Supplementary Information

Efficient photodegradation of carbamazepine by organocatalysts incorporating a third component with a more complementary absorption spectrum

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Text S1 Photocatalyst synthesis

The preparation of PM6 is referred to Zhang et al. [1]: First, BDT-F (450 mg, 0.5 mmol) and BDD (383 mg, 0.5 mmol) are dissolved in 12 ml of toluene and placed in a 50 ml double-neck round-bottom flask. The reaction vessel is purged with argon for 20 minutes to remove oxygen. Then, 25 mg of $Pd(PPh_3)_4$ is added as a catalyst, and the flask is flushed with argon for another 20 minutes. The mixture is heated to reflux and maintained for 12 hours. After cooling to room temperature, the reaction mixture is poured into 200 ml of methanol to precipitate the product, which is then filtered using a Soxhlet thimble. Soxhlet extraction is carried out sequentially with methanol, hexane, and chloroform. The polymer is recovered from the chloroform fraction by precipitation in methanol. Finally, the solid product is dried under vacuum.

The preparation of Y6 is referred to Yuan et al. [2]: Compound (12, 13-bis(2-ethylhex yl)-3, 9-diundecyl-12, 13-dihydro[1, 2, 5]thiadiazole[3, 4-e]thieno[2", 3":4, 5]thieno[2', 3 ':4, 5]pyrrolo[3, 2-g]thieno[2', 3':4, 5]thieno[3, 2-b]indole-2, 10-dicarbaldehyde (0.15g, 0. 15 mmol), 2-(5, 6-difluoro-3-oxo-2,3-dihydro-1H-inden-1-ylidene)malononitrile) (0.21g, 0.91mmol), pyridine (1 mL), and chloroform (45 mL) were dissolved in a round-bottom f lask under a nitrogen atmosphere. The solution was stirred at 65 °C overnight. After the r eaction mixture was cooled to room temperature, it was poured into methanol, and the res ulting precipitate was filtered. The residue was purified by column chromatography on sil ica gel, using a 1:1 (v/v) mixture of dichloromethane and petroleum ether as the eluent, yi elding a dark blue solid Y6.

The preparation of ITCPTC is referred to Xie et al. [3]: IT-CHO (129 mg, 0.12 mmol), CPTCN (100 mg, 0.5 mmol), and chloroform (10 mL) were placed in a two-neck round-

bottom flask. The mixture was purged with argon for 30 minutes to remove oxygen. Then, pyridine (0.1 mL) was added, and the reaction was refluxed at 80°C for 12 hours. After cooling to room temperature, the mixture was poured into 100 mL of methanol, and the resulting precipitate was filtered. The residue was purified by column chromatography on silica gel using petroleum ether/dichloromethane (1:1, v/v) as the eluent, yielding a dark blue solid (157 mg, 91% yield).

Text S2 Analysis and Characterizations

The surface morphology of the materials was visualized using scanning electron microscopy (SEM, Hitachi Regulus8100) and atomic force microscopy (AFM, Bruker Dimension ICON). The chemical composition of the material was analyzed using Raman spectroscopy (Raman, inVia Reflex, UK). The Brunauer–Emmett–Teller (BET) surface area was determined through nitrogen adsorption-desorption isotherms using the Micromeritics ASAP2460 system. The Ultraviolet-visible diffuse reflectance spectroscopy (UV-vis DRS, UV-2700i, Shimadzu, Japan) was utilized to examine the optical absorption characteristics of the photocatalyst in the UV-Vis range. The concentration of total organic carbon (TOC) was measured by a TOC analyzer (Shimadzu TOC-VSH, Shimadzu, Japan). Photoluminescence emission spectra (PL) and nanosecond timescale fluorescence decay kinetics of the photocatalyst were provided by a steady-state/transient fluorescence spectrometer (Edinburgh Instruments Ltd, FLS1000, UK). Absorbance measurements were conducted using a UV detector (Shimadzu Corporate Management China Ltd. UV-2700) at a wavelength of 285 nm. The identification of intermediate species during the degradation of carbamazepine was performed using liquid chromatography-mass spectrometry (LC-MS, Thermo Q-Exactive, USA). The charge transfer capability of the

