

Supplementary Information

Domino effect enables dynamic electronic structure evolution for stable and efficient water purification

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Supplementary Methods

Supplementary Method 1. Process of X-ray absorption spectroscopy data

The raw X-ray absorption spectroscopy (XAS) data was processed using the Athena software package. Energy calibration was first performed using a Co foil reference, with the maximum of the first derivative of the Co K-edge absorption spectra (7709 eV) defined as the reference energy to correct for any energy drift during data acquisition. Subsequently, pre-edge background subtraction and post-edge normalization were carried out to remove non-structural contributions and normalize the absorption intensity, yielding normalized X-ray absorption near-edge structure (XANES) spectra for further analysis. For EXAFS analysis, the normalized $\chi(E)$ data were converted into $\chi(k)$ functions and weighted by k^3 to enhance the contribution of high- k oscillations. Subsequently, Fourier transformation was performed to convert the $\chi(k)$ data into R-space, providing information on the local coordination environment surrounding the absorbing atom. EXAFS fitting was carried out using the Artemis software package. The amplitude reduction factor (S_0^2) was determined from the corresponding reference sample and fixed during the fitting process. Structural parameters, including coordination number (CN), bond distance (R), Debye–Waller factor (σ^2), and energy shift (ΔE_0), were optimized by nonlinear least-squares fitting. In

EXAFS fitting of metal foils and metal oxide standards, the coordination number was typically not treated as a free fitting parameter, instead, it was fixed according to the known crystallographic structure. Only in the case of synthesized or unknown samples was the coordination number released and refined during fitting.

Supplementary Method 2. Isotope liquid mass spectrometry testing method

The preparation of a solution containing 5 mM benzoic acid (BA) was to be undertaken, for which 1 mL of H_2^{16}O and 1 mL of H_2^{18}O are to be utilized. Subsequently, 1 mg 4Co/CN or 4MgCo/CN should be added, and the mixture thoroughly agitated. PMS should then be added for the reaction with visible light irradiation. The reaction solution must then be filtered through a 0.22 μm membrane. The mass-to-charge (m/z) value of *p*-hydroxybenzoic acid (*p*-HBA) was determined by means of mass spectrometry. In the control experiment, 2 mL of water was utilized to prepare a 5 mM benzoic acid solution, followed by the addition of 1 mg 4Co/CN or 4MgCo/CN. Following a thorough mixing process, PMS was added to initiate the reaction. The quantification of BA degradation and *p*-HBA formation was conducted through the utilization of high-performance liquid chromatography (HPLC), utilizing an apparatus equipped with a UV detector and a C18 column (4.6×250 mm, 5 μm diameter). For the analysis of BA, the mobile phase comprised a mixture of acetonitrile and 0.1% trifluoroacetic acid solution (volume ratio 35:65), with a flow rate of 1 mL/min, and the detector wavelength was set at 271 nm. The mobile phase employed for the determination of *p*-HBA consisted of a mixture of acetonitrile and 0.1% trifluoroacetic acid solution (35:65 v/v), with a flow rate of 1 mL/min and a detector wavelength set at 255 nm.

Supplementary Method 3. Quantification of H₂O₂ in-situ generation

The H₂O₂ concentration was detected by the iodometric method. A 0.01 M solution was prepared by dissolving H₂₄Mo₇N₆O₂₄·4H₂O in 5 mL of deionized water. Meanwhile, a 0.1 M KI solution was obtained by dissolving potassium iodide in 10 mL of deionized water. During different intervals, 0.5 mL of the reaction solution was collected and mixed with 2 mL of KI solution, followed by the addition of 50 µL ammonium molybdate tetrahydrate solution. The resulting mixture was vigorously shaken, allowed to stand for 4 min, and subsequently analyzed using a UV-Vis spectrophotometer at a maximum absorption wavelength of 352 nm.

Supplementary Method 4. Mass spectrometry detection method for degradation product

The degradation products were identified by the liquid chromatograph mass spectrometer (LC-MS). The mass spectrometer analysis was performed in a positive ion mode over the range of m/z 50-750 with an electrospray ionization (ESI) source under the following conditions: capillary voltage 3500 V, cone voltage 30 V, source temperature 110 °C, desolvation temperature 380 °C, cone gas flow 80 L/h and desolvation gas flow 600 L/h.

Supplementary Method 5. Theoretical toxicity evaluation of CBZ and its degradation products

The acute toxicity of *Daphnia magna* LC₅₀, Oral rat LD₅₀, developmental toxicity and mutagenicity for CBZ and its products were theoretically assessed by quantitative structure-activity relationship (QSAR) prediction using the Toxicity Estimation Software Tool (T.E.S.T.) in the consensus method with four evaluation criteria for acute toxicity of *Daphnia magna* and Oral rat toxicity, developmental toxicity and mutagenicity. The details were as follows:

(1) Acute toxicity to *Daphnia magna* was evaluated using the 48-h LC₅₀, defined as the concentration of a chemical that caused 50% of *Daphnia magna* to die after 48 h. An increase in the theoretical LC₅₀ value of the degradation products compared to the parent contaminant indicated a reduction in toxicity, whereas a decrease suggested the formation of more toxic intermediates.

