Supplementary Material to the ''Origins of curvature in meso-tetra(4-sulfonatophenyl) porphine aggregation: molecular dynamics and electronic spectroscopy''

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TECHNICAL INFORMATION OF Z1 AND Z2 MONOMERS REPARAMETRIZATION

Based on our theoretical calculations results of $TPPS_4$ Z1 and Z2 monomers, direct application of GAFF will lead to molecular structure, which obviously deviates from the QM optimized result. For this reason, the reparametrization has been performed. First of all, several atom types were changed (see Fig. 4 (c) and (d) in the main text). After the revision of atom types, several bond lengths (Table S1), several valence angles (Table S2) and several dihedral angles (Table S3) were also revised. The same parameters were used for both Z1 and Z2 monomers reparametrization (but different coordinates), because these monomers differ only one H atom position (Fig. 2 (a) and (b) inside blue rectangles in the main text). We performed several MM optimizations: without atom types revision, after atoms types (see Fig. 4 (c) and (d) in the main text) revision, after bonds (Table S1) revision, after valence angle (Table S2) revision and after dihedral angles (Table S3) revision. The final MM optimized structures of $TPPS_4$ Z1 and Z2 monomers with marked all atom types at MM level are presented in Fig. S1.

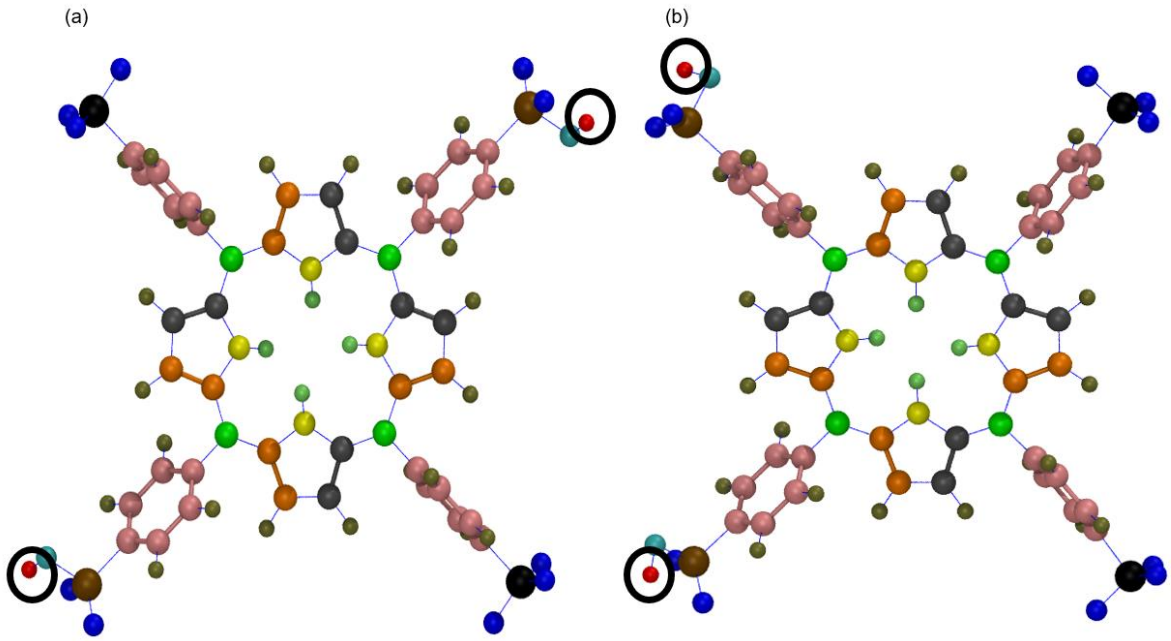

Fig. S1 MM optimized structures of $TPPS_4$ monomers: (a) Z1 monomer, (b) Z2 monomer. $TPPS_4$ monomers with marked new atom types at MM level: "ce''- green; "na''- yellow; "cc''- orange; "cd''- gray; "ca''- pink; "s6''- black; "sy''- ochre; "o''- blue; "oh''- cyan; "ha''- tan; "hn''- lime; "ho''- red. Hydrogens of SO_3H groups are surrounded by black oval.

