

Boosting Pollutant Degradation with Simultaneous H₂O₂ Production from its Electron Delocalization and Excitation Co-triggered by Microelectric field and Visible-light

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Fig. S11 (a) EPR trapping experiment of photocatalytic generation of $\bullet\text{OH}$, and (b) the absorbed energy of O_2 on the surface of RSN.

Text Captions

Text S1 Calculation of CO_2 selectivity.

Table Captions

Table S1 BET surface area of CN and RSN.

Table S2 The proportion of peaks of C-XPS.

Table S3 Atomic electron of BPA in optimal absorbed model RSN-BPA.

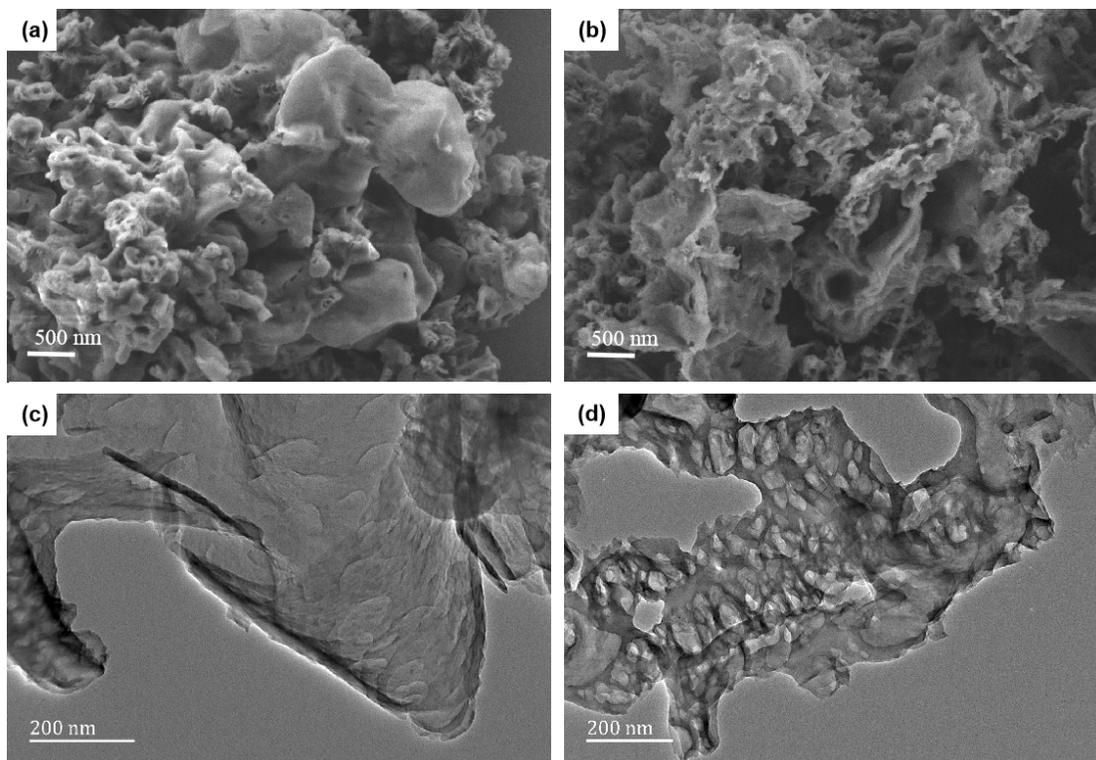


Fig. S1 SEM and TEM images of (a, c) CN and (b, d) RSN10.

