Supporting Information for "Time Resolved Photoelectron spectroscopy of Thioflavin T Photoisomerization; A Simulation Study"

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Table of contents

optimized xyz coordinates of the ground S_0 state Page 1
optimized xyz coordinates of the ground S_1 state Page 2
Fig S1 Page 3
Computational methods Page 4
References Page 4

39
ground S0 State

C	2.541677	0.690245	0.119208
C	2.754793	-0.669775	-0.122697
C	4.039637	-1.198595	-0.236322
C	5.133118	-0.343526	-0.110614
C	4.904665	1.027701	0.126970
C	3.629009	1.558811	0.244338
C	0.348054	-0.024342	0.035456
H	4.184337	-2.255736	-0.421994
H	5.755671	1.692953	0.219691
H	3.489599	2.616977	0.420052
C	-1.093809	-0.005679	0.039066
C	-1.810870	-1.118557	0.534215
C	-1.843919	1.056834	-0.513684
C	-3.186892	-1.159289	0.515040
H	-1.275329	-1.951852	0.974302
C	-3.220539	1.019801	-0.555185
H	-1.343037	1.903680	-0.964155
C	-3.946508	-0.085432	-0.029048
H	-3.683729	-2.023704	0.930673
H	-3.743531	1.847186	-1.012067
C	6.542958	-0.865743	-0.228729
H	6.555298	-1.940248	-0.415505
H	7.074595	-0.371101	-1.046685
H	7.107725	-0.672413	0.687853
N	1.179606	1.010992	0.227738
S	1.218676	-1.499630	-0.273139
C	0.760193	2.355072	0.656875
H	-0.239751	2.301262	1.075413
H	1.449324	2.698391	1.426126
H	0.777004	3.045811	-0.186389
N	-5.304319	-0.117154	-0.050574
C	-6.027691	-1.275190	0.471831
H	-7.095312	-1.098897	0.369673
H	-5.776315	-2.186646	-0.079651
H	-5.808393	-1.436354	1.531682
C	-6.063585	0.992707	-0.624056
H	-7.125129	0.781264	-0.525281
H	-5.852269	1.931029	-0.102550
H	-5.838314	1.125351	-1.687115

39
first excited state S1

C	-2.526394	0.702090	-0.012487
C	-2.790482	-0.678589	0.010371
C	-4.089010	-1.170325	0.019342
C	-5.171289	-0.277297	0.005152
C	-4.900575	1.097331	-0.017567
C	-3.600066	1.601597	-0.026511
C	-0.347962	-0.115855	0.000648
H	-4.266811	-2.239823	0.037174
H	-5.728628	1.798529	-0.028557
H	-3.428908	2.670402	-0.043885
C	1.123366	-0.089182	0.000201
C	1.851887	-0.123429	-1.211547
C	1.850837	-0.056080	1.212601
C	3.226041	-0.114997	-1.226231
H	1.309460	-0.158228	-2.147888
C	3.224924	-0.043859	1.227907
H	1.307607	-0.039655	2.148982
C	3.955819	-0.069903	0.000923
H	3.745490	-0.146158	-2.171888
H	3.743585	-0.018842	2.174169
C	-6.594837	-0.784732	0.014763
H	-6.625984	-1.875955	0.026254
H	-7.139506	-0.425394	0.893289
H	-7.144849	-0.443639	-0.867626
N	-1.179374	1.010402	-0.017837
S	-1.280173	-1.615383	0.024922
C	-0.696776	2.383341	-0.037019
H	0.390422	2.387818	-0.039883
H	-1.048556	2.901355	-0.933276
H	-1.044180	2.924954	0.847019
N	5.308851	-0.066496	0.001695
C	6.069848	-0.132479	-1.251945
H	7.125602	-0.030648	-1.026790
H	5.901022	-1.092969	-1.743189
H	5.770476	0.674509	-1.920324
C	6.068019	-0.047338	1.258060
H	7.122376	0.059483	1.028629
H	5.753899	0.791786	1.878236
H	5.913810	-0.980517	1.803834

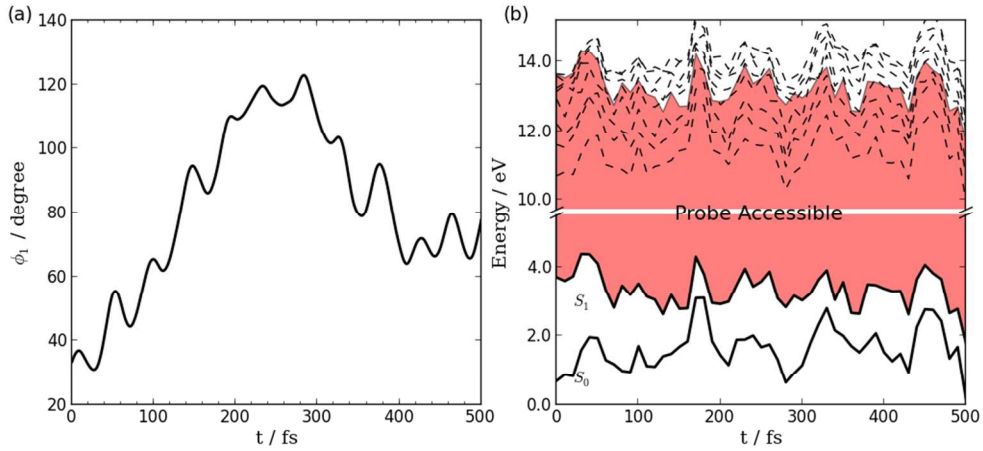

Fig S1: Time evolution of (a) ϕ_1 and (b) energy levels for the trajectory used in Fig. 5. N-electron states (S_0 and S_1, solid) and (N-1)-electron states (D_n, dashed) are presented. The accessible region by the 125 nm probe is shaded.

Computational Methods

The geometry of the ground and first excited state of ThT are optimized on the (TD)DFT/B3LYP level with the 6-311++G(d,p) basis set implemented in the Gaussian 09 package.[1] The conductor-like polarizable continuum model (CPCM)[2] is used to perform the self-consistent reaction field (SCRF) calculation to simulate the aqueous environment.

References:

[1] Gaussian 09, Revision **C.01**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

[2] Barone, V. and Cossi, M "Quantum calculation of molecular energies and energy gradients in solution by a conductor solvent model," *J. Phys. Chem. A*, **102** (1998) 1995-2001.