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Table S1. Revised bond lengths (Å) of Z1 and Z2 monomers

Bonds	Bond lengths (Å)
cc-ce	1.410
cd-ce	1.410
cc-na	1.400
cd-na	1.400

Table S2. Revised degrees (◦) of valence angles of Z1 and Z2 monomers

Valence angles	Degrees (◦)
cd-ce-cd	125.940
cc-ce-cc	125.940
cd-ce-cc	125.940
ca-ce-cc	118.130
ca-ce-cd	118.130

Table S3. Revised degrees (◦) of dihedral angles of Z1 and Z2 monomers

Dihedral angles	Degrees (◦)
ca-ca-ce-cd	180.000
ca-ca-ce-cc	180.000
cc-cc-ce-cd	180.000
na-cc-ce-cd	180.000
cc-cc-ce-cc	180.000
na-cc-ce-cc	180.000
na-cd-ce-cc	180.000
cd-cd-ce-cc	180.000
cd-cd-ce-cd	180.000
na-cd-ce-cd	180.000
ce-cd-na-hn	180.000
ce-cc-na-hn	180.000
cd-cd-na-hn	180.000
cc-cc-na-hn	180.000

Final Cartesian coordinates of MM optimized Z1 and Z2 monomers are presented in Table S4. It was obtained very precise results: QM and MM optimized structures of these monomers are very similar (Fig. 4 (c) and (d) in the main text).

Table S4. Final Cartesian coordinates of MM optimized Z1 and Z2 monomers

Z1 monomer				Z2 monomer			
Atom number	**X**	**Y**	**Z**	**Atom number**	**X**	**Y**	**Z**
S1	-5.350	7.855	0.222	C1	0.576	3.101	-0.095
C1	-4.346	6.385	0.067	N1	-0.429	2.140	0.019
C2	-4.211	5.718	-1.167	C2	-1.698	2.714	0.070
C3	-3.411	4.570	-1.272	C3	4.023	1.318	0.041
C4	-2.731	4.085	-0.142	C4	4.222	-0.049	0.031
C5	-2.855	4.746	1.091	C5	2.964	-0.693	-0.188
C6	-3.657	5.892	1.192	N2	2.043	0.340	-0.366
H1	-3.764	6.420	2.139	C6	2.632	1.592	-0.170
H2	-2.343	4.379	1.975	C7	-4.265	-1.366	0.029
C7	-1.906	2.866	-0.246	C8	-4.486	-0.001	0.026
C8	-2.626	1.644	-0.191	C9	-3.232	0.673	0.191
C9	-4.032	1.523	0.048	N3	-2.293	-0.339	0.371
C10	-4.353	0.183	0.137	C10	-2.863	-1.597	0.198
C11	-3.163	-0.591	-0.041	C11	1.207	-4.170	-0.087
N1	-2.152	0.338	-0.290	C12	-0.156	-4.366	0.022
H3	-1.349	0.095	-0.836	C13	-0.801	-3.088	0.071
C12	-3.000	-2.000	0.014	N4	0.229	-2.154	-0.003
C13	-1.765	-2.697	0.065	C14	1.480	-2.763	-0.103
N2	-0.513	-2.114	0.255	C15	-1.475	4.127	-0.003
C14	0.507	-3.060	0.204	C16	-0.117	4.357	-0.108
C15	-0.152	-4.320	0.044	H1	-0.259	1.160	0.097
C16	-1.513	-4.102	-0.042	H2	4.790	2.065	0.231
H4	-2.267	-4.869	-0.195	H3	5.170	-0.550	0.214
H5	0.345	-5.287	-0.027	H4	-5.021	-2.135	-0.125
C17	1.912	-2.861	0.252	H5	-5.447	0.487	-0.129
C18	2.651	-1.653	0.200	H6	1.949	-4.962	-0.153

Table S4 continues on the next page

Table S4 (continued)