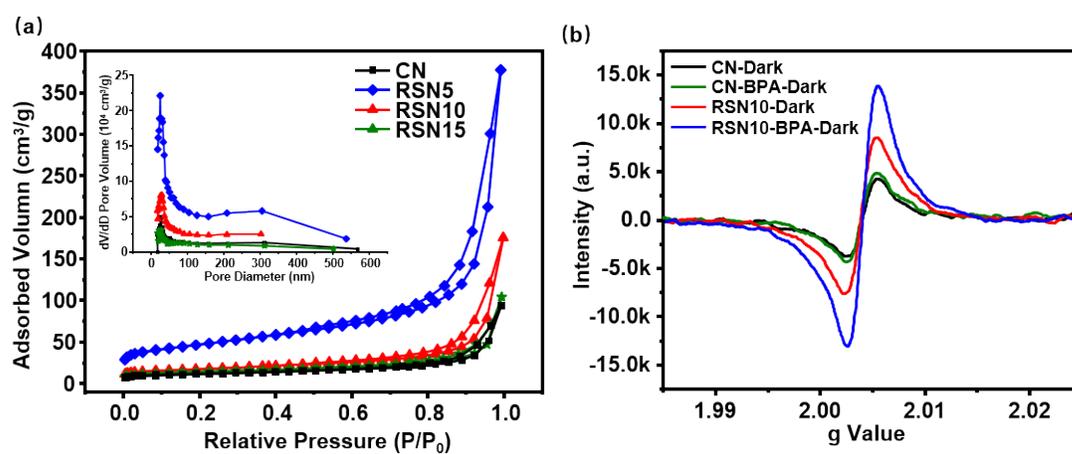


Fig. S2 (a) BET and pore distribution of CN and RSN; (b) EPR signal of the as-prepared samples in dark conduction.

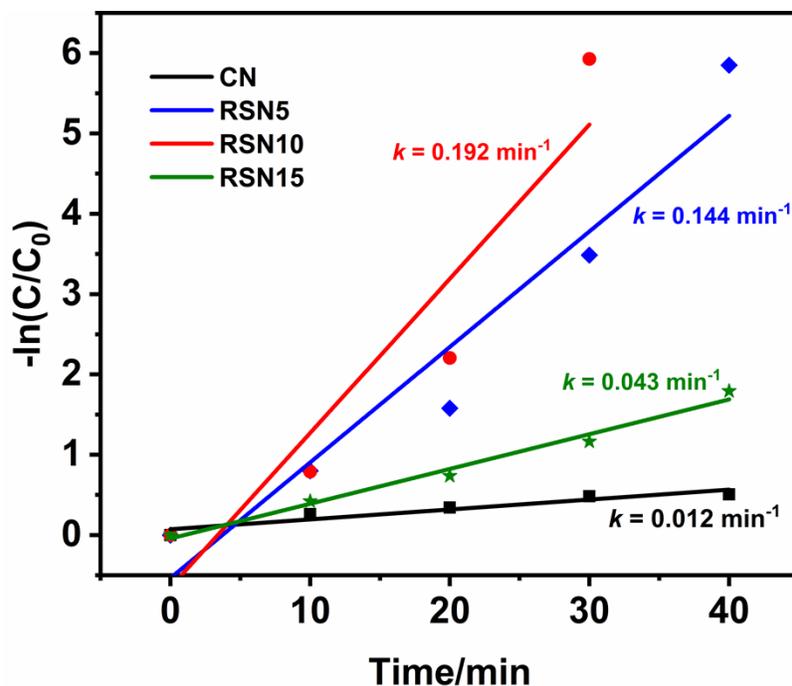


Fig. S3 Pseudo-first-order kinetics of BPA degradation with CN and RSN under light irradiation.

