Electronic supplementary information

High efficiency photo-oxidation of thioethers over C_{60}@PCN-222 under air

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- **Fig. S1**. A linear relationship between the C_{60} concentration and its UV absorbance.
- **Fig. S2**. UV analysis of C_{60} content in a series of C_{60}@PCN-222 composites.
- **Fig. S3** DFT pore size distribution for C_{60}@PCN-222 photocatalysts.
- **Fig. S4** Solid-state UV-*vis* spectra of C_{60}@PCN-222 samples.
- **Fig. S5** Room-temperature PL excitation and emission spectra of C_{60}@PCN-222 samples.
- **Fig. S6** Time course of the products distribution for the photocatalytic oxidation of thioanisole.
- **Fig. S7-S8** Recycling experiments of the 3%-C_{60}@PCN-222 photocatalyst.
- **Scheme S1** Proposed mechanism for the selective oxidation of sulfides into sulfoxides.
- **Table S1** Comparison of the photocatalytic oxidation activities of thioanisole to phenyl methyl sulfoxide.

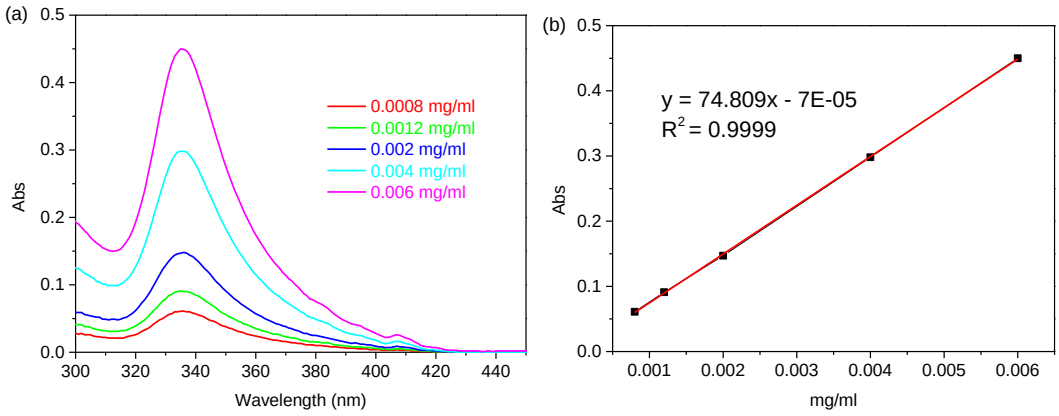


Fig. S1 A linear relationship between the C60 concentration and its UV absorbance.

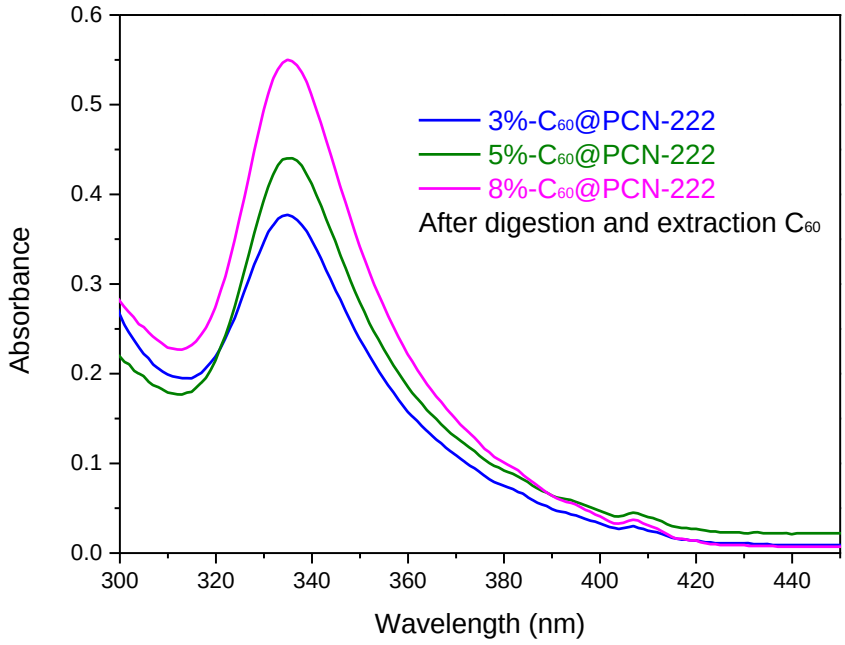


Fig. S2 UV analysis of C_{60} content in a series of C_{60}@PCN-222 composites.

