Supporting information for:

XFEL Radiation Damage Through the S-state Cycle of the Oxygen-Evolving Complex of Photosystem II

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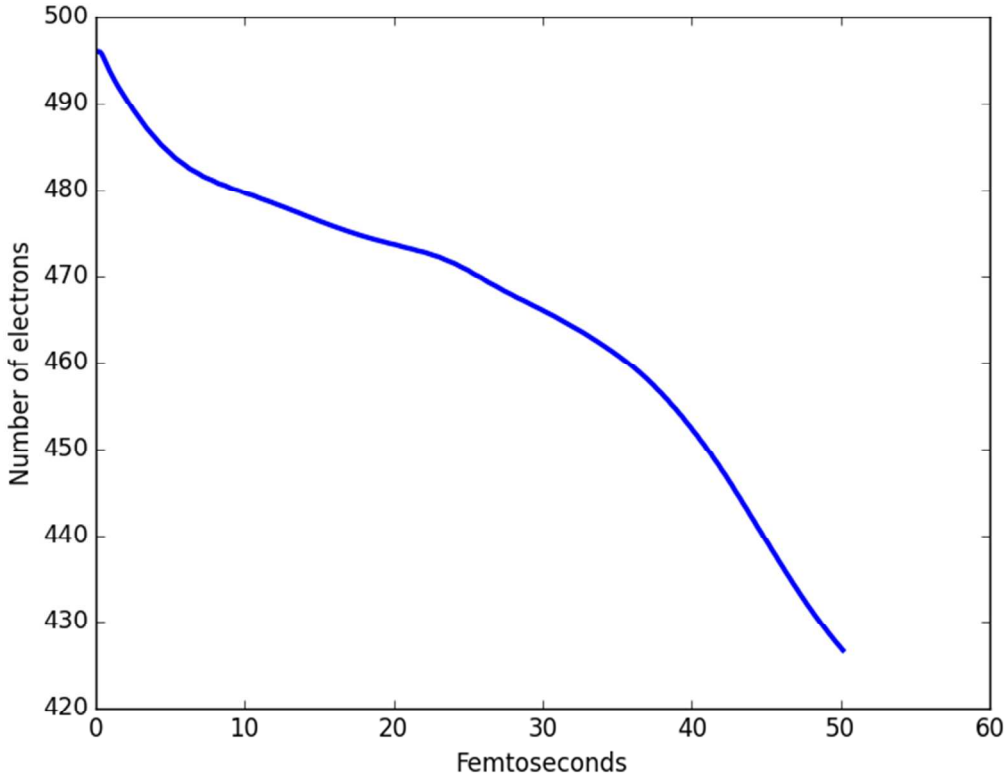

Figure SI1. The electron loss through pulse duration of 50 femtoseconds.