photocatalyst was assessed through electrochemical impedance spectroscopy (EIS) and photocurrent response (PCR) tests using the CHI660E electrochemical workstation (Shanghai Chenhua Instruments Co., Ltd.). The types of free radicals were identified using electron spin resonance (ESR, Bruker-A300, Germany). The photogenerated charge behavior was measured using the PL-SPV1000 Stable surface photovoltage (SPV) spectrometer (Beijing Perfectlight Technology Co., Ltd.).

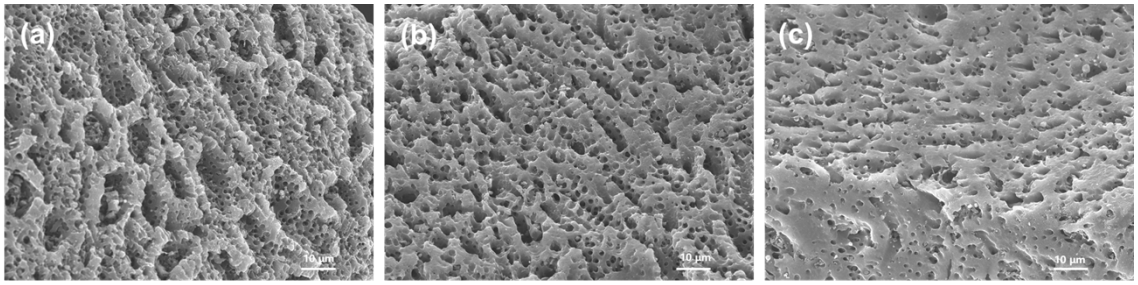


Fig.S1. SEM images. (a) PM6:Y6, (b) PM6:ITCPTC, and (c) PM6:Y6:ITCPTC.

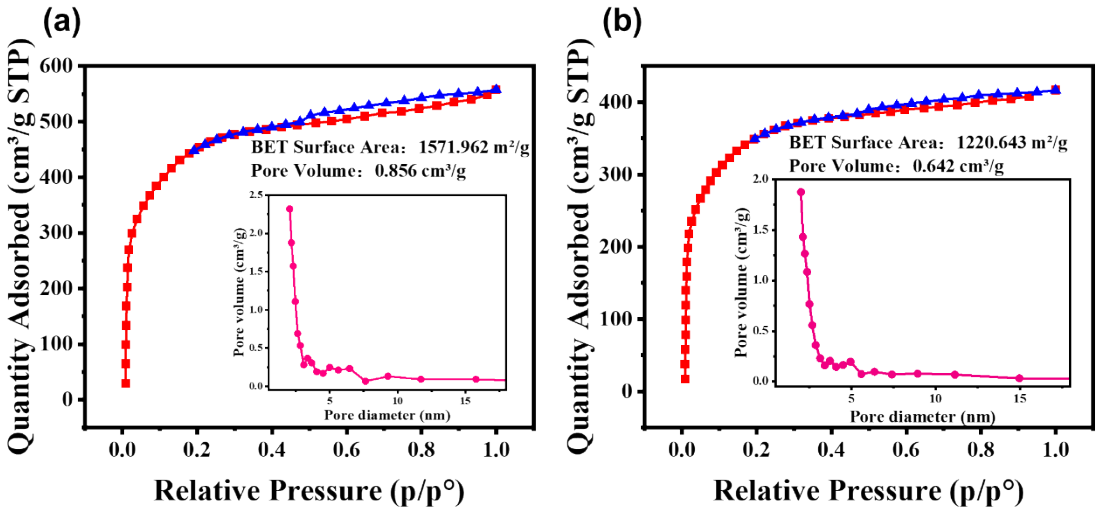


Fig.S2. N_2 adsorption-desorption isotherms of (a) pure CSC and (b) CSC-loaded PM6:Y6:ITCPTC.