C_{60} content calculation: C_{60}@PCN-222 samples were digested by 1 mol/L KOH solution, then 100 mL toluene were used to extract C_{60} for several times, and then the extraction solution was analyzed by UV spectrum based on working curve in Fig. S1.

Sample name	Sample usage (mg)	Toluene (mL)	UV-*vis* absorbance	*c*. (mg/mL)	C_{60}/C_{60}@PCN-222
3%-C_{60}@PCN-222	15	100	0.37	0.0049	0.032
5%-C_{60}@PCN-222	12	100	0.43	0.0059	0.049
8%-C_{60}@PCN-222	9	100	0.55	0.0073	0.081

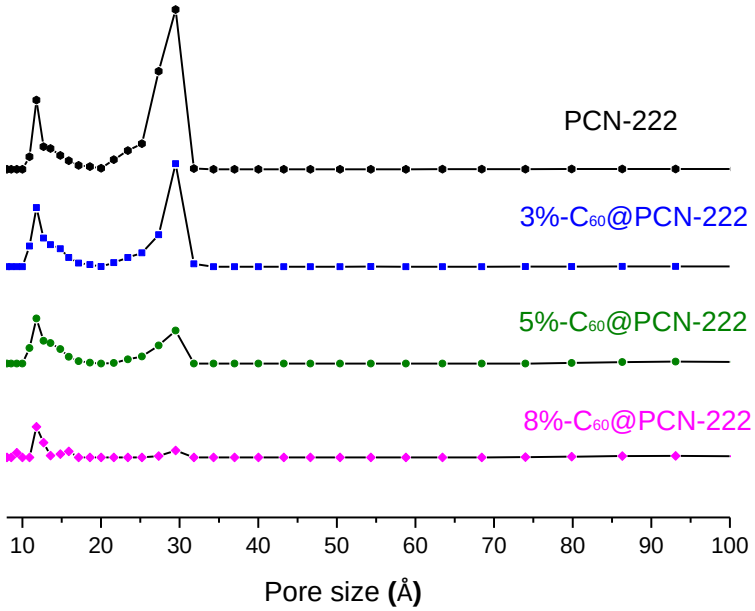


Fig. S3 DFT pore size distribution for as-synthesized PCN-222 and C_{60}@PCN-222 composites with different C_{60} contents based on N_2 adsorption isotherms at 77 K.

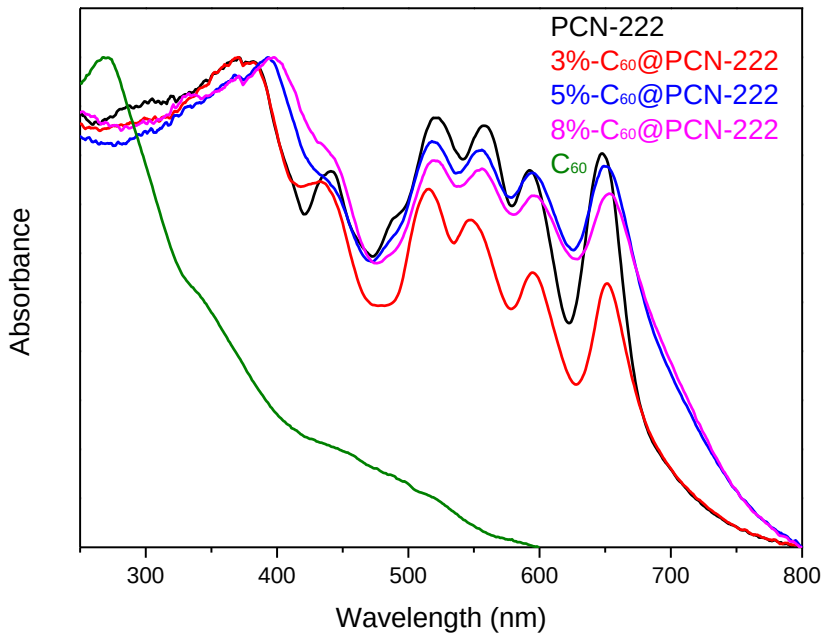


Fig. S4 Solid-state UV-vis spectra of PCN-222 and 3%/5%/8%-C_{60}@PCN-222 at room temperature.