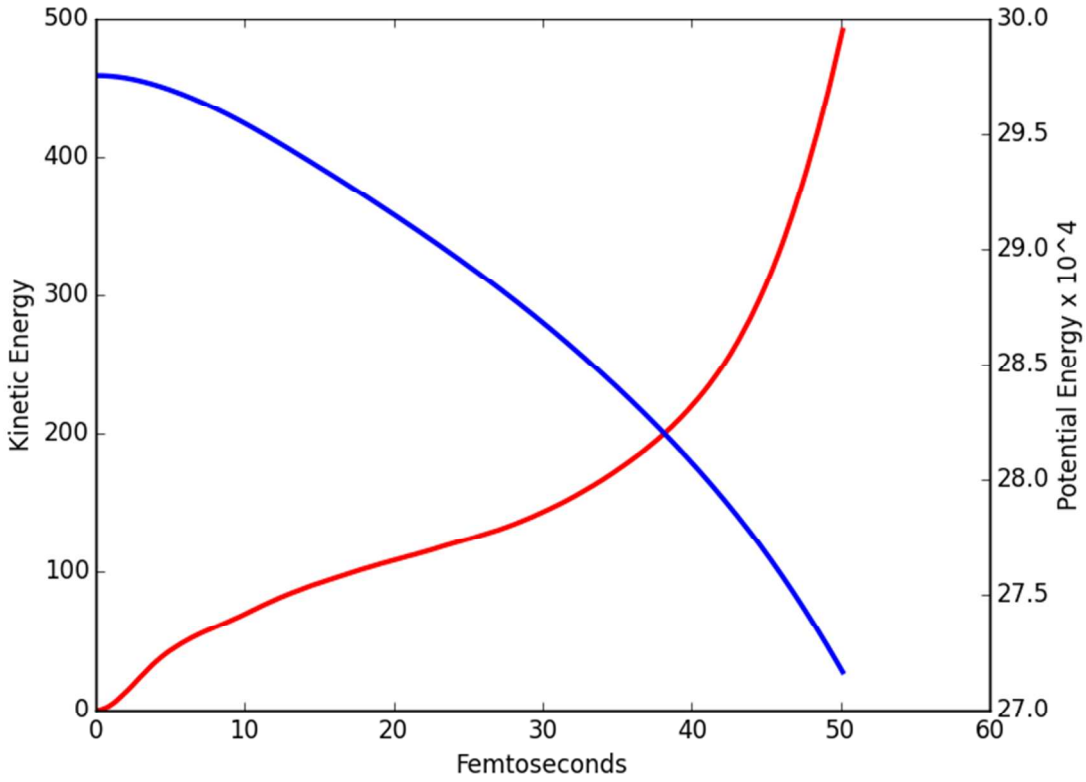

Figure SI2. The evolution of the kinetic and potential energy of the atoms in the S_1 structure.

The S_1 structure:

C	-6.189294	4.267072	0.466009
C	-4.779784	4.864185	0.593832
C	-4.108275	4.880466	-0.784289
O	-4.231630	3.851508	-1.505930
O	-3.491511	5.938477	-1.129663
H	-4.836554	5.871344	1.012315
H	-4.173965	4.226612	1.246711
C	-4.008691	-0.418863	-6.575470
C	-3.255603	-1.614968	-5.959998
C	-2.544709	-1.267098	-4.655943
O	-2.120802	-2.229609	-3.935253
O	-2.348607	-0.056718	-4.387688
H	-3.305050	0.328781	-6.875518
H	-3.939581	-2.456804	-5.812915
H	-2.467053	-1.965622	-6.637933
C	7.476440	-2.255067	-5.376144
C	5.964474	-2.094778	-5.223914

C	5.697463	-1.078669	-4.124410
C	4.239928	-0.799054	-3.842009
O	3.296854	-1.184006	-4.558252
O	4.097958	-0.097299	-2.773844
H	7.964861	-1.871917	-4.505067
H	5.521217	-1.770118	-6.166837
H	5.515875	-3.044353	-4.928631
H	6.154825	-1.459527	-3.206383
H	6.167651	-0.113982	-4.350357
C	4.405230	6.528547	-1.123255
C	4.449055	5.356830	-2.117881
C	4.227987	3.990698	-1.571878
C	3.257200	3.057475	-1.848975
N	5.045947	3.387500	-0.636455
C	4.581248	2.154555	-0.379738
N	3.488983	1.917189	-1.100171
H	4.586600	7.445377	-1.643989
H	3.658149	5.534005	-2.850970
H	5.405958	5.396872	-2.644305
H	5.866951	3.786112	-0.173759
H	2.416530	3.125724	-2.523315
H	5.052251	1.456481	0.289392
C	1.029416	6.494736	0.765266
C	0.402167	5.116478	0.564911
C	-0.253914	4.952886	-0.795698
C	-0.461457	3.526508	-1.242802
O	-0.243352	2.552937	-0.431581
O	-0.855419	3.401515	-2.429579
H	0.276278	7.186717	1.080712
H	1.174462	4.365716	0.677750
H	-0.369254	4.966677	1.311586
H	-1.234427	5.443798	-0.774926
H	0.336023	5.432491	-1.580737
C	1.446453	1.852395	6.542266
C	2.785438	1.684112	5.808038
C	2.663045	1.790438	4.323646
C	2.290363	0.867848	3.383566
N	2.881297	2.970195	3.630843
C	2.648783	2.783375	2.335362
N	2.286673	1.511444	2.160118
H	1.061990	0.890408	6.808113
H	3.485245	2.437401	6.177399
H	3.191262	0.698501	6.070592
H	3.108077	3.880920	4.059477
H	2.054356	-0.181854	3.479798