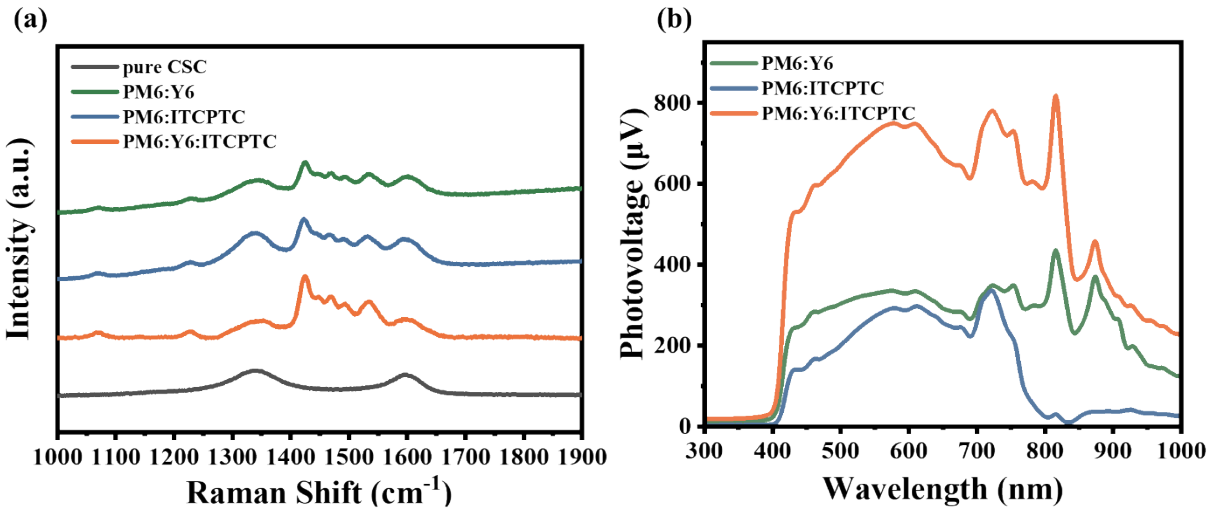


Fig.S3. The Raman (a) and SPV (b) spectra of the materials.

Table S1. The first-order kinetics constant (k_1) and the second kinetics constant (k_2) for photodegradation of different samples.

Samples	k_1 (min^{-1})	R_1^2	k_2 ($g\cdot(mg\cdot min)^{-1}$)	R_2^2
PM6:Y6	0.10111	0.95995	0.13184	0.9962
PM6:ITCPTC	0.10436	0.95335	0.06385	0.99896
PM6:Y6:ITCPTC	0.20418	0.8644	0.02477	0.99397

