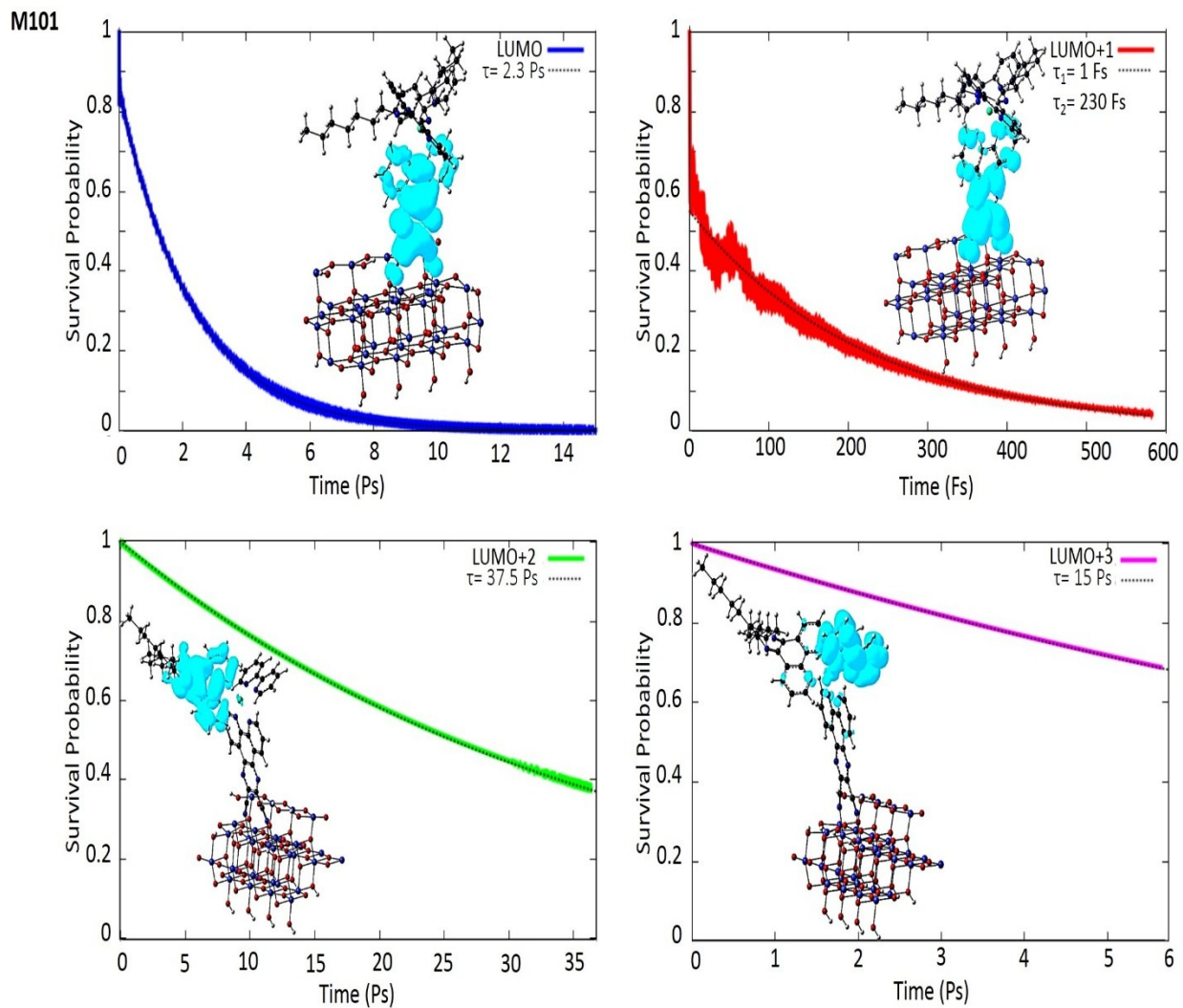


Fig. S7. Computed survival probabilities corresponding to photoexcited surface M101. Each curve represents the probability of the electron to remain in the respective photoexcited surface complex. Estimated life time of LUMO-LUMO+3 of M101 is obtained from the fitting of the survival probability with the bi-exponential decay model.