(2) Acute toxicity to Oral rat was assessed based on the LD₅₀, which was the dosage of chemical that caused the death of 50% of rats after oral ingestion. Predicted LD₅₀ values were categorised into four toxicity classes: very toxic, toxic, harmful, and non-toxic. An ideal theoretical result for degradation products relative to the parent contaminant was a shift in toxicity classification toward the non-toxic one.

(3) Developmental toxicity was assessed to evaluate the potential for causing developmental abnormalities. The parent contaminant and its degradation products were classified as either a developmental toxicant or a non-developmental toxicant. The

ideal theoretical result was a non-toxicant, indicating a reduction in toxicity of degradation product compared to the parent contaminant.

(4) Mutagenicity was used to evaluate the potential for causing genetic mutations. According to the T.E.S.T. classification standard, a predicted value greater than 0.5 indicated a positive result, while a value below 0.5 indicated a negative result. Therefore, the ideal theoretical result of the degradation process was to achieve the negative mutagenicity.

Supplementary Method 6. The experimental method for bean sprouts and evaluation method for mean length

Mung bean seeds were purchased from a local market in Changchun, China. Seeds were surface-disinfected by soaking in a 0.5% sodium hypochlorite solution for 10 min, rinsed five times with deionized water, and then dried on filter paper for germination testing. 5 mL sample obtained from the 4Co/CN SACs/PMS/vis system and 4MgCo/CN DSACs/PMS/vis system, reacted for 4, 12, and 24 min respectively, were poured into 90 mm diameter Petri dishes. Ten selected seeds were evenly distributed on each dish. Place in an artificial climate incubator for dark cultivation at 25 °C and 70% relative humidity. Germination was determined when the root tip extended beyond half the seed length. After 5 days of cultivation, record the stem and mean length of all germinated seeds.

Supplementary Method 7. Electrical energy per order calculation

The economic feasibility was evaluated by electrical energy per order (EE/O), which was defined as “electric energy in kWh consumed to oxidize the contaminant by 1 m³ of wastewater. The corresponding EE/O value in the PMS/vis system was calculated according to the Eq. 1:

$$EE/(O_{vis+oxidant}) = \frac{P \times t \times 1000}{V \times \log(C_0/C)} + \frac{Eq_{oxidant} \times [oxidant] \times 1000}{\log(C_0/C)} \quad (1)$$

Where P (kW) was electrical power, t (h) was degradation time, V (L) was solution volume, C₀ and C were initial and reaction concentration, respectively. Eq_{oxidant} represented equivalent electric energy consumption to generate per mole of PMS. [oxidant] was the PMS concentration in units of mol/L.

The equivalent electric energy consumption to generate per molar of oxidant was evaluated by Eq. 2.

$$Eq_{oxidant} = \frac{Price \times Mass}{10^6 \times Purity \times EC} \quad (2)$$

where Price was the average price of oxidant (\$ ton⁻¹); Mass was the molar mass of oxidant (g mol⁻¹); Purity is the purity of oxidant (%); EC was the average electricity cost (\$ kWh⁻¹). The average price of potassium persulfate (PMS, 99.0% by weight) in Alibaba.com was \$32.4, respectively. Given the average electricity cost is around 12 cent/kWh in the U.S., one mole PMS could be transformed into 0.084 kWh.

Supplementary Method 8. Linear combination fitting of Co and Mg K-edge XANES spectra

Linear combination fitting (LCF) of the normalized Co and Mg K-edge XANES spectra was performed to estimate the apparent average oxidation states of Co and Mg in 4MgCo/CN. For Co K-edge LCF, Co foil, CoO, and Co₂O₃ were selected as reference compounds for Co⁰, Co²⁺, and Co³⁺, respectively. For Mg K-edge LCF, Mg foil and MgO were selected as reference compounds for Mg⁰ and Mg²⁺, respectively.

All XANES spectra were first energy calibrated and normalized using the same procedure. The LCF analysis was conducted in the XANES region based on the normalized $\mu(E)$ spectra. During fitting, the sum of all weighting factors was constrained to unity, all weighting factors were constrained between 0 and 1, and the energy shift, E_0 , of each reference spectrum was fixed at 0 eV. The fitting quality was evaluated using the R-factor, chi-square, and reduced chi-square values.