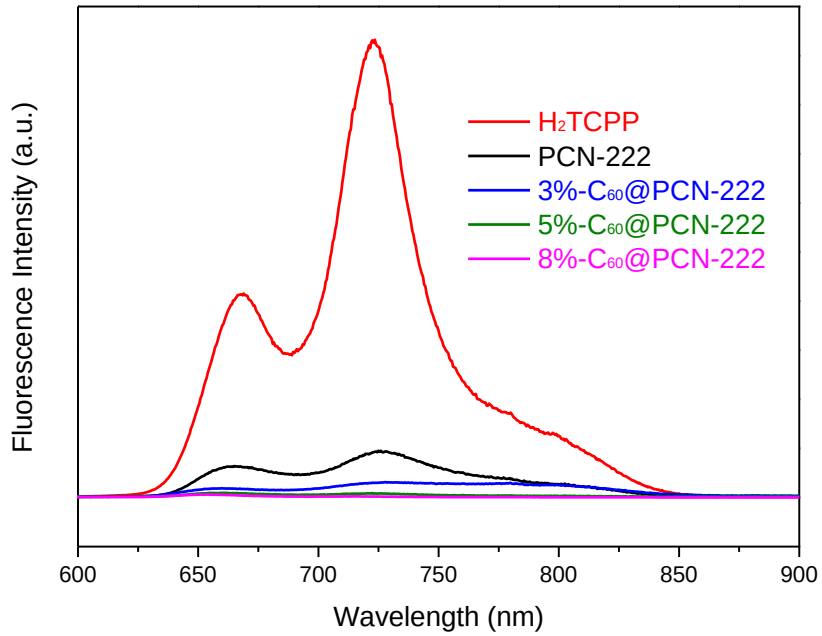


Fig. S5 Room-temperature PL spectra of H_2TCPP, PCN-222, 3%/5%/8%-C_{60}@PCN-222 composites (λ_{ex} = 380 nm).

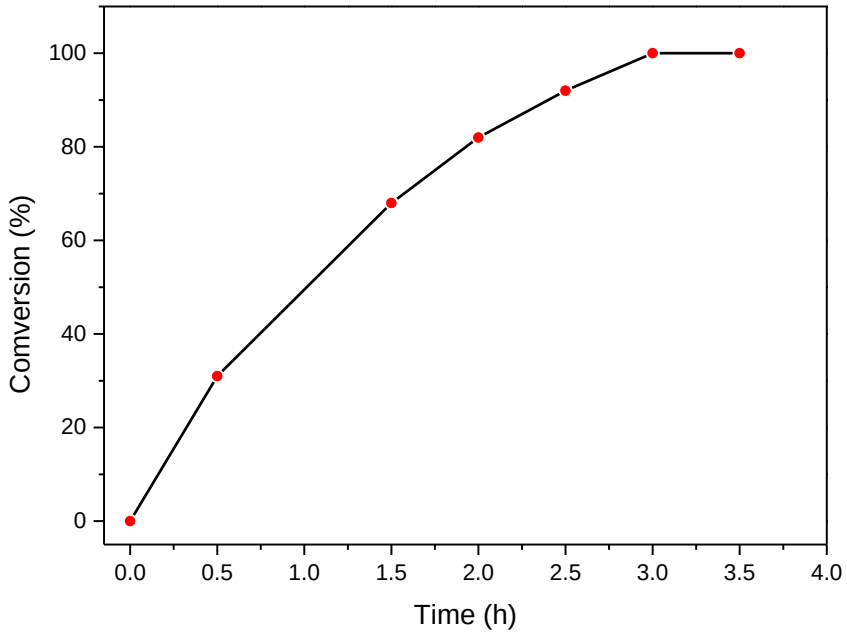


Fig. S6 Time course of the products distribution for the photocatalytic oxidation of thioanisole.

