SUPPLEMENTARY INFORMATIONS

Quantum Chemical Calculations.

Optimized geometries used for unperturbed calculations

B3LYP/cc-PVTZ
C,0,1.2315247763,1.4226542904,0.
C,0,1.2060718638,2.8206298206,0.
C,0,0.0009050836,3.5084676776,0.
C,0,-1.204579259,2.8212472642,0.
C,0,-1.2303775314,1.423198284,0.
C,0,0.0004284167,0.7102938126,0.
H,0,2.1414789107,3.3653726165,0.
H,0,0.0013552949,4.5902039156,0.
H,0,-2.139858073,3.3661571805,0.
C,0,-2.4538198993,0.6780099953,0.
C,0,-0.0005497289,-0.7104039736,0.
C,0,2.4543151822,0.6767621815,0.
C,0,1.2308449238,-1.4235581654,0.
C,0,-1.2311375575,-1.4220794016,0.
C,0,1.2046987812,-2.821245291,0.
C,0,2.4536037936,-0.6781714335,0.
H,0,3.3886741317,-1.2239049332,0.
H,0,3.3894614239,1.2221385196,0.
C,0,-0.0014232705,-3.5084323836,0.
H,0,2.139744386,-3.3665337175,0.
H,0,-0.0018104265,-4.5901511541,0.
C,0,-1.2061614426,-2.8205945781,0.
H,0,-2.141573997,-3.365360371,0.
C,0,-2.4543606719,-0.6768410646,0.
H,0,-3.3893041911,-1.2225816572,0.
H,0,-3.3880682196,1.2250373917,0.

PBEPBE/6-31+G(d)
C,0,1.2436202641,1.4363087426,0.
C,0,1.218290747,2.8490025256,0.
C,0,0.0008970791,3.5449635995,0.
C,0,-1.2168169418,2.8495902102,0.
C,0,-1.242421368,1.4368439233,0.
C,0,0.0004582944,0.7162339699,0.
H,0,2.1665313013,3.3996619473,0.
H,0,0.0013425218,4.6405699503,0.
H,0,-2.1649538089,3.4003824948,0.
C,0,-2.4739596408,0.6870809949,0.
C,0,-0.0005320424,-0.7163884466,0.
C,0,2.4744941328,0.6858814848,0.
C,0,1.2429075051,-1.4372194248,0.
C,0,-1.2431959384,-1.4357155359,0.
C,0,1.2168971407,-2.849666263,0.
C,0,2.4737223525,-0.6872519709,0.

H,0,3.4200085234,-1.241544702,0.
H,0,3.4208394539,1.2398442345,0.
C,0,-0.0014294735,-3.5449272763,0.
H,0,2.1647702127,-3.4008869812,0.
H,0,-0.0018477199,-4.6405148063,0.
C,0,-1.2184065012,-2.8488710836,0.
H,0,-2.1666672243,-3.3995296212,0.
C,0,-2.4745240523,-0.685950002,0.
H,0,-3.4206773244,-1.2402614646,0.
H,0,-3.4193552819,1.2427862608,0.

VSXC/6-31+G(d)
C,0,1.2397893051,1.4329014024,0.
C,0,1.2167624551,2.8435882338,0.
C,0,0.0008236356,3.5400773977,0.
C,0,-1.2153827585,2.8441376023,0.
C,0,-1.2385015435,1.4334155582,0.
C,0,0.0005452558,0.7151366615,0.
H,0,2.1664644416,3.381880275,0.
H,0,0.0012198795,4.6286038787,0.
H,0,-2.165084405,3.3824103162,0.
C,0,-2.469885837,0.6865115935,0.
C,0,-0.0004665924,-0.7153182603,0.
C,0,2.4704641853,0.6852440078,0.
C,0,1.2390294907,-1.4338739731,0.
C,0,-1.2393448375,-1.4322265535,0.
C,0,1.2154319505,-2.8443024445,0.
C,0,2.4696598815,-0.6866568188,0.
H,0,3.4062369758,-1.2478460593,0.
H,0,3.4071418283,1.2460553086,0.
C,0,-0.0014601169,-3.540038524,0.
H,0,2.1648170022,-3.3830859997,0.
H,0,-0.0019146583,-4.6285481995,0.
C,0,-1.2169560466,-2.8433945106,0.
H,0,-2.1667413613,-3.3815738213,0.
C,0,-2.4704529244,-0.6852702728,0.
H,0,-3.4068629919,-1.246544184,0.
H,0,-3.4056097286,1.2490618877,0.