For Co K-edge LCF, the fitted spectrum was expressed as:

$$\mu_{\text{fit}}(E) = w_{\text{Co foil}} \mu_{\text{Co foil}}(E) + w_{\text{CoO}} \mu_{\text{CoO}}(E) + w_{\text{Co}_2\text{O}_3} \mu_{\text{Co}_2\text{O}_3}(E) \quad (3)$$

where $w_{\text{Co foil}}$, w_{CoO} , and $w_{\text{Co}_2\text{O}_3}$ are the fitted weighting factors of Co foil, CoO, and Co₂O₃, respectively. The weighting factors were constrained as:

$$w_{\text{Co foil}} + w_{\text{CoO}} + w_{\text{Co}_2\text{O}_3} = 1 \quad (4)$$

The apparent average Co valence was calculated according to the assigned valence states of the reference compounds:

$$\text{Co valence} = 0 \times w_{\text{Co foil}} + 2 \times w_{\text{CoO}} + 3 \times w_{\text{Co}_2\text{O}_3} \quad (5)$$

For Mg K-edge LCF, the fitted spectrum was expressed as:

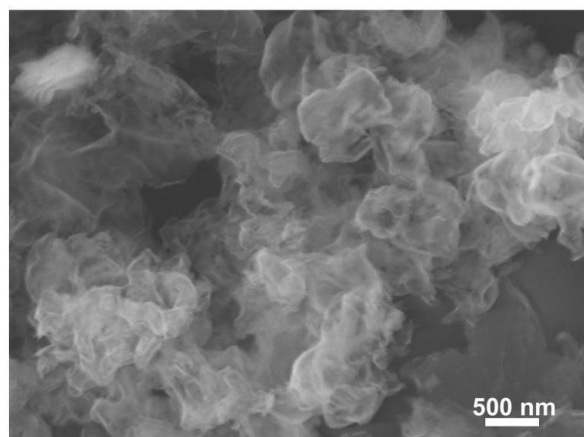
$$\mu_{\text{fit}}(E) = w_{\text{Mg foil}} \mu_{\text{Mg foil}}(E) + w_{\text{MgO}} \mu_{\text{MgO}}(E) \quad (6)$$

where $w_{\text{Mg foil}}$ and w_{MgO} are the fitted weighting factors of Mg foil and MgO, respectively. The weighting factors were constrained as:

$$w_{\text{Mg foil}} + w_{\text{MgO}} = 1 \quad (7)$$

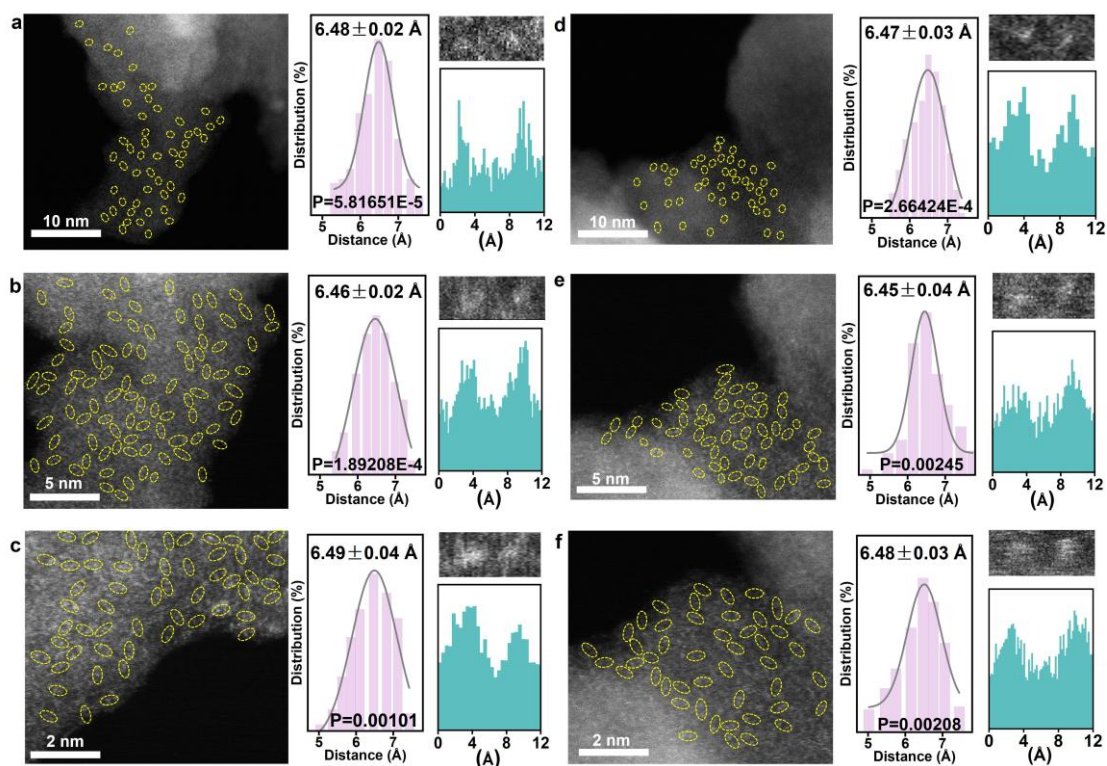
The apparent average Mg valence was calculated according to the assigned valence states of the reference compounds:

$$\text{Mg valence} = 0 \times w_{\text{Mg foil}} + 2 \times w_{\text{MgO}} \quad (8)$$