H	2.794975	3.520925	1.566198
H	1.997170	1.076147	1.259284
C	4.671284	-3.330752	2.606273
C	5.037374	-2.177053	1.677954
C	3.896002	-1.647839	0.847296
O	2.725013	-2.084187	1.059945
O	4.204965	-0.738543	0.011133
H	3.608365	-3.377906	2.714335
H	5.407640	-1.345262	2.285559
H	5.870965	-2.455429	1.030239
C	0.645337	-5.740660	-0.624233
C	0.423797	-4.268391	-0.914347
O	0.002850	-3.908888	-2.017637
C	-0.694314	-6.384058	-0.267184
O	0.679227	-3.500874	0.098116
H	1.052830	-6.218839	-1.489981
H	-1.155633	-5.856770	0.573741
H	-1.374417	-6.328340	-1.120393
H	-0.584334	-7.445377	-0.005192
C	-3.224186	-1.666384	4.512060
C	-1.929875	-1.788227	3.707864
C	-1.277584	-0.430802	3.404245
C	-0.671721	-0.442710	2.014085
O	0.182686	-1.375495	1.774801
O	-1.030500	0.455233	1.205155
H	-3.582723	-0.659589	4.460362
H	-2.470165	-1.764201	2.784484
H	-2.016425	0.371295	3.463076
H	-0.500076	-0.229115	4.150212
C	-7.356672	-4.688561	0.941255
C	-5.965752	-5.347760	1.063352
C	-5.025400	-5.026041	-0.101011
N	-4.740432	-3.605839	-0.173823
C	-3.938022	-3.057005	-1.108917
N	-3.165094	-3.826745	-1.875555
N	-3.911376	-1.729420	-1.243969
H	-7.821150	-5.002026	0.029718
H	-7.247883	-3.624109	0.938441
H	-5.491395	-5.054785	1.998066
H	-6.087108	-6.428277	1.067072
H	-4.104988	-5.593288	0.066446
H	-5.481654	-5.408671	-1.022037
H	-5.404173	-2.955989	0.241378
H	-3.260835	-4.839477	-1.875013
H	-2.702539	-3.398414	-2.680240

H	-4.572935	-1.141066	-0.742777
H	-3.155800	-1.266181	-1.738160
O	3.425663	-3.985468	-2.005072
H	4.403099	-3.881995	-1.999249
H	3.047629	-3.101603	-1.771125
O	1.736754	-3.405464	-4.232771
H	2.384413	-2.852033	-4.708274
H	2.285425	-3.833731	-3.542802
O	0.385485	-0.952474	-5.487407
H	1.249955	-0.888543	-5.940616
H	-0.193678	-0.362976	-6.012848
O	-0.729605	2.208657	-4.953019
H	-1.056326	1.779795	-5.769565
H	-0.876225	3.194160	-5.037474
O	-3.174331	2.625091	-3.573843
H	-3.543394	3.150628	-2.798529
H	-3.923860	2.217953	-4.104211
O	-0.838081	4.900952	-5.010157
H	-0.105731	4.932472	-4.369741
H	-1.619183	5.183965	-4.454677
O	-4.752688	1.146010	-1.228282
H	-3.797843	0.991050	-1.082603
H	-4.799859	2.116221	-1.095996
O	-3.576183	1.704370	1.420074
H	-2.693274	1.308414	1.429346
H	-3.960100	1.471788	2.280805
O	6.686712	0.022839	-1.169383
H	5.876097	-0.289667	-0.729748
H	6.348337	0.348914	-2.009571
O	1.070145	-3.791460	3.336657
H	1.530683	-3.209016	3.974554
H	0.693811	-3.150653	2.714424
O	1.994119	-1.646936	-1.569360
Ca	0.133369	-1.789487	-3.182877
Mn	2.779852	0.004949	-1.383709
O	-0.492795	-1.219009	-0.846389
Mn	1.005124	-1.647445	0.005046
O	1.421800	0.195091	-0.066032
Mn	-0.453905	0.634445	-0.815762
O	-2.073115	0.831619	-1.525894
Mn	-1.534178	1.529603	-3.144912
O	0.088328	0.722809	-2.527479
H	7.807403	-1.714556	-6.238278
H	7.715205	-3.291867	-5.492103
H	1.323817	-5.845509	0.196287

