Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Photoresponsive Sulfone-Based Molecules: Photoinduced Electron Transfer and Heat/Air-Stable Radical in the Solid State

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Index:

Additional graphics and table

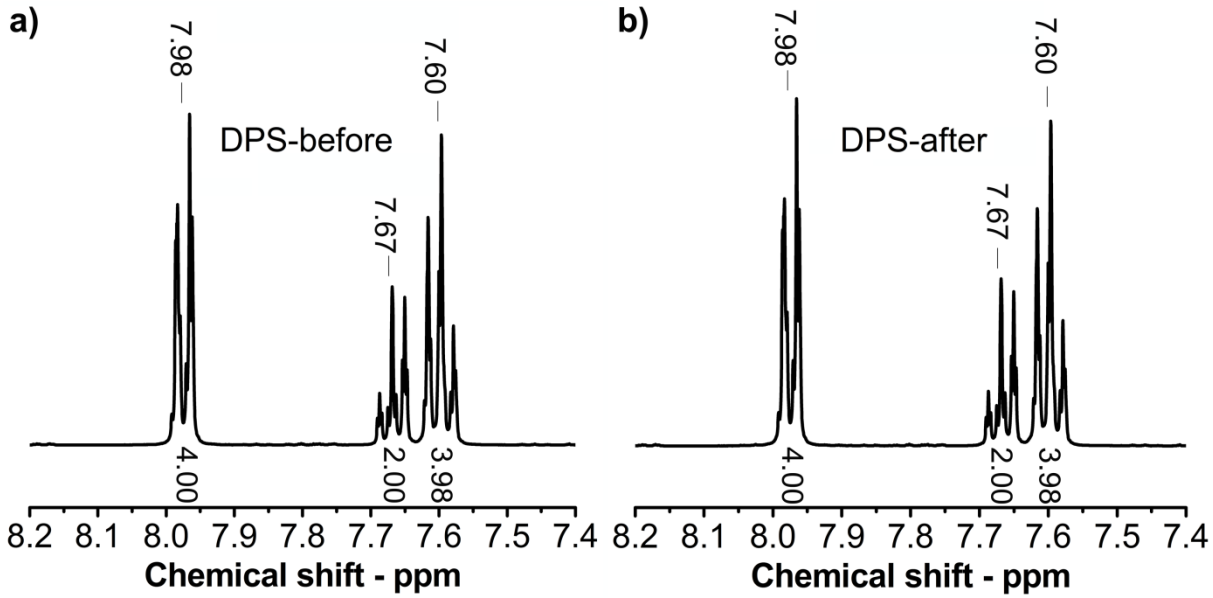


Fig. S1 ^{1}H-NMR spectra of **DPS** in CH_3CN-d_3 before and after irradiation.