Z1 monomer				Z2 monomer			
Atom number	**X**	**Y**	**Z**	**Atom number**	**X**	**Y**	**Z**
C19	4.059	-1.497	-0.017	H7	-0.660	-5.332	0.061
C20	4.361	-0.152	-0.101	H8	0.086	-1.167	0.020
C21	3.151	0.590	0.065	H9	-2.250	4.893	0.014
N3	2.154	-0.355	0.298	H10	0.346	5.337	-0.193
H6	1.336	-0.130	0.826	C17	-4.141	2.955	0.061
C22	3.000	1.999	-0.007	C18	-4.942	3.176	1.194
C23	1.759	2.684	-0.073	C19	-4.414	3.640	-1.136
C24	1.546	4.094	0.015	C20	-5.984	4.115	1.142
C25	0.188	4.333	-0.068	H11	-4.741	2.658	2.126
C26	-0.505	3.087	-0.203	C21	-5.457	4.576	-1.185
N4	0.498	2.122	-0.243	H12	-3.810	3.474	-2.023
H7	0.371	1.215	-0.639	C22	-6.240	4.832	-0.043
H8	-0.291	5.311	-0.012	H13	-6.589	4.321	2.024
H9	2.316	4.849	0.152	H14	-5.663	5.137	-2.096
C27	4.241	2.818	-0.045	C23	-3.058	-4.055	0.078
C28	4.501	3.668	-1.138	C24	-3.104	-4.810	-1.107
C29	5.678	4.436	-1.179	C25	-3.767	-4.487	1.211
C30	6.608	4.359	-0.126	C26	-3.822	-6.014	-1.144
C31	6.353	3.512	0.969	H15	-2.569	-4.486	-1.995
C32	5.175	2.746	1.007	C27	-4.483	-5.694	1.172
H10	4.988	2.103	1.864	H16	-3.737	-3.918	2.136
H11	7.072	3.458	1.786	C28	-4.504	-6.472	-0.002
S2	8.121	5.340	-0.192	H17	-3.844	-6.624	-2.046
O1	9.225	4.277	-0.654	H18	-5.007	-6.055	2.055
H12	9.830	4.602	0.038	C29	3.941	-2.965	-0.125
O2	8.673	5.553	1.139	C30	4.839	-2.994	-1.209
O3	8.117	6.374	-1.219	C31	4.208	-3.751	1.013
H13	5.881	5.089	-2.028	C32	5.990	-3.799	-1.159
H14	3.800	3.729	-1.967	H19	4.642	-2.401	-2.099
H15	5.344	0.266	-0.303	C33	5.360	-4.554	1.068
H16	4.765	-2.318	-0.141	H20	3.529	-3.737	1.862
C33	2.733	-4.082	0.139	C34	6.254	-4.577	-0.018
C34	3.342	-4.625	1.282	H21	6.683	-3.822	-2.002
C35	4.134	-5.779	1.170	H22	5.568	-5.160	1.951
C36	4.329	-6.392	-0.084	C35	2.862	4.048	-0.109
C37	3.711	-5.840	-1.222	C36	2.832	4.919	0.998
C38	2.918	-4.689	-1.115	C37	3.757	4.307	-1.164
H17	2.458	-4.276	-2.007	C38	3.689	6.032	1.052
H18	3.864	-6.327	-2.184	H23	2.153	4.731	1.827
S3	5.319	-7.871	-0.247	C39	4.615	5.418	-1.114
O4	5.998	-7.604	-1.504	H24	3.785	3.654	-2.033
O5	4.255	-8.857	-0.306	C40	4.586	6.280	-0.003
O6	6.114	-7.841	0.969	H25	3.664	6.704	1.910
H19	4.604	-6.214	2.050	H26	5.306	5.619	-1.934
H20	3.205	-4.167	2.256	C41	-2.201	-2.852	0.153
H21	-0.410	-1.217	0.681	C42	2.736	-2.098	-0.177
C39	-4.241	-2.819	0.050	C43	1.976	2.855	-0.159
C40	-4.476	-3.713	1.113	C44	-2.963	2.067	0.149
C41	-5.653	-4.481	1.151	O1	-5.846	-8.078	-1.389
C42	-6.608	-4.362	0.125	O2	6.852	7.177	1.061

Table S4 continues on the next page

Table S4 (continued)

Z1 monomer				Z2 monomer			
Atom number	**X**	**Y**	**Z**	**Atom number**	**X**	**Y**	**Z**
C43	-6.378	-3.472	-0.941	O3	-7.993	5.960	-1.444
C44	-5.200	-2.704	-0.976	O4	7.297	-6.931	-0.716
H22	-5.033	-2.029	-1.812	S1	7.735	-5.600	0.067
H23	-7.116	-3.385	-1.738	S2	-5.311	-8.065	-0.039
S4	-8.120	-5.344	0.188	S3	-7.479	6.116	-0.094
O7	-9.212	-4.299	0.716	S4	5.707	7.689	0.061
H24	-9.832	-4.596	0.026	O5	5.183	8.734	0.930
O8	-8.094	-6.417	1.173	O6	6.379	7.966	-1.202
O9	-8.703	-5.504	-1.137	O7	-6.617	7.266	0.118
H25	-5.837	-5.168	1.978	O8	-8.346	5.749	1.013
H26	-3.757	-3.807	1.923	O9	-6.248	-7.960	1.066
H27	-5.341	-0.216	0.351	O10	-4.148	-8.908	0.180
H28	-4.723	2.355	0.180	O11	8.074	-6.026	1.418
H29	-3.322	4.071	-2.232	O12	8.736	-5.136	-0.886
H30	-4.736	6.108	-2.038	H27	-1.471	-0.204	0.927
O10	-4.301	8.858	0.184	H28	1.214	0.225	-0.923
O11	-5.957	7.631	1.523	H29	8.127	-6.950	-1.221
O12	-6.207	7.763	-0.948	H30	6.819	8.012	1.560