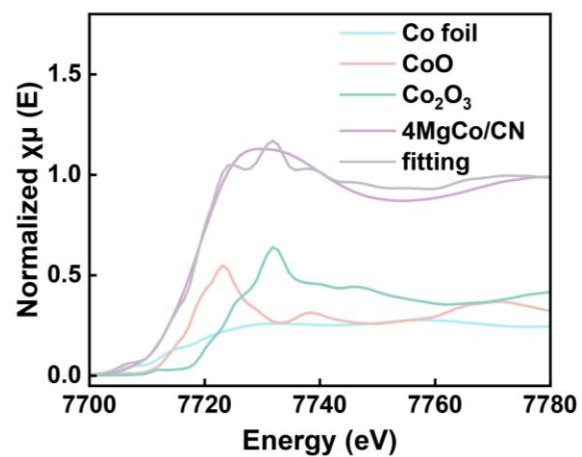


Supplementary Fig. 1. Scanning electron microscope (SEM) image of MgCo/CN DSACs. Image is representative of three independent measurements with similar results.

Scale bar: 500 nm

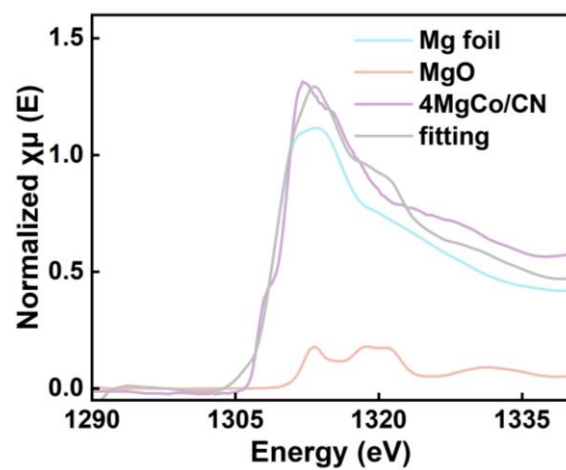


Supplementary Fig. 2. Aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (AC-HAADF-STEM) images of 4MgCo/CN DSACs with different magnifications at different regions and corresponding atomic distance distribution, respectively. Images are representative of three independent measurements with similar results. Scale bar is 10 nm (a,d), 5 nm (b,e) and 2 nm (c,f), respectively. The unedited AC-HAADF-STEM is added into the Source Data file.



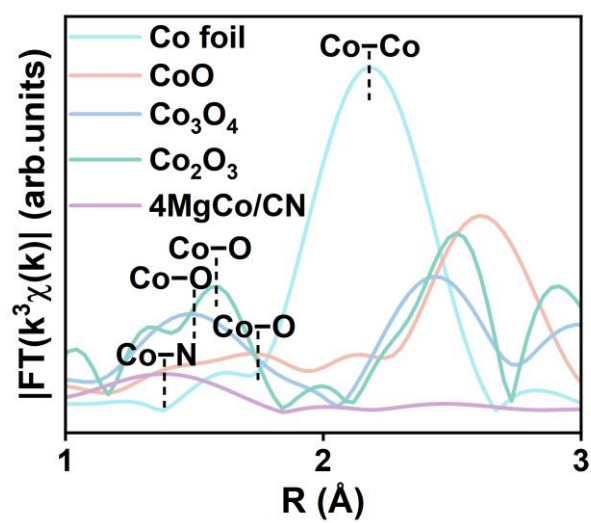
Supplementary Fig. 3. The linear combination fitting result for 4MgCo/CN DSACs.

Source data are provided as a Source Data file.

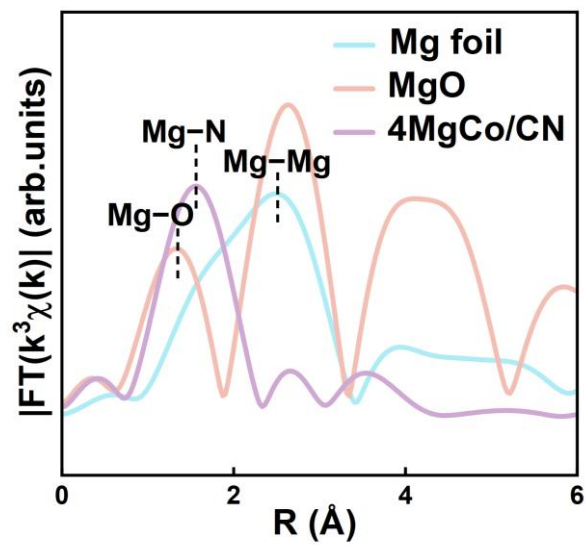


Supplementary Fig. 4. The linear combination fitting result for 4MgCo/CN DSACs.