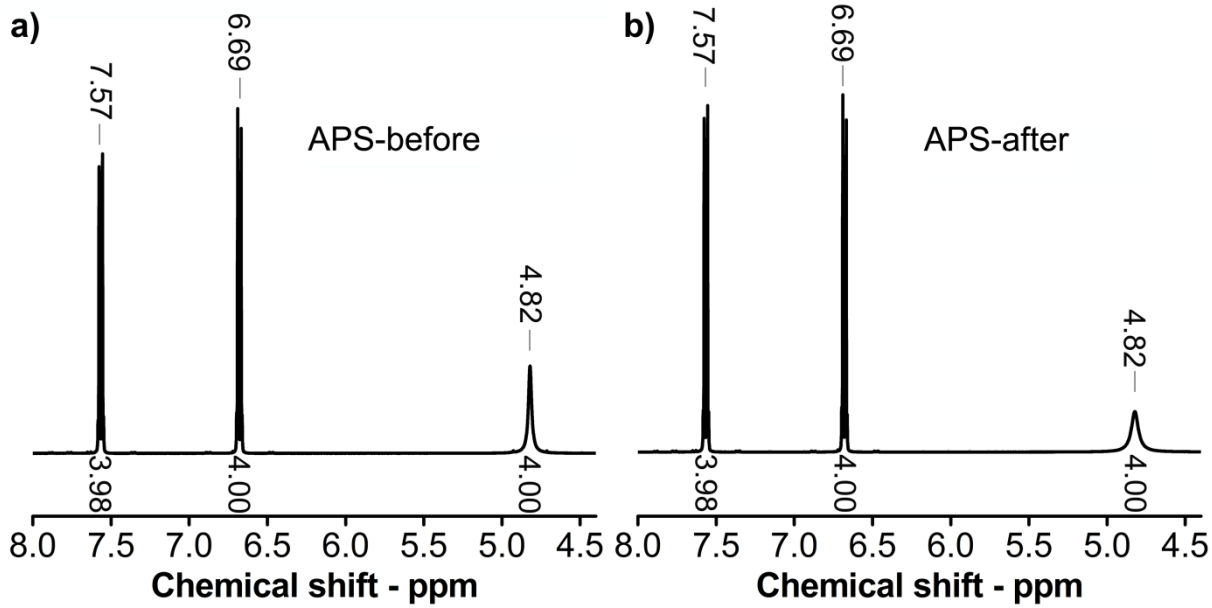


Fig. S2 ^{1}H-NMR spectra of **APS** in CH_3CN-d_3 before and after irradiation.

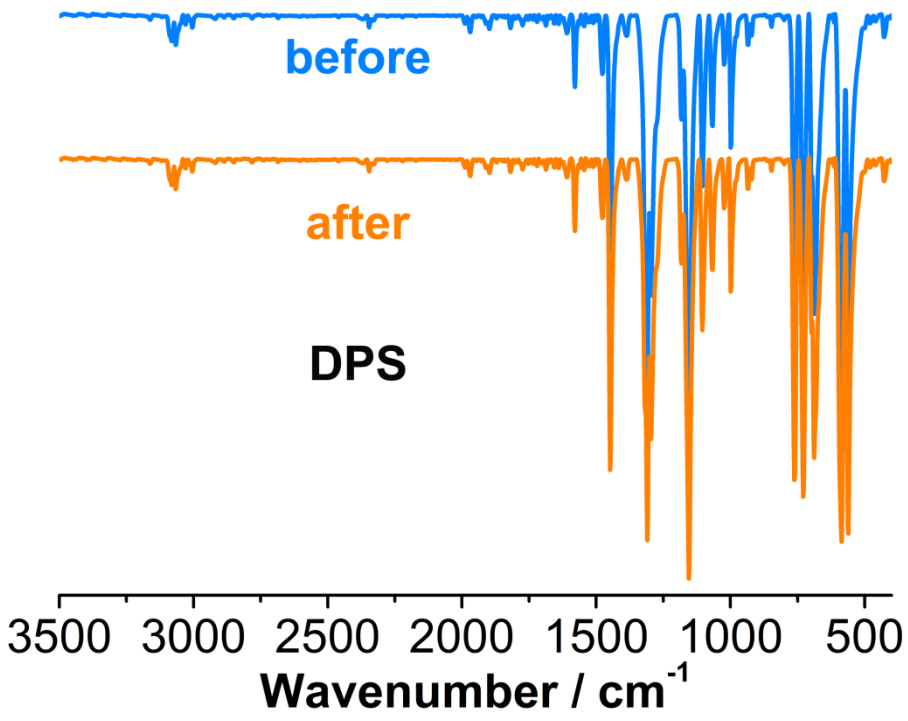


Fig. S3 IR spectra of **DPS** in the KBr matrix before and after irradiation.