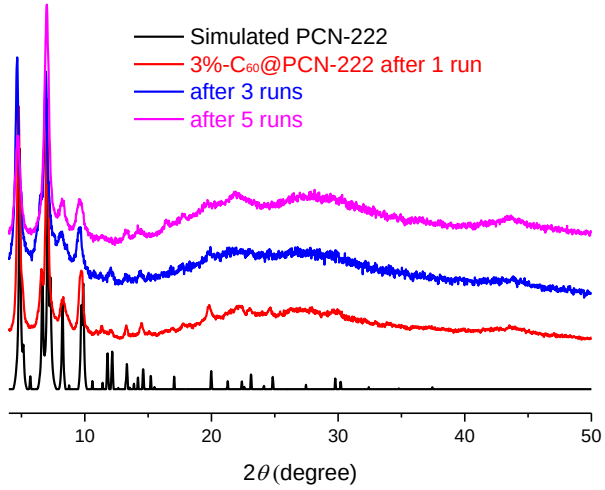


Fig. S7 PXRD profiles of 3%-C_{60}@PCN-222 after catalytic reaction

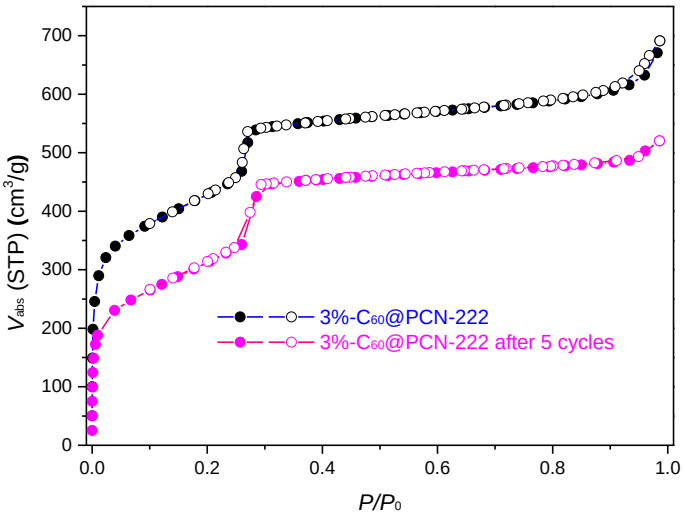
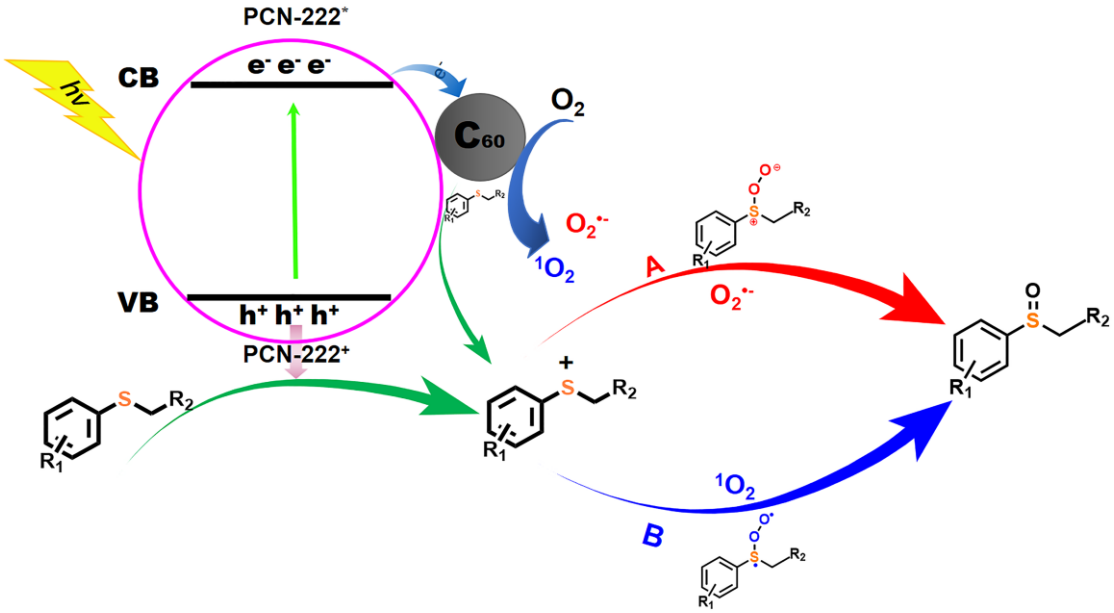


Fig. S8 N_2 sorption isotherms for 3%-C_{60}@PCN-222 before reaction and after 5 catalytic cycles at 77 K



Scheme S1. The proposed mechanism for the selective oxidation of sulfides into sulfoxides with air in the merger of visible light photocatalysis of C_{60}@PCN-222.