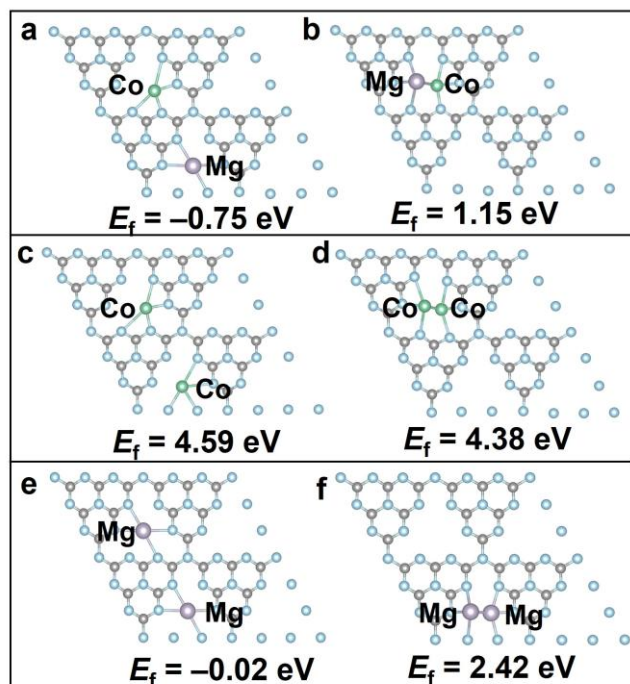
Source data are provided as a Source Data file.



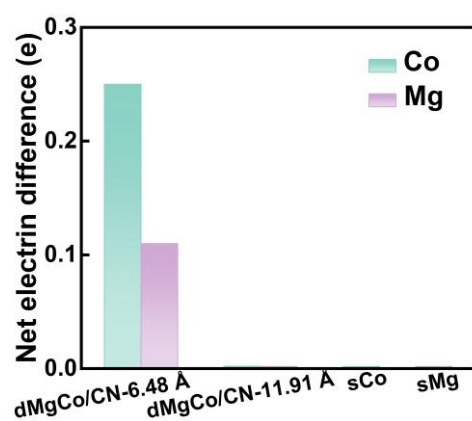
Supplementary Fig. 5. Fourier transformed (FT) k^3 -weighted Co K-edge extended X-ray absorption fine structure (EXAFS) spectra of 4MgCo/CN DSACs. Source data are provided as a Source Data file.



Supplementary Fig. 6. Fourier transformed (FT) k^3 -weighted Mg K-edge extended X-ray absorption fine structure (EXAFS) spectra of 4MgCo/CN DSACs. Source data are provided as a Source Data file.

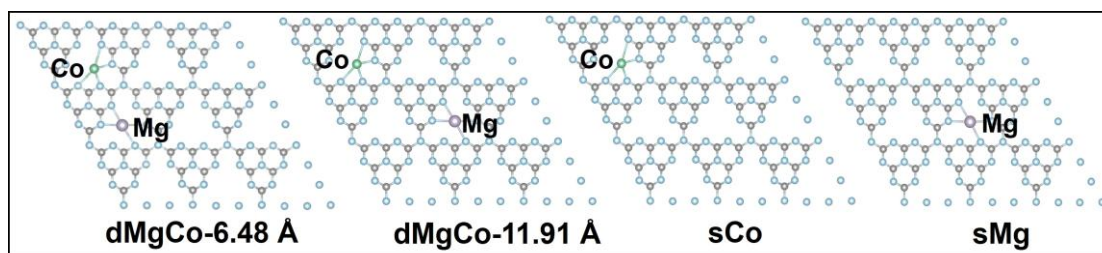


Supplementary Fig. 7. The formation energies for different catalysts. (a) MgCo/CN without the Mg–Co bond, (b) MgCo/CN with the Mg–Co bond, (c) CoCo/CN without Co–Co bond, (d) CoCo/CN with Co–Co bond, (e) MgMg/CN without Mg–Mg bond and (f) MgMg/CN with Mg–Mg bond.

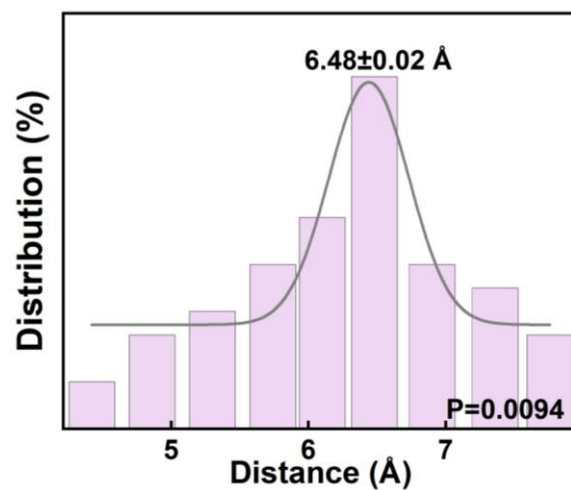


Supplementary Fig. 8. Net electron difference of Mg and Co in different catalysts.