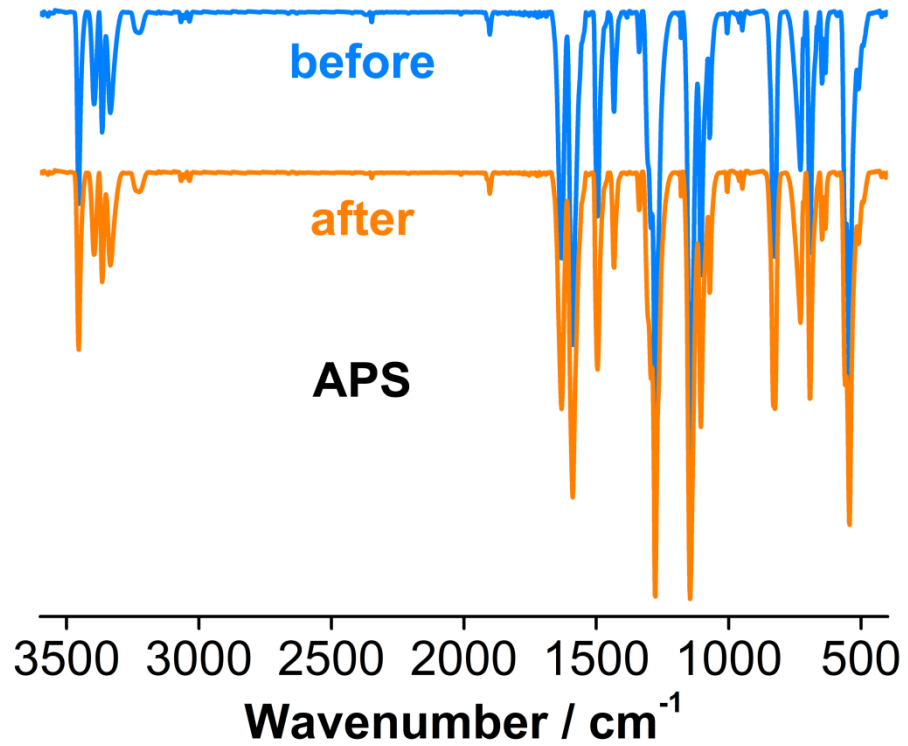


Fig. S4 IR spectra of **APS** in the KBr matrix before and after irradiation.

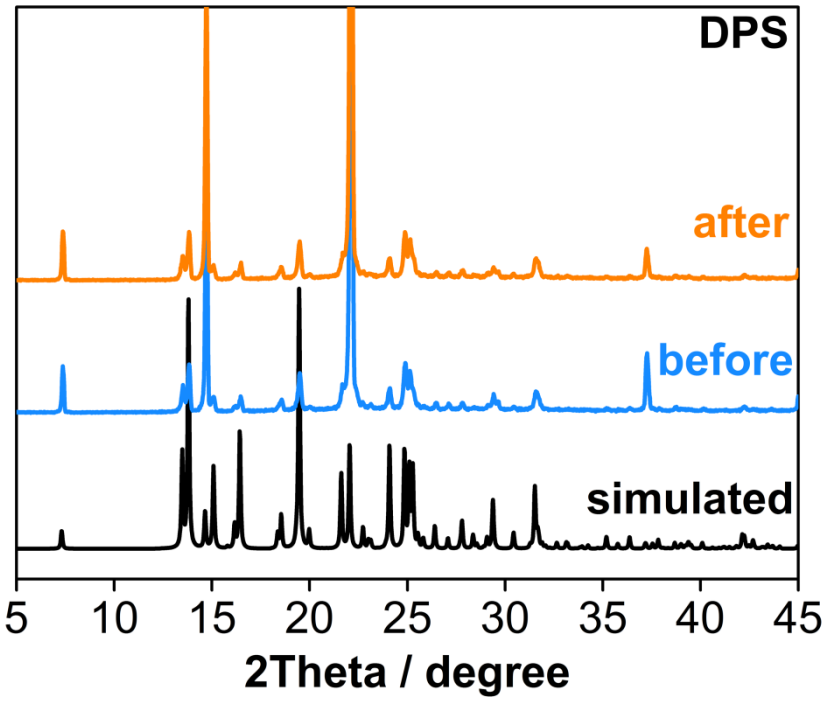


Fig. S5 PXRD spectra of **DPS** before and after irradiation. The simulated pattern was derived from the X-ray single crystal diffraction data.