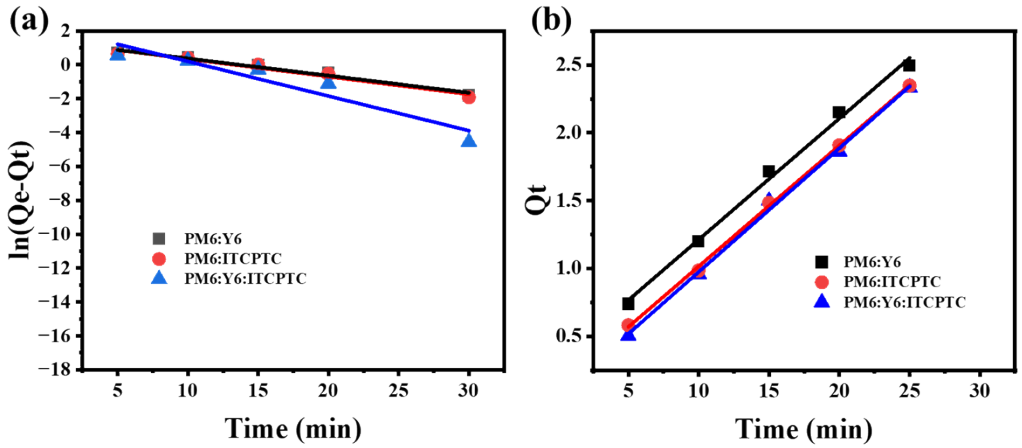
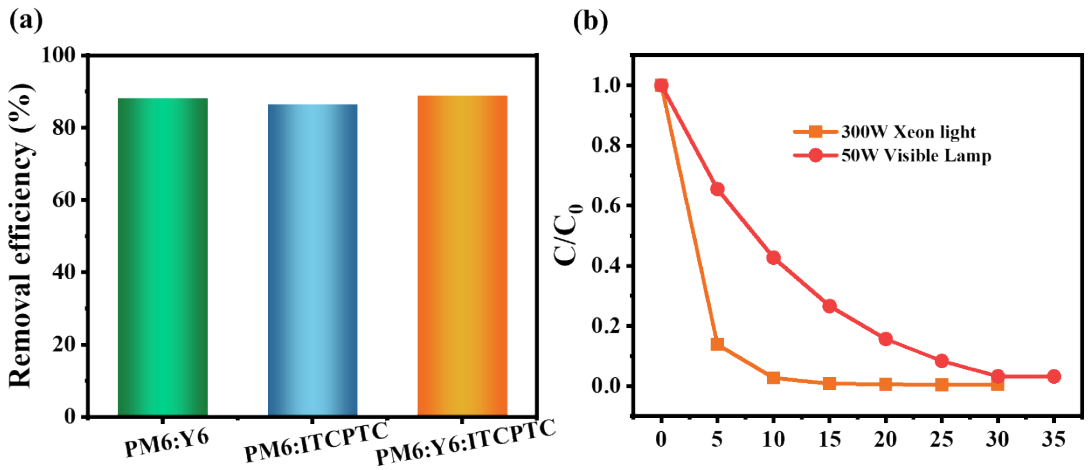


Fig.S4. Pseudo-first-order kinetics (a) and pseudo-second-order kinetics (b) of carbamazepine degradation for the prepared samples.



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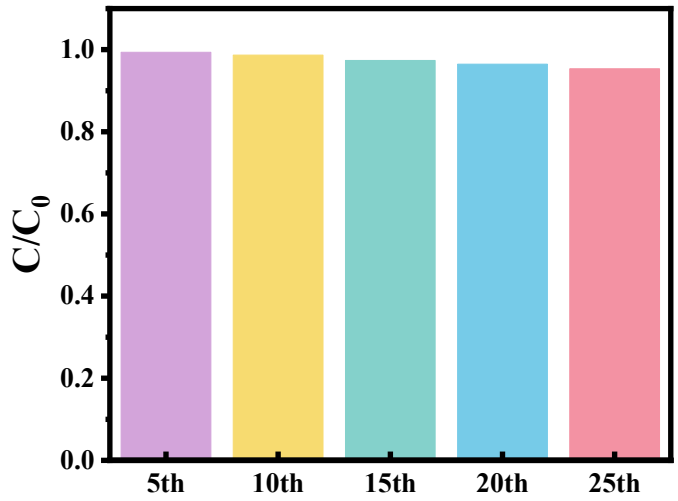
68 **Fig.S5**. TOC removal efficiencies using various photocatalysts (a). Comparison of

69 PM6:Y6:ITCPTC degradation of carbamazepine under different light intensities (b).



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71 **Fig. S6**. Recycling tests of PM6:Y6:ITCPTC photocatalyst for carbamazepine

72 degradation.

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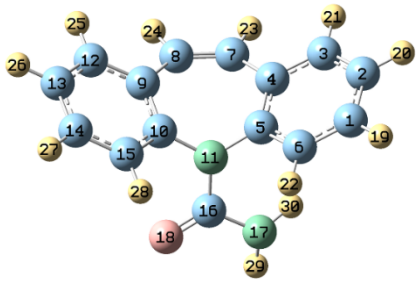
Table S2. Photocatalytic performance comparison of carbamazepine over various photocatalysts under 300 W Xenon light source.