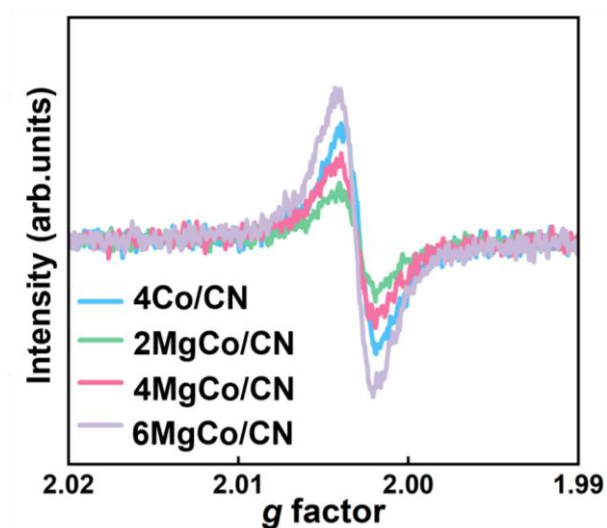
Source data are provided as a Source Data file.



Supplementary Fig. 9. Different catalyst modes for net electron difference evaluation.

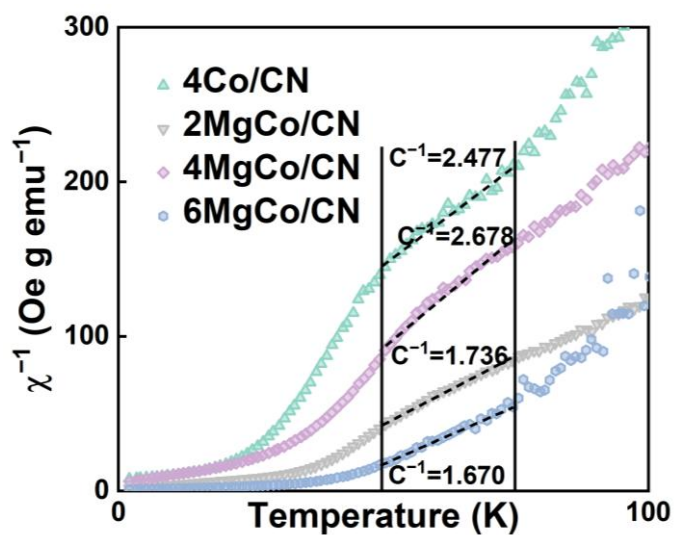


Supplementary Fig. 10. Histogram of the observed atomic distance of 4MgCo/CN DSACs obtained by the kernel method of frequency statistic and Gauss fitting of diatomic distances. Source data are provided as a Source Data file.

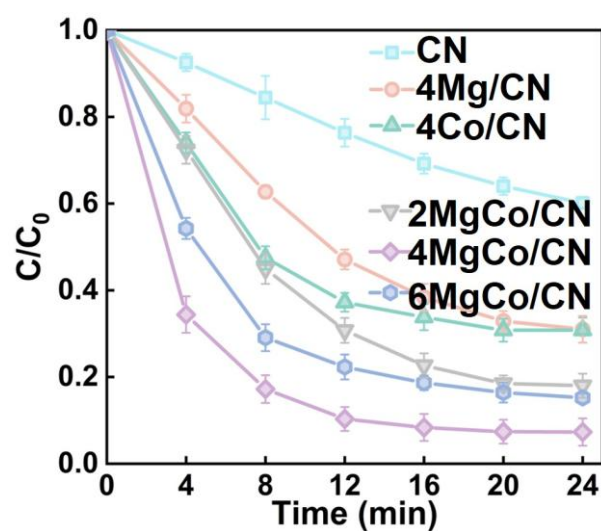


Supplementary Fig. 11. Electron paramagnetic resonance (EPR) spectra of catalysts.