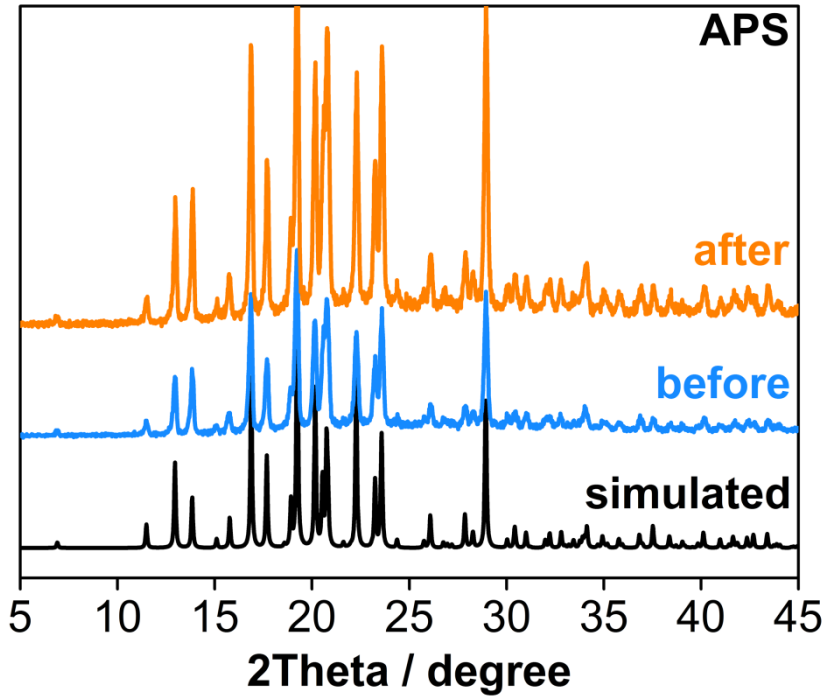


Fig. S6 PXRD spectra of **APS** before and after irradiation. The simulated pattern was derived from the X-ray single crystal diffraction data.

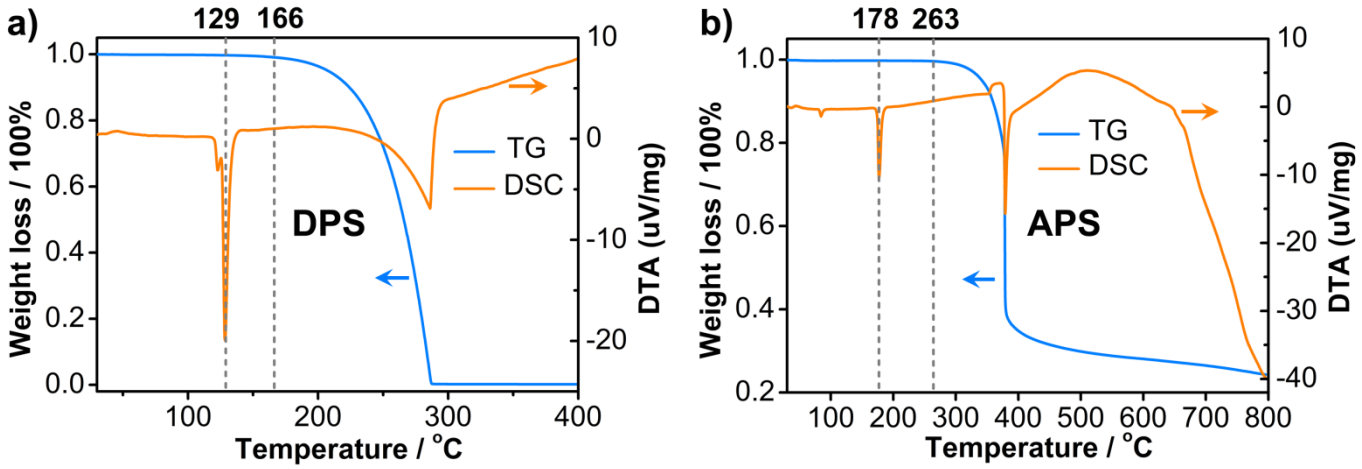


Fig. S7 TG curves of **DPS** and **APS** under N_2.