H	-3.035230	-1.926322	5.533109
H	-3.960831	-2.328013	4.105116
H	-1.519658	-2.723252	3.388483
H	-6.657212	4.643243	-0.419946
H	-6.121006	3.201189	0.407607
H	-6.772177	4.541072	1.321142
H	5.156892	6.389061	-0.374565
H	3.441478	6.566821	-0.659044
H	1.793377	6.434007	1.511927
H	1.458083	6.829252	-0.156855
H	1.596180	2.433419	7.428236
H	0.748759	2.350661	5.902522
H	5.028927	-4.249827	2.191098
H	5.120722	-3.174316	3.564717
H	-4.565144	-0.748139	-7.428236
H	-4.679016	-0.007629	-5.849174
O	2.829596	-0.973152	-7.215049
H	2.450744	-1.869437	-7.354979
H	3.269806	-1.030767	-6.336131
H	-7.964861	-4.982736	1.770994
O	-2.946200	5.958780	-3.680735
H	-3.109394	5.829130	-2.681890
H	-3.624354	5.400330	-4.091358

The S_2 structure:

Ca	1.053162	-1.669562	-3.187236
O	2.240750	-1.564447	-1.091593
O	-0.363992	-1.098739	-0.834446
O	1.383910	0.318740	0.270627
O	-1.690903	1.171967	-1.760277
O	0.571113	0.870418	-2.331595
Mn	2.952130	0.108330	-0.754906
Mn	0.990537	-1.516904	0.265208
Mn	-0.299599	0.692131	-0.709010
Mn	-0.775734	1.804672	-3.127000
C	-5.917270	4.645815	-0.333428
C	-4.506675	5.138097	0.013414
C	-3.590357	5.047908	-1.210867
O	-3.606924	3.973776	-1.893557
O	-2.870659	6.052986	-1.475694
H	-5.873101	4.017374	-1.198304
H	-4.552170	6.164457	0.383183
H	-4.081423	4.494823	0.787872
C	-2.851966	-0.022023	-6.764711

C	-2.161311	-1.129984	-5.948278
C	-1.626782	-0.677585	-4.594488
O	-1.348308	-1.534018	-3.725849
O	-1.422662	0.584276	-4.467044
H	-2.133004	0.723156	-7.034346
H	-2.841499	-1.976768	-5.812935
H	-1.279682	-1.508319	-6.480614
C	7.887768	-2.585420	-4.015484
C	6.382418	-2.311214	-4.118354
C	6.034179	-1.238761	-3.097038
C	4.583284	-0.841074	-2.982135
O	3.666229	-1.224819	-3.738137
O	4.403240	-0.046099	-1.985498
H	8.083466	-3.180362	-3.147932
H	6.123296	-1.989178	-5.126728
H	5.820508	-3.214153	-3.875443
H	6.336519	-1.623106	-2.117452
H	6.603242	-0.320069	-3.275352
C	4.962324	6.474570	-0.403367
C	5.080101	5.267858	-1.352520
C	4.663376	3.944544	-0.818179
C	3.669881	3.080224	-1.210367
N	5.278886	3.317378	0.246842
C	4.685387	2.138855	0.470759
N	3.689007	1.961240	-0.394562
H	4.269661	7.181683	-0.809703
H	4.440858	5.472664	-2.213767
H	6.110694	5.216407	-1.708884
H	6.054715	3.672218	0.814839
H	2.953407	3.185629	-2.011699
H	5.001485	1.430765	1.216947
C	1.376025	6.449917	1.013875
C	0.936268	5.019657	0.703547
C	0.094822	4.967534	-0.559276
C	-0.112539	3.553266	-1.006769
O	-0.102967	2.606747	-0.178741
O	-0.298637	3.414743	-2.268089
H	0.514495	7.053207	1.210615
H	1.814827	4.394489	0.556932
H	0.350034	4.599820	1.514569
H	-0.881214	5.428531	-0.362792
H	0.566122	5.521917	-1.373445
C	0.068743	2.254083	6.664356
C	1.530525	1.875868	6.328780
C	1.840067	1.868787	4.873021