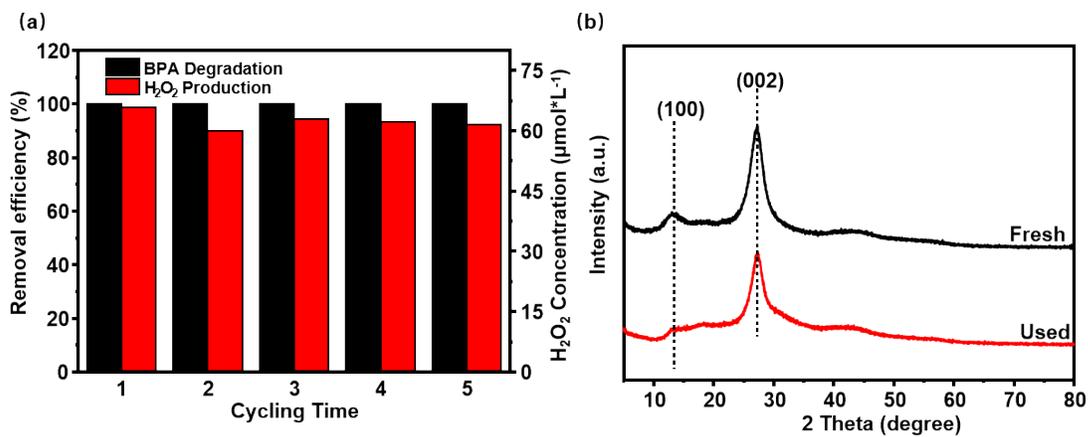


Fig. S4 (a) Cycling photocatalytic degradation of BPA with in-situ H₂O₂ production and (b) XRD patterns of RSN10 before and after cycling experiments.

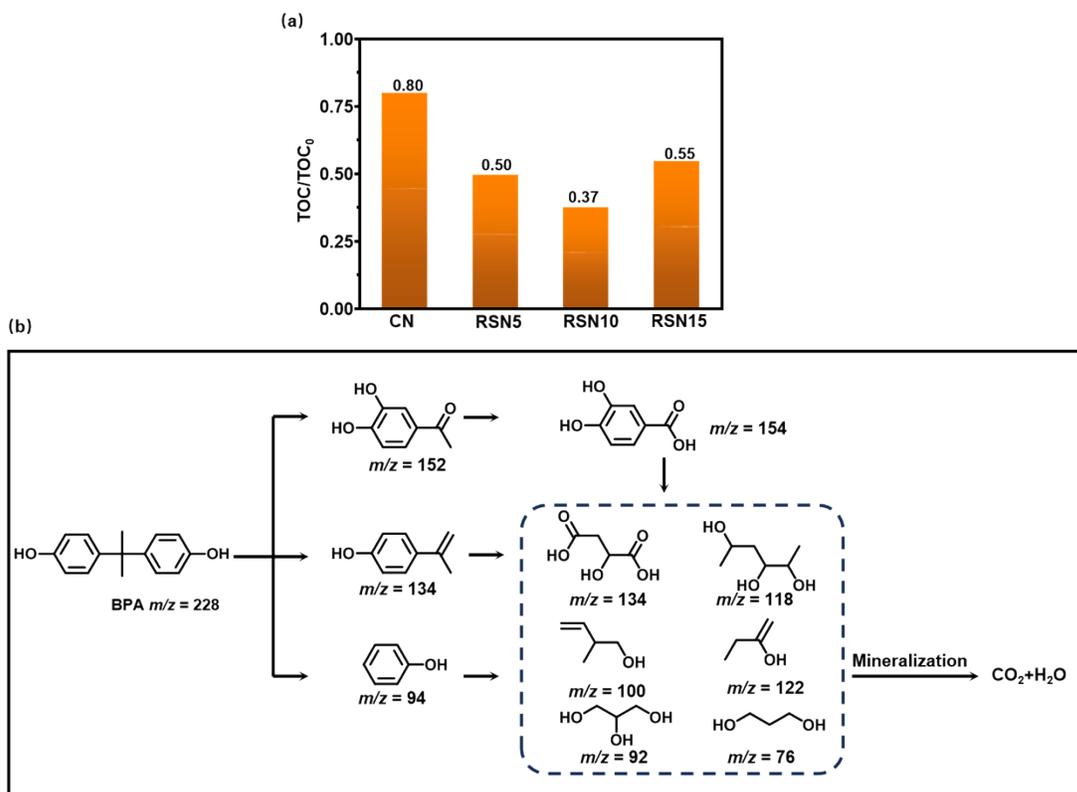


Fig. S5 (a) TOC removal of BPA and (b) its corresponding photocatalytic degradation route.

Text S1 Calculation of CO₂ selectivity.