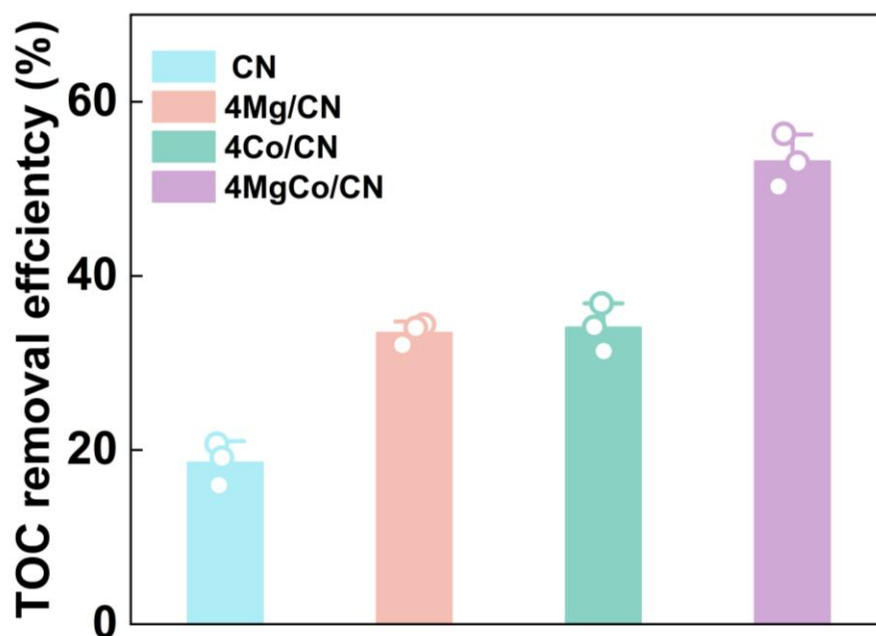
Source data are provided as a Source Data file.



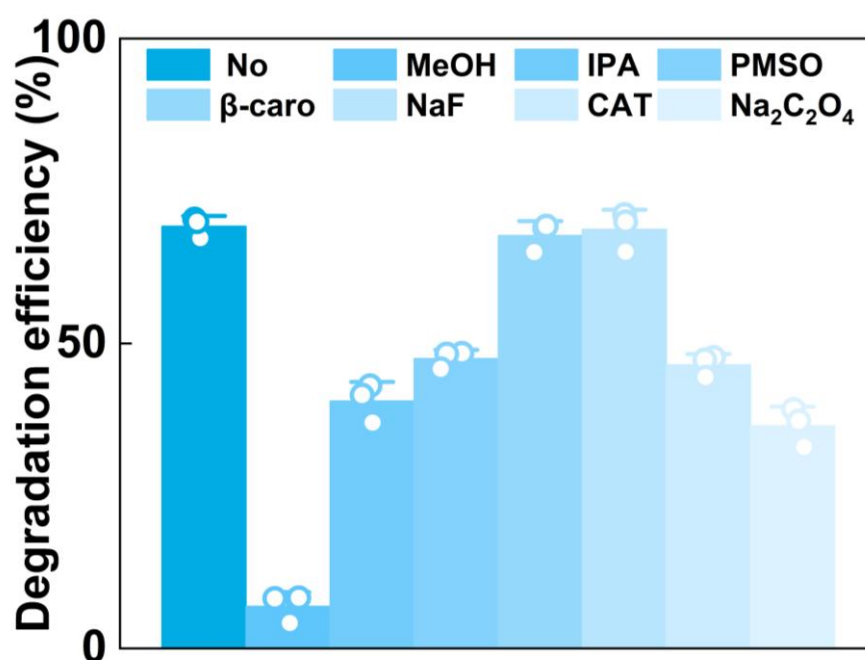
Supplementary Fig. 12. Temperature-dependent inverse susceptibilities fitted by Curie-Weiss law over different catalysts. Source data are provided as a Source Data file.



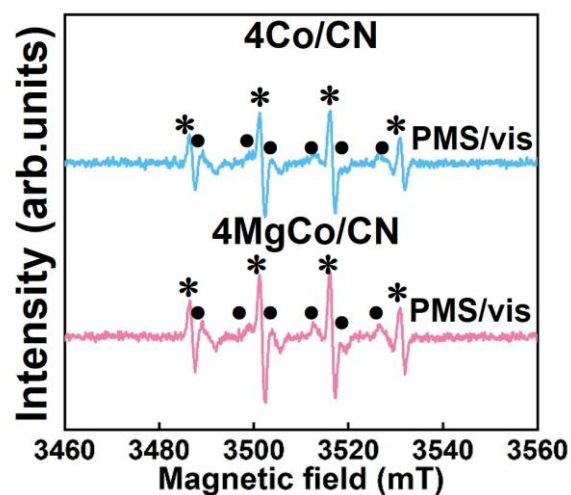
Supplementary Fig. 13. Degradation of carbamazepine (CBZ) by different catalysts in photo-Fenton-like system. Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



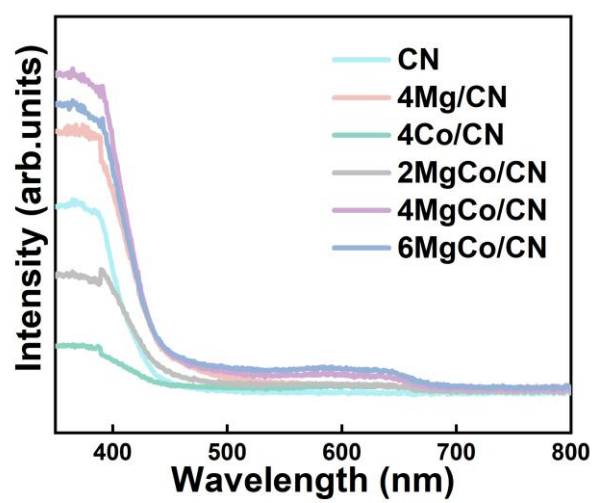
Supplementary Fig. 14. TOC removal of carbamazepine (CBZ) by different catalysts in the peroxymonosulfate (PMS)/visible light (vis) system. Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