ZINDO/6-31+G(d)
C,0,1.2216420188,1.4217559839,0.
C,0,1.2010680371,2.8128739842,0.
C,0,-0.0000949538,3.499655,0.
C,0,-1.2011769629,2.8128630158,0.
C,0,-1.2216579812,1.4216690161,0.
C,0,0.0000000094,0.715114,0.
H,0,2.1297030443,3.3551119719,0.
H,0,-0.0000819397,4.574524,0.
H,0,-2.1298509557,3.3550260281,0.
C,0,-2.4546979912,0.6699140324,0.
C,0,-0.0000270094,-0.715116,0.

C,0,2.4547050088,0.6699709676,0.
C,0,1.2217149812,-1.4217610161,0.
C,0,-1.2215970188,-1.4216619839,0.
C,0,1.2011799629,-2.8128070158,0.
C,0,2.4547199912,-0.6699060324,0.
H,0,3.383648984,-1.2114510446,0.
H,0,3.383613016,1.2115419554,0.
C,0,-0.0000370462,-3.499649,0.
H,0,2.1297919557,-3.3550820281,0.
H,0,0.0000559397,-4.574519,0.
C,0,-1.2010700371,-2.8129299842,0.
H,0,-2.1297560443,-3.3550709719,0.
C,0,-2.4546770088,-0.6699869676,0.
H,0,-3.383530016,-1.2116459554,0.
H,0,-3.383558984,1.2115680446,0.

EOM-CCSD/6-31G//HF/6-31G

C	6.0	1.4214765210	-1.2215420868	0.0000000000
C	6.0	2.8121099574	-1.2013749247	0.0000000000
C	6.0	3.4988004764	-0.0000151970	0.0000000000
C	6.0	2.8121437537	1.2013553934	0.0000000000
C	6.0	1.4214916501	1.2215381915	0.0000000000
C	6.0	0.7160021076	0.0000080510	0.0000000000
H	1.0	3.3562251472	-2.1300507472	0.0000000000
H	1.0	4.5746041023	0.0000511200	0.0000000000
H	1.0	3.3562092489	2.1300593137	0.0000000000
C	6.0	0.6690208114	2.4564700812	0.0000000000
C	6.0	-0.7159977128	0.0000081698	0.0000000000
C	6.0	0.6690097191	-2.4564893265	0.0000000000
C	6.0	-1.4214781566	-1.2215328167	0.0000000000
C	6.0	-1.4214703685	1.2215437002	0.0000000000
C	6.0	-2.8121170983	-1.2013774687	0.0000000000
C	6.0	-0.6690390763	-2.4564990785	0.0000000000
H	1.0	-1.2123264947	-3.3854574536	0.0000000000
H	1.0	1.2123142730	-3.3854419056	0.0000000000
C	6.0	-3.4987770529	0.0000052078	0.0000000000
H	1.0	-3.3562208365	-2.1300568946	0.0000000000
H	1.0	-4.5745832232	0.0000093531	0.0000000000
C	6.0	-2.8121243883	1.2013735833	0.0000000000
H	1.0	-3.3562178700	2.1300599874	0.0000000000
C	6.0	-0.6690284800	2.4564991168	0.0000000000
H	1.0	-1.2123319440	3.3854469918	0.0000000000
H	1.0	1.2123223378	3.3854260480	0.0000000000