C	1.707007	0.887592	3.928511
N	2.240245	3.001152	4.192329
C	2.321375	2.749302	2.896666
N	2.007012	1.463897	2.709180
H	-0.590156	1.791416	5.959592
H	2.196950	2.566883	6.854748
H	1.726410	0.873438	6.733750
H	2.395497	3.924532	4.624395
H	1.434428	-0.151869	4.024863
H	2.671209	3.441964	2.152852
H	1.877355	1.023084	1.788995
C	3.958680	-3.439250	3.361194
C	4.582530	-2.312477	2.536624
C	3.634579	-1.643145	1.581454
O	2.412292	-1.997712	1.593758
O	4.101058	-0.711387	0.850291
H	3.014117	-3.117634	3.747540
H	4.944900	-1.540078	3.225311
H	5.478030	-2.663616	2.019187
C	0.421070	-5.581760	-0.464938
C	0.424184	-4.092854	-0.787189
O	0.260426	-3.684010	-1.945225
C	-1.009449	-6.130604	-0.432695
O	0.595693	-3.352654	0.263228
H	0.981471	-6.104364	-1.211755
H	-1.641625	-5.546470	0.241595
H	-1.445695	-6.089199	-1.433148
H	-1.034346	-7.181683	-0.114547
C	-3.901447	-1.299979	4.216474
C	-2.517004	-1.538142	3.603810
C	-1.789364	-0.228229	3.265315
C	-1.013971	-0.323290	1.969030
O	-0.152321	-1.264190	1.865461
O	-1.243260	0.552494	1.078677
H	-4.169686	-0.270456	4.102316
H	-1.911357	-2.148353	4.274063
H	-2.659639	-2.096277	2.676828
H	-2.493620	0.600004	3.191675
H	-1.088388	0.017089	4.068972
C	-7.700524	-4.113240	0.118011
C	-6.347223	-4.779430	0.444305
C	-5.243357	-4.549590	-0.600227
N	-4.891927	-3.147591	-0.748361
C	-3.771993	-2.697844	-1.342605
N	-2.832326	-3.576687	-1.744731

N	-3.552558	-1.393770	-1.482677
H	-8.047892	-4.458580	-0.833291
H	-7.577116	-3.050792	0.088429
H	-5.992429	-4.447350	1.415520
H	-6.500360	-5.853866	0.498465
H	-4.370681	-5.116929	-0.267261
H	-5.580322	-4.994291	-1.543414
H	-5.605173	-2.442851	-0.569671
H	-3.120896	-4.521162	-2.000936
H	-2.029660	-3.219041	-2.253485
H	-4.212456	-0.658291	-1.230822
H	-2.684322	-1.076509	-1.902709
O	3.609486	-4.001338	-1.488985
H	4.553479	-4.061121	-1.205146
H	3.272067	-3.125516	-1.189536
O	2.332424	-3.690146	-3.917213
H	2.963686	-3.596846	-4.649165
H	2.898343	-3.924791	-3.143455
O	1.178064	-0.848816	-5.468917
H	2.069106	-0.905251	-5.887687
H	0.748215	-0.095982	-5.930308
O	0.475192	2.512655	-4.627068
H	0.208606	2.258488	-5.533206
H	0.619701	3.510512	-4.581995
O	-2.227083	3.031591	-3.813926
H	-2.722879	3.488866	-3.030268
H	-2.922525	2.598375	-4.408402
O	-4.506614	1.398716	-1.276378
H	-4.216376	1.538196	-0.330773
H	-4.172862	2.237421	-1.658585
O	-3.668105	2.010080	1.070771
H	-2.768596	1.733260	1.308339
H	-4.168568	1.935025	1.906861
O	6.736110	-0.336437	0.019098
H	5.855526	-0.500825	0.399842
H	6.524669	0.098262	-0.812235
O	0.307995	-3.697600	3.731378
H	0.741897	-3.184013	4.445069
H	0.089107	-3.009003	3.088070
O	3.771137	-1.239946	-6.465848
H	3.430435	-2.132537	-6.694194
H	3.984986	-1.278874	-5.502210
H	-6.548721	5.485828	-0.534794
H	-6.314064	4.090813	0.490845
H	-3.277259	-0.444525	-7.651005