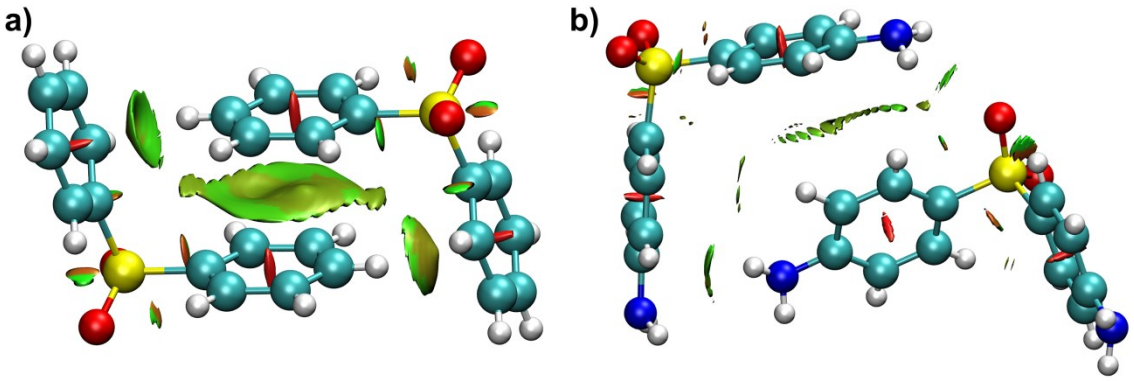


Fig. S8 Gradient isosurfaces (s = 0.5 a.u.) for dimers of **DPS** (a) and **APS** (b). The surfaces are colored on a blue-green-red (BGR) scale according to values of sign(λ_2)ρ, ranging from –0.04 to 0.02 a.u.. Blue indicates strong attractive interactions, and red indicates strong nonbonded overlap.

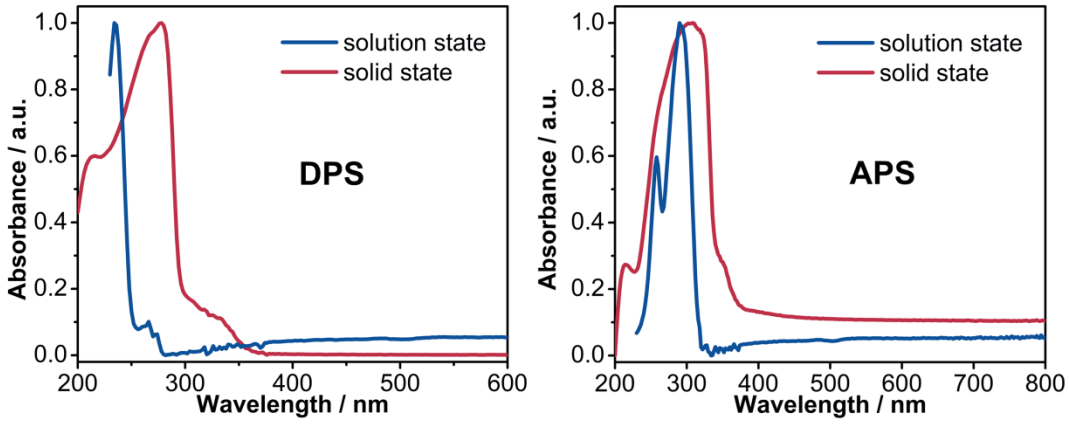
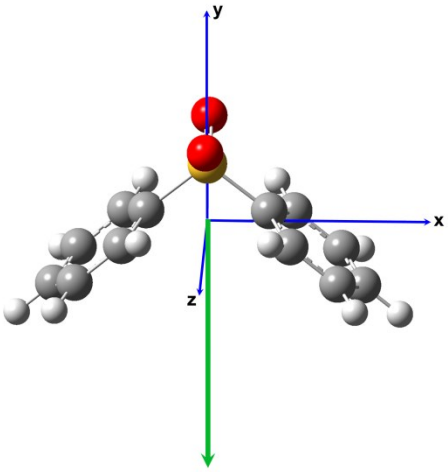
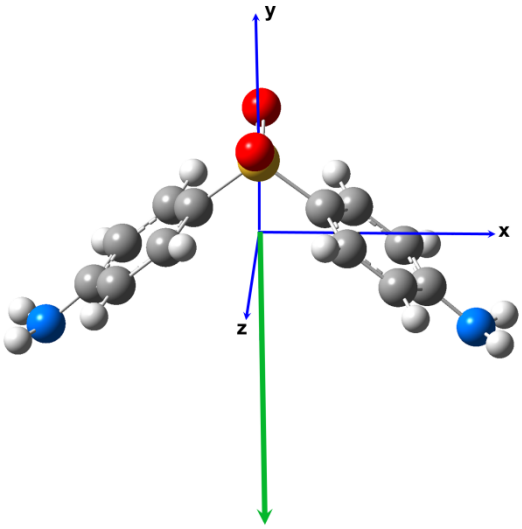