Molecular Dynamics Simulations

B3LYP/6-311g(d,p) atomic charges (atomic units) using Merz and Kollman fitting procedure

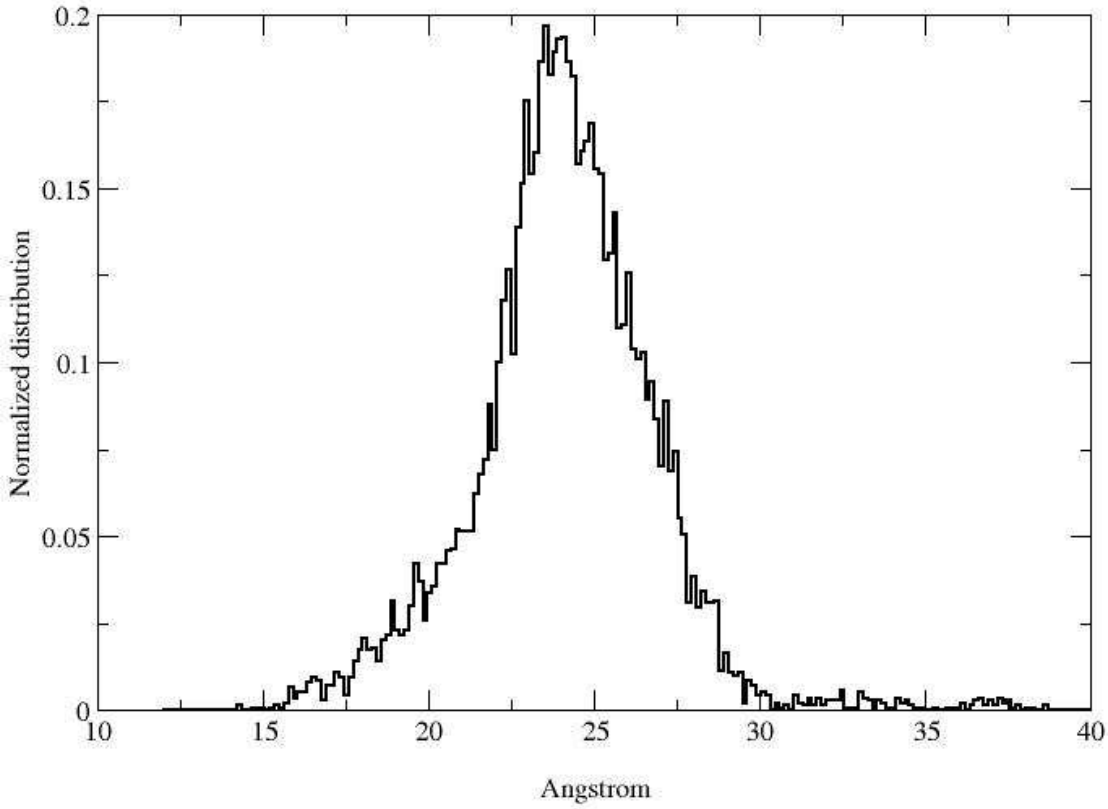
Pyrene Charges		
1	C	-0.11
2	C	-0.16
3	C	0.085
4	C	0.03
5	C	0.085
6	C	-0.16
7	C	-0.16
8	C	-0.16
9	C	0.085
10	C	0.03
11	C	0.085
12	C	-0.16
13	C	-0.16
14	C	-0.16
15	C	-0.11
16	C	-0.16
17	H	0.11
18	H	0.11
19	H	0.11
20	H	0.11
21	H	0.11
22	H	0.11
23	H	0.11
24	H	0.11
25	H	0.11
26	H	0.11