H	-3.625551	0.425192	-6.176098
H	0.878430	-5.735820	0.490043
H	8.215297	-3.109734	-4.888822
H	8.414850	-1.657481	-3.937924
H	4.614471	6.143602	0.552854
H	5.920996	6.936973	-0.293682
H	2.014113	6.448449	1.872794
H	1.907377	6.849534	0.175501
H	-0.045104	3.316846	6.614610
H	-0.169728	1.915624	7.651005
H	-3.878830	-1.549426	5.256745
H	-4.622409	-1.913774	3.718107
H	4.609416	-3.689671	4.172817
H	3.816017	-4.298817	2.740153
H	-8.414850	-4.368457	0.872665
O	-1.693562	6.016577	-3.815342
H	-2.112044	5.929533	-2.895155
H	-2.078334	5.277973	-4.316310
O	0.776369	5.165276	-4.527400
H	1.435806	5.604280	-3.944065
H	-0.102871	5.470461	-4.171310

The S_3 structure:

Ca	-1.201779	-1.541250	3.194518
O	-1.976277	-1.593321	0.895910
O	0.718253	-1.038095	0.743437
O	-1.074900	0.397987	-0.245975
O	2.220411	1.195668	1.570184
O	-2.338645	0.669762	2.274225
Mn	-2.719079	0.071966	0.645655
Mn	-0.629352	-1.466112	-0.347528
Mn	0.718033	0.759398	0.638647
Mn	1.473529	1.834047	3.056825
O	0.079633	2.367622	4.645497
H	0.618307	2.963586	5.268847
H	-0.592507	2.985356	4.276409
C	6.436094	4.416823	0.279720
C	5.094167	5.042868	-0.129164
C	4.165918	5.069474	1.075919
O	4.014559	3.856855	1.585854
O	3.641460	6.082239	1.527578
H	6.364054	3.350715	0.223834
H	5.248179	6.051604	-0.511491
H	4.631185	4.409884	-0.889394
C	3.028406	-0.179218	6.740437

C	2.290040	-1.224343	5.881431
C	1.817194	-0.722884	4.515336
O	1.179884	-1.497444	3.778177
O	2.128579	0.496649	4.234527
H	2.362696	0.625346	6.973694
H	2.924228	-2.107324	5.744289
H	1.378295	-1.563283	6.387422
C	-8.059847	-2.231058	3.714009
C	-6.551178	-2.008470	3.775872
C	-6.145467	-0.838782	2.893962
C	-4.666384	-0.866362	2.583193
O	-3.817681	-1.207484	3.427471
O	-4.406452	-0.518481	1.362737
H	-8.440528	-1.840611	2.793394
H	-6.236316	-1.822728	4.802379
H	-6.048778	-2.904651	3.408567
H	-6.719185	-0.900986	1.971526
H	-6.372706	0.112281	3.386016
C	-4.360533	6.579664	0.068149
C	-4.583726	5.384379	1.013698
C	-4.273177	4.020683	0.501173
C	-3.433810	3.059892	1.006542
N	-4.855016	3.433948	-0.606388
C	-4.383219	2.183552	-0.746129
N	-3.511176	1.921206	0.222610
H	-3.943383	5.538793	1.885910
H	-5.618958	5.423198	1.360352
H	-5.538584	3.851111	-1.243913
H	-2.800291	3.115461	1.877299
H	-4.700297	1.490027	-1.506746
C	-0.728464	6.509291	-1.238512
C	-0.262995	5.099503	-0.868873
C	0.464912	5.054714	0.466975
C	0.664452	3.640882	0.950370
O	0.542991	2.680407	0.146982
O	0.971726	3.525177	2.192156
H	0.123547	7.126727	-1.432804
H	-1.133605	4.452269	-0.794012
H	0.402021	4.704423	-1.629884
H	1.440007	5.541853	0.360915
H	-0.098414	5.600370	1.228298
C	0.558263	2.091185	-6.790087
C	-0.916126	1.778311	-6.448304
C	-1.236572	1.821482	-4.993800