Photocatalyst	Carbamazepine concentration (mg/L)	Catalyst dosage (g/L)	Reaction time (min)	Removal (%)	Kinetic rate (min^{-1})	Ref.
Single-atom Ba embedded g-C_3N_4 (MBs) 20	1	0.4	60	~100	0.0485	4
10% novel Ag_3PO_4 modified tubular porous carbon nitride (Ag_3PO_4@$TPCN_{12}$)	2	0.5	45	~100	0.0927	5
0.1 wt% Au-BiOBr	5	1	30	95.8	0.0901	6
0.1 La doped $BiFeO_3$ composites (La-BFOs)	5	0.2	30	94.5	0.101	7
Defective TiO_2	10	0.5	300	69.3	0.0034	8
Meso-$Bi_{12}O_{17}Cl_2$/BiOCl-O_V	10	1	30	83	unknown	9
PM6:Y6:ITCPTC	**10**	**0.1**	**20**	**99.58**	**0.02477**	**This study**



Atom	Charge (0) (e/Å^3)	Charge (+1) (e/Å^3)	Charge (-1) (e/Å^3)	f^0	f^+	f^-
C1	-0.2342	-0.33439	-0.15857	**0.08791**	0.10019	0.07563
C2	-0.23607	-0.26074	-0.21011	0.025315	0.02467	0.02596
C3	-0.21163	-0.24786	-0.17988	0.03399	0.03623	0.03175
C4	-0.07499	-0.10586	-0.06523	0.020315	0.03087	0.00976
C5	0.14942	0.09943	0.17322	0.036895	0.04999	0.0238
C6	-0.23481	-0.24264	-0.23307	0.004785	0.00783	0.00174
C7	-0.22579	-0.31247	-0.13199	**0.09024**	0.08668	0.0938
C8	-0.19874	-0.31491	-0.13547	**0.08972**	0.11617	0.06327
C9	-0.08265	-0.08494	-0.04599	0.019475	0.00229	0.03666
C10	0.18622	0.14753	0.21536	0.033915	0.03869	0.02914
N11	-0.52174	-0.50484	-0.45255	0.026145	-0.0169	0.06919
C12	-0.20923	-0.24753	-0.17782	0.034855	0.0383	0.03141
C13	-0.23709	-0.25579	-0.20765	0.02407	0.0187	0.02944
C14	-0.22721	-0.31187	-0.13609	**0.08789**	0.08466	0.09112
C15	-0.21484	-0.2226	-0.21516	0.00372	0.00776	-0.00032
C16	0.83174	0.83227	0.81974	-0.006265	-0.00053	-0.012
N17	-0.898	-0.90548	-0.87374	0.01587	0.00748	0.02426
O18	-0.64686	-0.6791	-0.5865	0.0463	0.03224	0.06036

Fig. S7. chemical structure (upper) and Fukui index of carbamazepine (lower).

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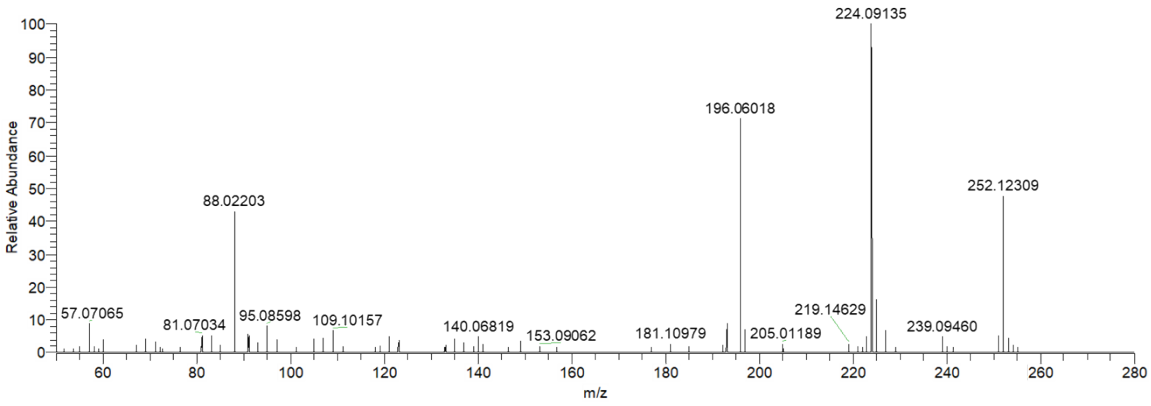