BBPA : BPA concentration before irradiation

ABPA : BPA concentration after irradiation

BTOC : TOC value before irradiation

ATOC : TOC value after irradiation

$$TTOC : \text{Theoretical TOC value after irradiation} = \frac{ABPA \times BTOC}{BBPA}$$

$$\text{CO}_2 \text{ selectivity} = \frac{BTOC - ATOC}{BTOC - TTOC} \times 100\%$$

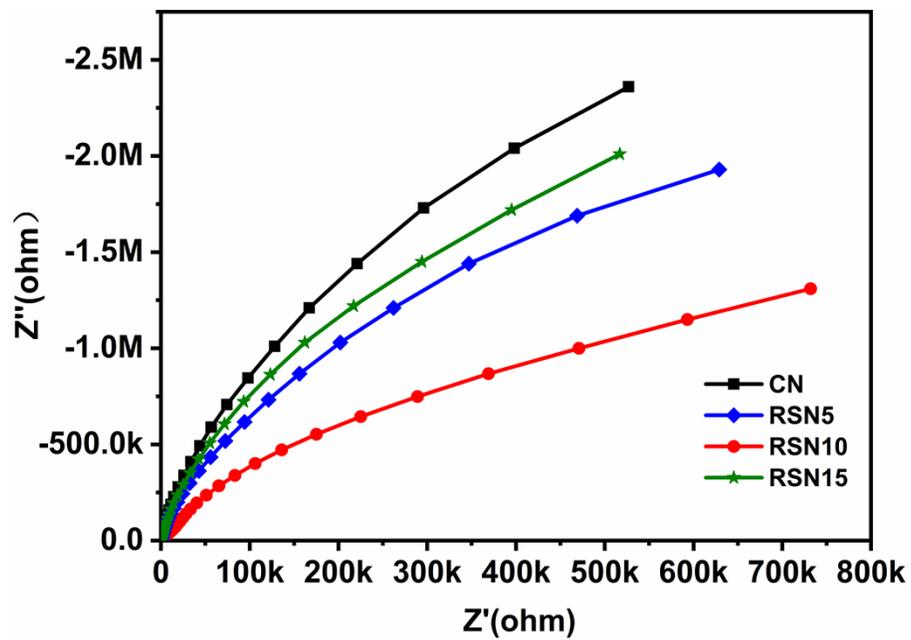


Fig. S6 EIS curves of as-prepared samples.