Table S1. Comparison of the photocatalytic oxidation activities of thioanisole to phenyl methyl sulfoxide.

Catalytic	Oxid.	T. (h)	Abs. (nm)	Photo intensity	Con. (%)	Sel. (%)	TOF (h^{-1})	Ref.
3%-C_{60}@PCN-222	air	3	$\lambda > 400$	50 mW/cm^2	100	100	80[b]	This work
5%-C_{60}@PCN-222	air	2	$\lambda > 400$	50 mW/cm^2	100	100	71.4[b]	This work
8%-C_{60}@PCN-222	air	2	$\lambda > 400$	50 mW/cm^2	100	100	45.5[b]	This work
MOF-6	air	22	--	26 W fluorescent lamp	73	100	16.6	*J. Am. Chem. Soc.* 2011, 133, 13445
Ru^{II}_{chro}–Cu^{II}_{cat}[a]	air	20	--	blue LEDs		90	2	*ChemSusChem* 2017, 10, 3358
pTCT	air	12	--	26 W white CFL	> 99	97	0.007	*J. Mater. Chem. A* 2018, 6, 15154
1 (MOF)	H_2O_2	4	$\lambda > 420$	300 W Xe lamp	99	95	16.7	*ACS Appl. Mater. Interfaces* 2019, 11, 3016.
RuII(TMP)(CO)[a]	PhI(OAc)$_2$	100	λmax= 420	--	100	99	31.25	*Applied Catalysis A: General* 2014, 478, 275.
4%C_{60}/g-C_3N_4	O_2	6	$\lambda > 400$	1 W /cm^2	100	100	20	*ChemSusChem* 2018, 11, 2444
$TBA_4H[\gamma$-$PV_2W_{10}O_{40}]$	O_2	24	$\lambda > 400$	xenon lamp	100	92	0.0004	*Chem. Commun.* 2018, 54, 7127
DBFL[a]	O_2	8.3	--	110 W /m^2	100	100	0.005	*ACS Sustainable Chem. Eng.* 2018, 6, 15254
SnPor@PAF	O_2	0.5	--	90 mW/cm^2	31	99	19872	*Adv. Synth. Catal.* 2018, 360, 4402

$Au_{38}S_2(SAdm)_{20}$	O_2	12	532	~34 mW/cm 2	58	100	20.83	*ACS Catal*. 2017, 7, 3368
ARS-TiO_2	O_2	10	$\lambda > 450$	300 W Xe lamp	81	91	75	*Angew. Chem.* 2016, 128, 4775
Degussa P_{25} TiO_2	O_2	22	$\lambda > 400$	300 W Xe lamp	81	93	0.05	*Chem. Sci.* 2015, 6, 5000
TiO_2	O_2	4	$\lambda > 400$	300 W Xe lamp	83	92	0.15	*Chem. Sci.* 2015, 6, 1075
0.5 wt.% $Pt/BiVO_4$	O_2	5.5	$\lambda > 420$	300 W Xe lamp	96	98	36	*Journal of Catalysis* 2015, 332, 95
1 (MOF)	O_2	12	--	350 W Xe lamp	> 99.9	> 99.9	0.84	*Inorg. Chem.* 2011, 50, 5318
cdcn(30)	O_2	6	--	white LEDs	61.8	99	2.1	*Catal. Sci. Technol.* 2017, 7, 587
mpg-C_3N_4	O_2	4	$\lambda > 420$	a mercury lamp (150 W)	97	98	0.62	*Green Chem.* 2012, 14, 1904

[a] homogeneous photocatalyst

[b] Turnover frequency (TOF) = [moles of **1b**] / [(moles of C_{60}) × (reaction time)]