C	-1.229892	0.855682	-4.024992
N	-1.541213	3.004595	-4.348425
C	-1.698050	2.791718	-3.050927
N	-1.515457	1.487783	-2.825328
H	1.076543	1.179345	-7.001823
H	-1.553574	2.483438	-6.990620
H	-1.153656	0.778469	-6.832275
H	-1.553499	3.927935	-4.799645
H	-1.052444	-0.206151	-4.092455
H	-2.022759	3.526196	-2.337288
H	-1.491922	1.067288	-1.886444
C	-3.721875	-3.147216	-3.621937
C	-4.178077	-1.941836	-2.801798
C	-3.161716	-1.462824	-1.800973
O	-2.018610	-1.999024	-1.745269
O	-3.520350	-0.470039	-1.083789
H	-2.660302	-3.253247	-3.539950
H	-4.377064	-1.111033	-3.488084
H	-5.127797	-2.137016	-2.295650
C	-0.389127	-5.501196	0.464133
C	-0.263875	-4.015405	0.767471
O	-0.208093	-3.577957	1.923283
C	0.982372	-6.174093	0.320730
O	-0.227930	-3.291893	-0.316765
H	-0.927347	-5.974301	1.258734
H	1.611908	-5.639626	-0.395617
H	1.498167	-6.196029	1.283790
H	0.882219	-7.217014	-0.007198
C	4.270215	-1.565463	-4.193578
C	2.876925	-1.698789	-3.571305
C	2.217227	-0.335866	-3.319922
C	1.387132	-0.322732	-2.056552
O	0.483341	-1.222699	-1.944717
O	1.597950	0.587207	-1.199215
H	4.964783	-1.241417	-3.446938
H	2.242525	-2.318505	-4.204212
H	2.995207	-2.201975	-2.609050
H	2.966512	0.452008	-3.257699
H	1.561131	-0.094507	-4.162299
C	7.808935	-4.538301	0.018538
C	6.435247	-5.140538	-0.342784
C	5.320815	-4.865542	0.678429
N	5.014569	-3.450652	0.812552
C	3.861746	-2.965856	1.305486
N	2.884261	-3.817975	1.678035

N	3.650056	-1.657453	1.384988
H	8.118139	-4.903964	0.975400
H	7.733053	-3.471516	0.051891
H	6.116675	-4.790410	-1.319533
H	6.539786	-6.221653	-0.395467
H	4.435620	-5.401260	0.329091
H	5.619515	-5.318206	1.630352
H	5.751841	-2.764935	0.649780
H	3.141704	-4.754139	1.990820
H	2.044700	-3.436133	2.105502
H	4.325021	-0.919476	1.132569
H	2.726851	-1.336837	1.661720
O	-3.421018	-3.980684	1.115600
H	-4.386764	-3.957993	0.909059
H	-3.071608	-3.080822	0.917556
O	-2.464006	-3.641675	3.744820
H	-3.216098	-3.725499	4.361855
H	-2.850174	-3.902936	2.876559
O	-1.152205	-0.215595	5.248179
H	-2.002617	-0.203310	5.742274
H	-0.788697	0.695761	5.267066
O	0.054716	0.993316	2.294741
H	-1.447331	1.118804	2.277698
O	2.816093	2.932820	3.744798
H	3.472358	3.806074	2.423241
H	3.463078	2.436371	4.323660
O	-1.056101	4.746266	3.740150
H	-1.483696	5.583271	3.422789
H	-0.197017	4.716355	3.285249
O	1.654817	4.147608	5.759655
H	2.202779	3.916387	4.963692
H	2.179442	3.771025	6.521267
O	4.819890	0.900359	1.232579
H	3.977259	1.173154	1.641334
H	4.676319	1.272906	0.317492
O	4.070703	1.798555	-1.102908
H	3.156464	1.563094	-1.336614
H	4.565470	1.684033	-1.936093
O	-3.713550	-0.923401	6.196412
H	-3.283158	-1.777939	6.422297
H	-3.959028	-1.007945	5.244536
O	-6.453479	-0.056584	-0.287348
H	-5.619738	-0.263369	0.178030
H	-6.719080	0.773214	0.109979
O	-0.098888	-3.747016	-3.809790