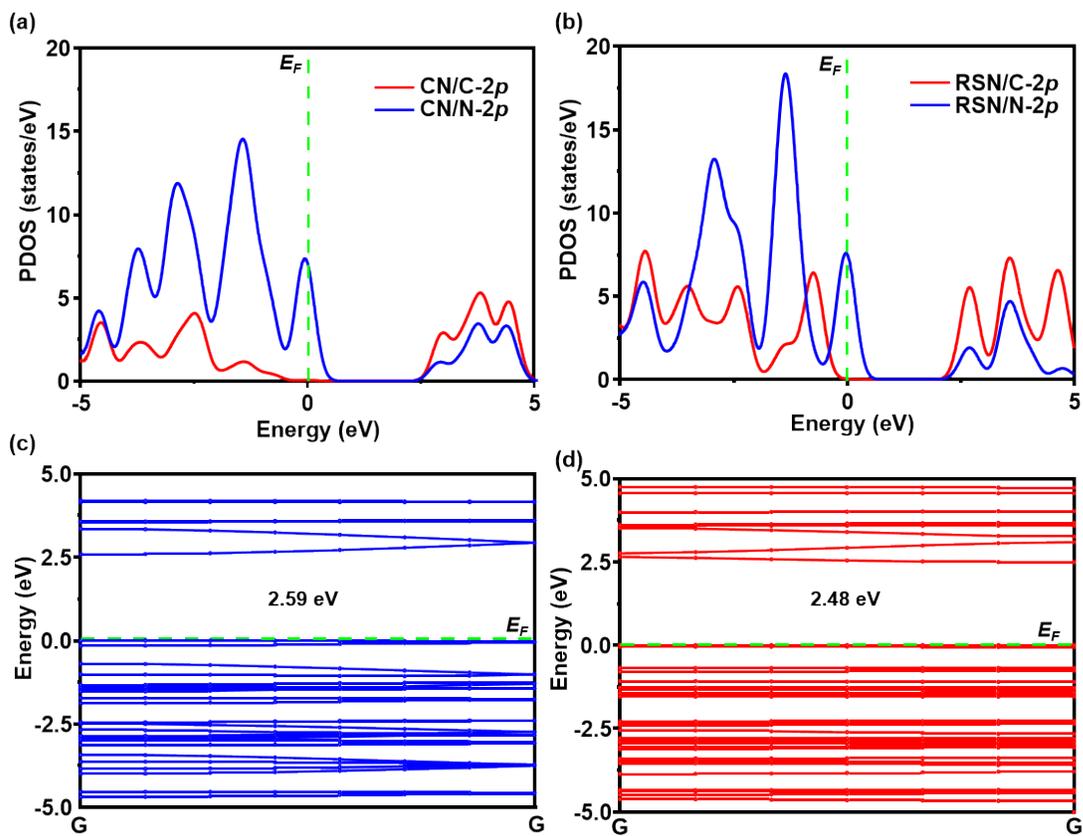


Fig. S7 PDOS distribution of (a) CN model and (b) RSN model, and the corresponding HOMO-LUMO energy level of (c) CN model and (d) RSN model.

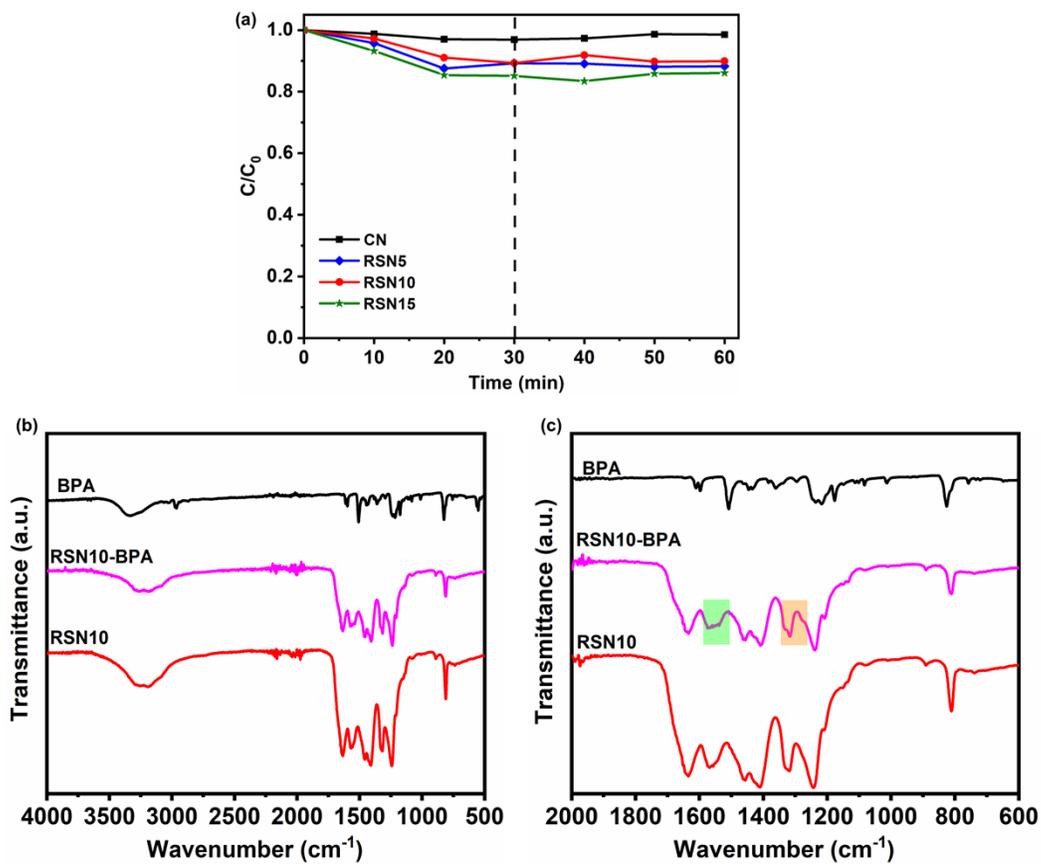


Fig. S8 (a) The adsorption-desorption equilibrium of BPA and (b-c) corresponding FTIR spectra of RSN10 and the absorbed samples.