Fig. S9 Comparison of electronic absorption spectra of **DPS** and **APS** in CH_3CN and the solid state.

Table S1 Dipole moments and Cartesian coordinates for the optimized molecular structures of **DPS** and **APS**. The green arrows denote the dipole directions.

Compounds	Dipole moment	
	Direction	Value
DPS		**5.85 Debye**
APS		**6.66 Debye**

Cartesian coordinates of the optimized molecular structure of DPS:

	X	Y	Z
S	-0.00001668	1.35648496	-0.00133123
O	0.00000641	2.05762984	-1.27577846
O	-0.00001623	2.06021349	1.27166888
C	-1.39735931	0.24273613	-0.00020666

C	-1.91757777	-0.18168619	1.21566229
C	-1.91686244	-0.18493086	-1.21527196
C	-2.98642473	-1.06947041	1.20930967
H	-1.50242162	0.20029748	2.14065714
C	-2.98567652	-1.07271208	-1.20722046
H	-1.50121978	0.19461779	-2.14105018
C	-3.51439248	-1.51578859	0.00148155
H	-3.41132279	-1.40769156	2.14639592
H	-3.40998775	-1.41348320	-2.14365327
H	-4.34945977	-2.20592763	0.00214975
C	1.39731194	0.24266976	-0.00020222
C	1.91755583	-0.18174026	1.21566678
C	1.91683796	-0.18494671	-1.21526316
C	2.98645098	-1.06944009	1.20931476
H	1.50237472	0.20017968	2.14067417
C	2.98571226	-1.07268410	-1.20721227
H	1.50117833	0.19462619	-2.14102102
C	3.51445465	-1.51572207	0.00146699
H	3.41142235	-1.40765423	2.14636900
H	3.41001882	-1.41338838	-2.14367116
H	4.34958082	-2.20578925	0.00217425

Cartesian coordinates of the optimized molecular structure of APS:

	X	Y	Z
S	-0.00000638	1.65055340	0.00000435
O	-0.00000714	2.35685368	-1.27417547
O	0.00005098	2.35687816	1.27415936
C	-1.39947211	0.55777386	0.00003657

C	-1.93136564	0.12297609	1.20894857
C	-1.93153349	0.12322640	-1.20886365
C	-2.99880032	-0.75682805	1.20869216
H	-1.52002258	0.49689009	2.13922679
C	-2.99899187	-0.75659916	-1.20865083
H	-1.52035217	0.49735672	-2.13912708
C	-3.54532785	-1.21348841	-0.00000373
H	-3.42168590	-1.09798576	2.14711871
H	-3.42195468	-1.09753456	-2.14712349
C	1.39940938	0.55769807	-0.00001207
C	1.93131312	0.12295164	-1.20892512
C	1.93149422	0.12315062	1.20888677
C	2.99877772	-0.75683705	-1.20869675
H	1.51996545	0.49687312	-2.13919912
C	2.99898012	-0.75662694	1.20863903
H	1.52028651	0.49723534	2.13915625
C	3.54534916	-1.21346474	-0.00002711
H	3.42162748	-1.09797229	-2.14714696
H	3.42198628	-1.09756967	2.14709010
N	-4.57612683	-2.13512736	0.00004222
H	-5.12750882	-2.18711698	0.84202455
H	-5.12755415	-2.18717791	-0.84190514
N	4.57620606	-2.13509127	-0.00004999
H	5.12767276	-2.18691088	-0.84200113
H	5.12774179	-2.18685979	0.84185717