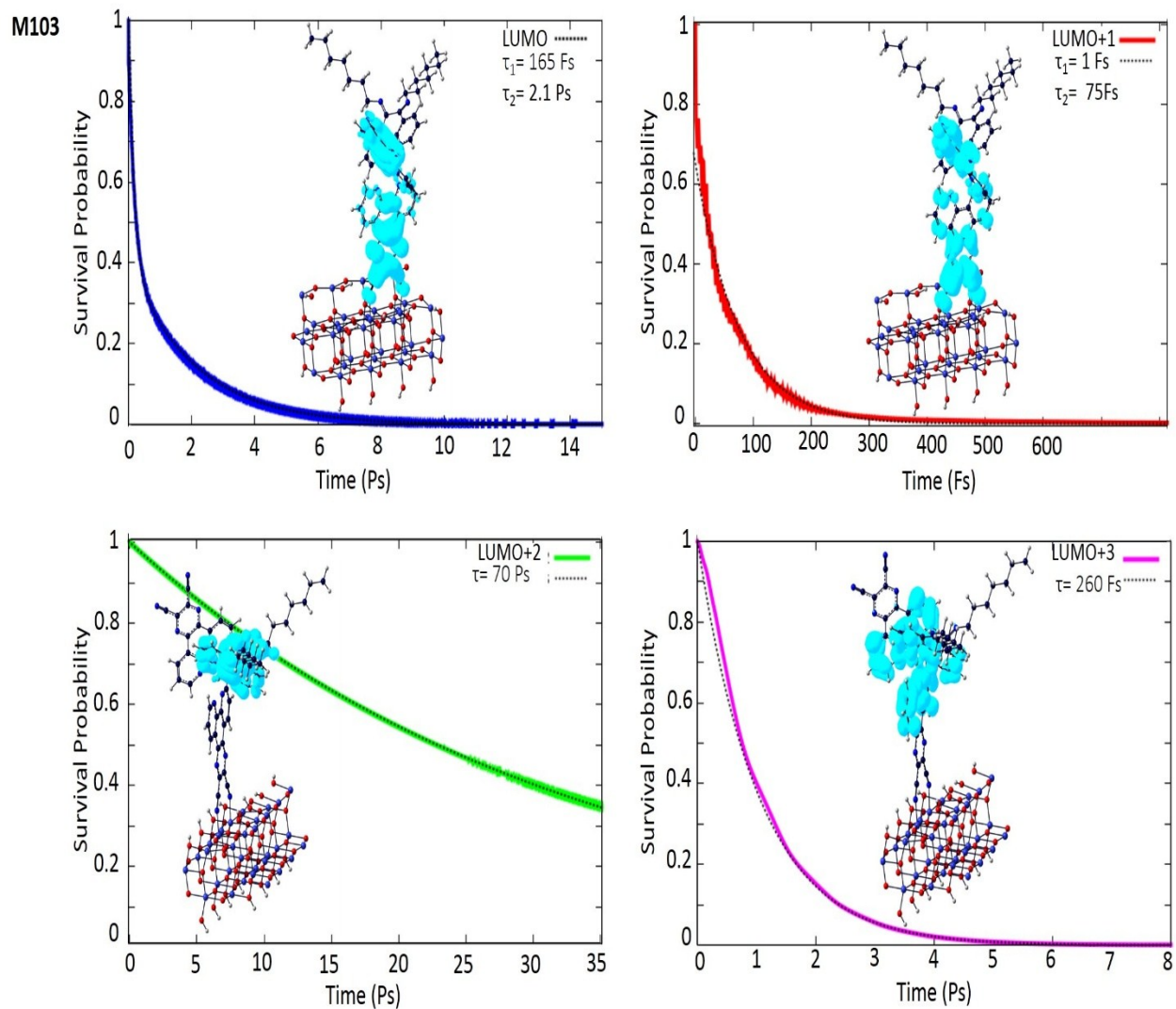


Fig. S8. Computed survival probabilities corresponding to photoexcited surface M103. Each curve represents the probability of the electron to remain in the respective photoexcited surface complex. Estimated life time of LUMO-LUMO+3 of M103 is obtained from the fitting of the survival probability with the bi-exponential decay model.