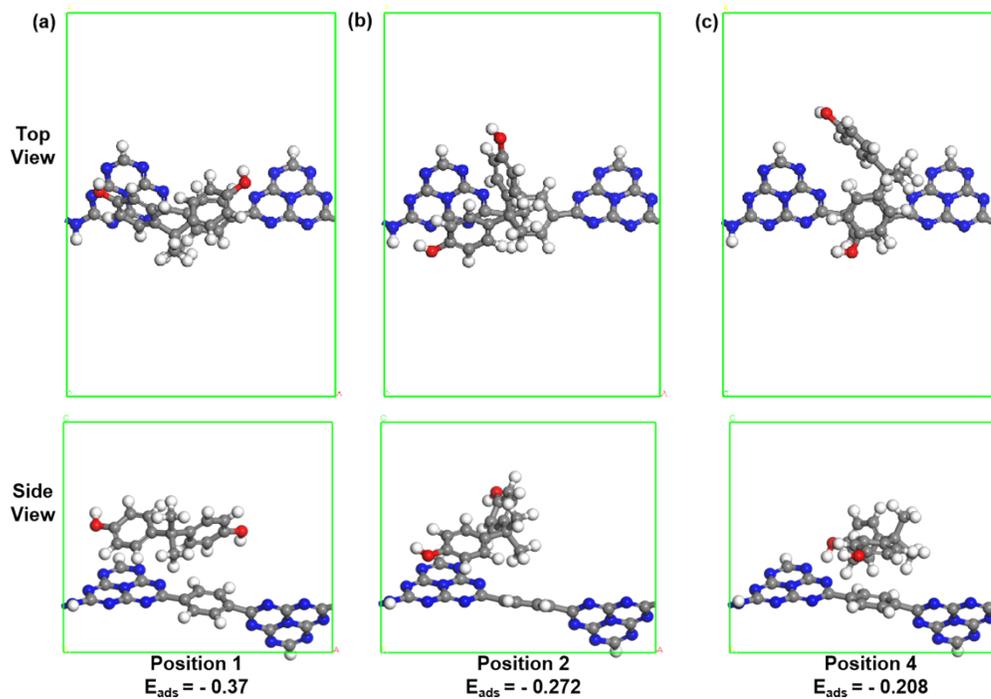


Fig. S9 The adsorbed model of BPA on the surface of RSN and the corresponding absorbing energy.