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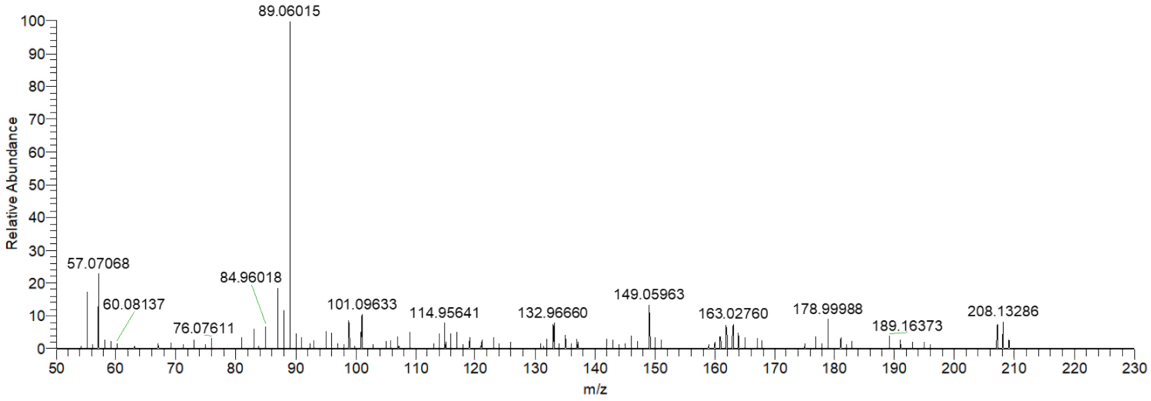

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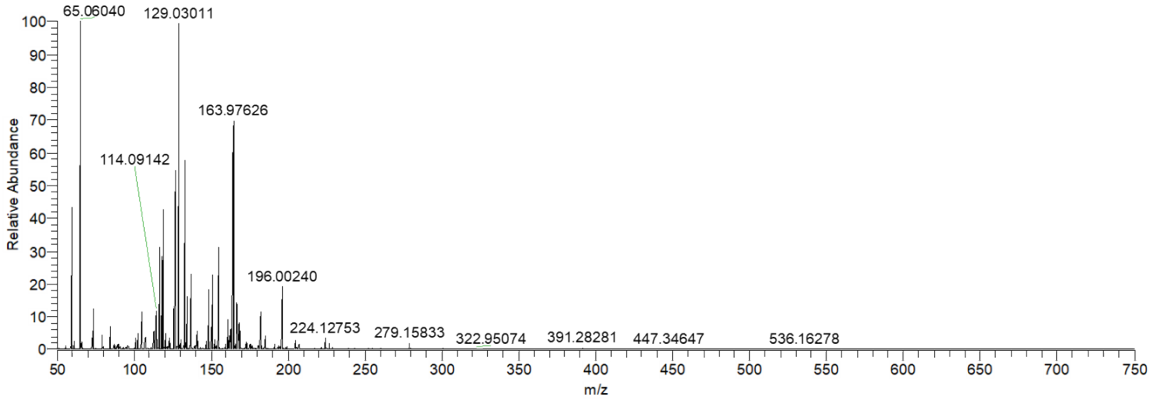

84 **Fig. S8**. LCMS (ESI) data of degraded carbamazepine solutions scanned in the range of

85 50-750 m/z show signals of intermediate formation of carbamazepine.

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