H	-0.445896	-3.192476	-4.539242
H	0.178177	-3.085328	-3.161900
H	-8.528322	-1.729579	4.534954
H	-8.268362	-3.279033	3.770311
H	8.528322	-4.821747	-0.721084
H	-3.499897	7.130171	0.386186
H	-4.206936	6.222126	-0.928583
H	-5.219723	7.217014	0.090008
H	-1.343093	6.464090	-2.113205
H	-1.291377	6.923007	-0.428038
H	4.579860	-2.513443	-4.581333
H	4.239283	-0.848394	-4.987149
H	0.597752	2.731084	-7.646749
H	1.021269	2.579741	-5.958320
H	7.204929	4.757521	-0.381882
H	6.673988	4.706176	1.282008
H	3.366202	-0.636811	7.646749
H	3.868932	0.199396	6.197237
H	-4.198215	-4.031111	-3.252167
H	-3.987570	-3.001570	-4.648140
H	-0.934546	-5.625243	-0.448024

Input file for AIMD calculations:

```
CalculationMode = td
Units = eV_angstrom
FromScratch = yes
%Species
  'Mn' | 55 | spec_ps_psf | 25 | 3 | 0 | 0.2 | 5
  'Ca' | 41 | spec_ps_psf | 20 | 3 | 0 | 0.2 | 5
%
XYZCoordinates = 'S1.xyz'
ExcessCharge = 2
BoxShape = minimum
Spacing = 0.14
Extrastates =10
SmearingFunction = fermi_dirac
Smearing = 0.005
TypeOfMixing = linear
Mixing = 0.005
LCAOStart = lcao_states
PoissonSolver = isf
EigenSolver = rmmdiis
EigensolverTolerance = 1e-12
```

```
MaximumIter = -1
spinComponents = spin_polarized
ConvRelDens = 1e-5
T  = 33
dt = 0.0013
AbsorbingBoundaries=mask
TDPropagator = aetrs
TDMaximumIter = T/dt
TDTimeStep = dt
MoveIons=Yes
amplitude = 10.0
omega = 5000
tau0 = 7
t0 = 25
TDDynamics=ehrenfest

%TDExternalFields
 electric_field | 1 | 0 | 0 | omega | "envelope_cos"
 electric_field | 1 | 0 | 0 | omega+20 | "envelope_cos1"
 electric_field | 1 | 0 | 0 | omega+10 | "envelope_cos2"
 electric_field | 1 | 0 | 0 | omega-10 | "envelope_cos3"
 electric_field | 1 | 0 | 0 | omega-20 | "envelope_cos4"
%

%TDFunctions
 "envelope_cos" | tdf_gaussian | amplitude | tau0 | t0
 "envelope_cos1" | tdf_gaussian | 1.5*amplitude | 3 | 1
 "envelope_cos2" | tdf_gaussian | 0.8*amplitude | 4 | 9
 "envelope_cos3" | tdf_gaussian | 0.3*amplitude | 2 | 16
 "envelope_cos4" | tdf_gaussian | 1.3*amplitude | 5 | 30
%

Output = density+potential
OutputHow = cube + dx

OutputInterval = 100
```