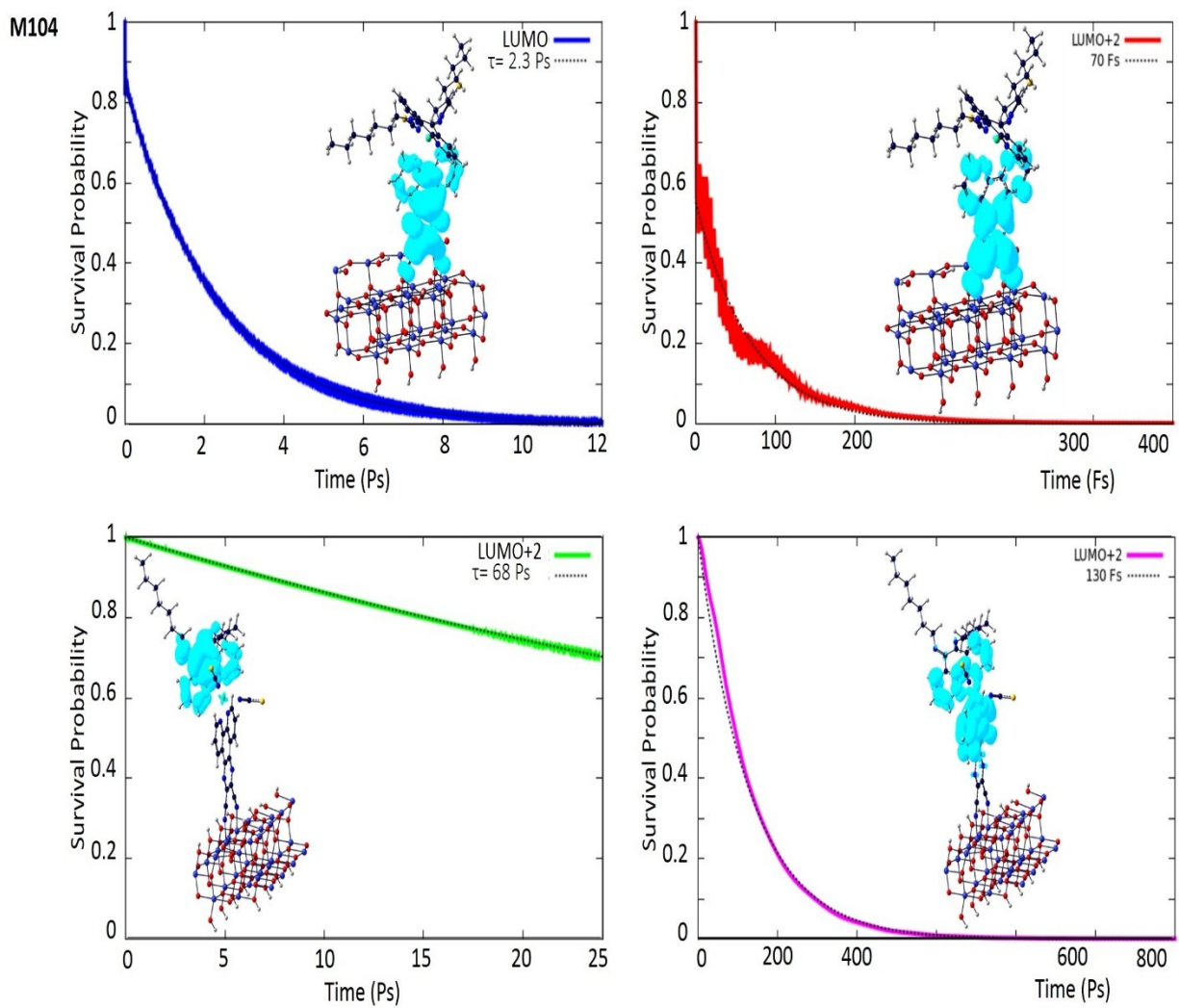


Fig. S9. Computed survival probabilities corresponding to photoexcited surface M104. Each curve represents the probability of the electron to remain in the respective photoexcited surface complex. Estimated life time of LUMO-LUMO+3 of M104 is obtained from the fitting of the survival probability with the bi-exponential decay model.