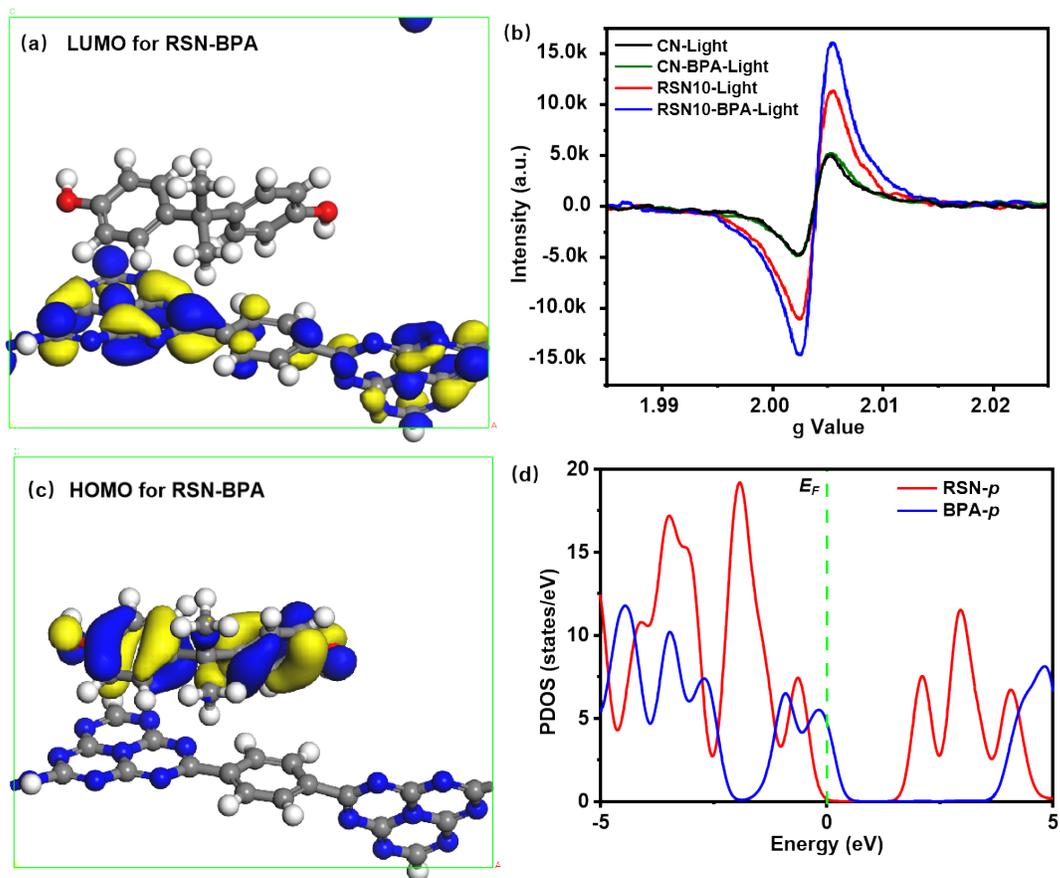


Fig. S10 (a) LOMO distribution of RSN-BPA model, (b) EPR spectra of CN and RSN10 with and without BPA absorption under light irradiation LUMO distribution; (c) HUMO distribution of RSN-BPA model, and (d) PDOS distribution distribution of RSN-BPA model.

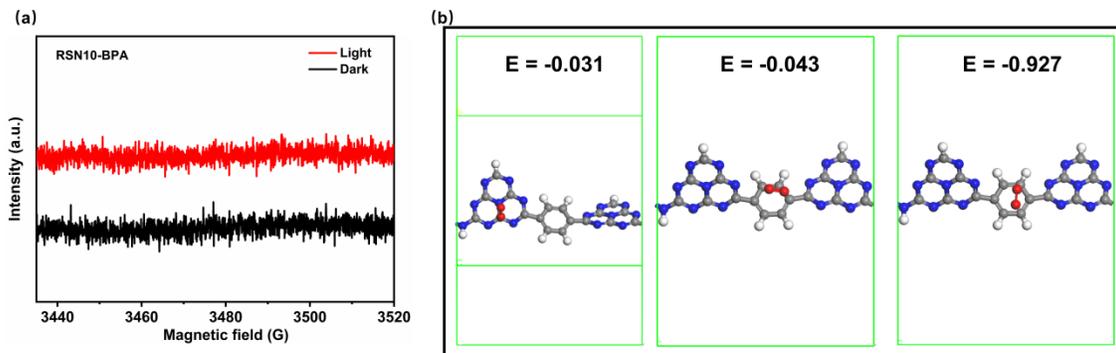


Fig. S11 (a) EPR trapping experiment of photocatalytic generation of $\bullet\text{OH}$, and (b) the absorbed energy of O_2 on the surface of RSN.

Table S1 BET surface area of CN and RSN.

Sample	ABET (m^2/g)	Vpore (cm^3/g)	dpore(nm)
CN	42.4435	0.141233	18.0356
RSN5	167.2043	0.574007	16.3569
RSN10	63.1741	0.118827	9.6088
RSN15	43.7187	0.150442	22.8219

Table S2 The proportion of peaks of C-XPS.

Sample	Peak area content (%)		
	C-C/C=C	C-NH _x /C=O	N-C=N
CN	14.90	13.82	71.28
RSN10	18.71	10.03	71.26

Table S3 Atomic electron of BPA in optimal absorbed model RSN-BPA.

C	0.349
C	-0.151
C	-0.099
C	0.067
C	-0.091
C	-0.185
C	0.062
C	-0.11
C	-0.169
C	0.351
C	-0.17
C	-0.077
O	-0.513
H	0.283
H	0.094
H	0.091
H	0.1
H	0.105
C	-0.202
C	-0.29
C	-0.314
O	-0.519
H	0.284
H	0.114
H	0.11
H	0.111
H	0.15
H	0.108
H	0.111
H	0.098
H	0.132
H	0.095
H	0.086
Total electron	0.011