Coordinates (nm) used for the simulation

Pyrene

C	1	1.420	2.014	1.649
C	2	1.349	1.898	1.683
C	3	1.378	1.776	1.622
C	4	1.479	1.764	1.526
C	5	1.550	1.879	1.489
C	6	1.525	1.999	1.557
C	7	1.345	1.665	1.702
C	8	1.394	1.538	1.670
C	9	1.487	1.524	1.566
C	10	1.537	1.639	1.504
C	11	1.656	1.629	1.431
C	12	1.726	1.743	1.392
C	13	1.671	1.869	1.420
C	14	1.539	1.398	1.536
C	15	1.645	1.386	1.445
C	16	1.707	1.503	1.398
H	17	1.417	2.102	1.712
H	18	1.328	1.893	1.790
H	19	1.335	1.694	1.806
H	20	1.386	1.461	1.747
H	21	1.494	1.309	1.580
H	22	1.653	1.295	1.386
H	23	1.776	1.496	1.314
H	24	1.823	1.735	1.342
H	25	1.717	1.961	1.383
H	26	1.620	2.027	1.602

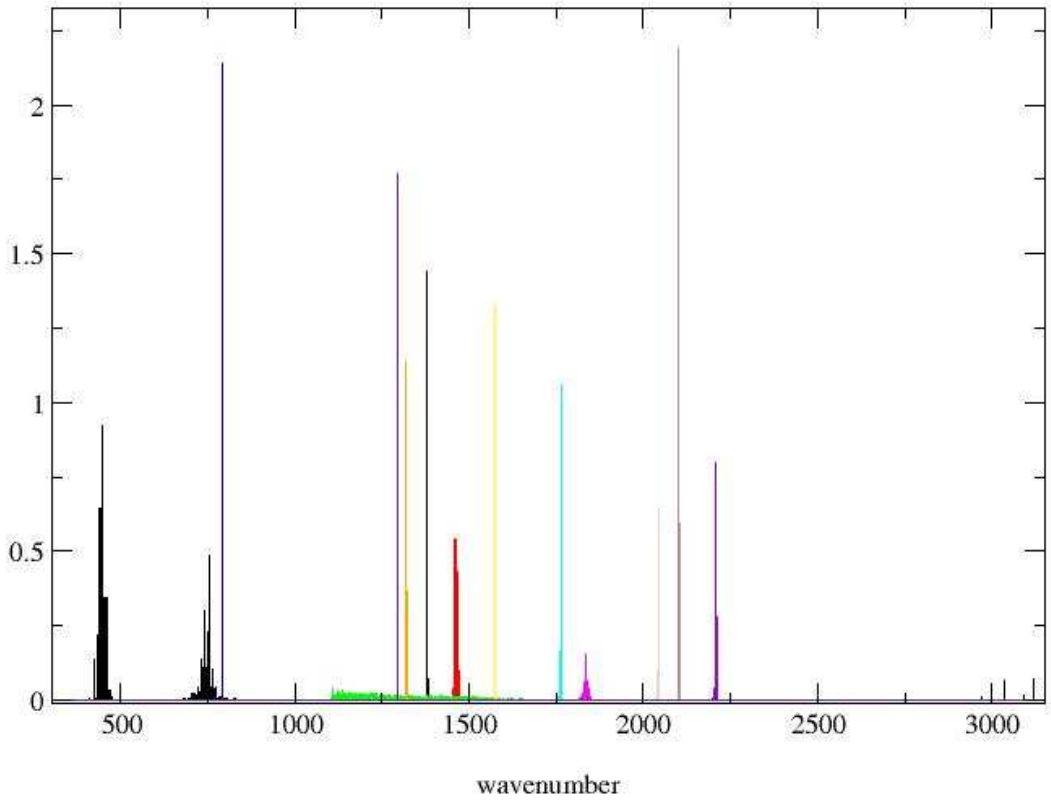
Analysis of trajectory in POPC



Normalized Distribution of Pyrene center of mass along the 'z' quota in POPC (see text for schematic view)

Perturbed Matrix Method

Perturbed frequency distributions from CIS/3-21G calculations.



Perturbed frequency (CIS/3-21G) distributions for S2 state in water.

EXPERIMENTAL SPECTRA