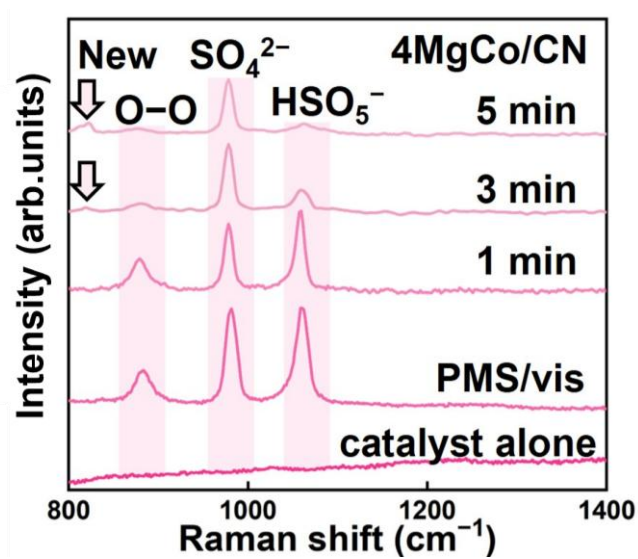
Supplementary Fig. 15. Degradation of carbamazepine (CBZ) by Co/CN SACs in the peroxymonosulfate (PMS)/visible light (vis) system. (MeOH: methanol, IPA: isopropyl alcohol, PMSO: methyl phenyl sulfoxide, β -caro: β -carotene, NaF: sodium fluoride, CAT: catalase, Na₂C₂O₄: sodium oxalate). Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



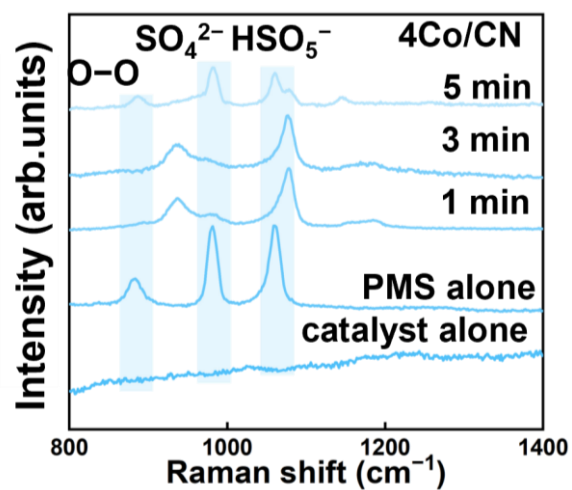
Supplementary Fig. 16. ESR spectra of sulfate radical ($\bullet\text{SO}_4^-$)-DMPO and hydroxyl radical ($\bullet\text{OH}$)-DMPO by 4MgCo/CN DSACs and Co/CN SACs in the peroxymonosulfate(PMS)/ visible light (vis) system. Solid circle represents the characteristic signal of $\bullet\text{SO}_4^-$ -DMPO and fancy symbol represents the characteristic signal of $\bullet\text{OH}$ -DMPO. Source data are provided as a Source Data file.



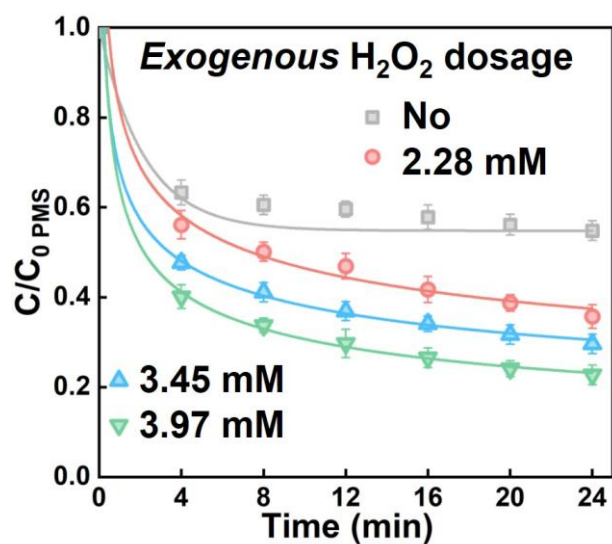
Supplementary Fig. 17. Diffuse reflectance spectroscopy (DRS) of catalysts. Source data are provided as a Source Data file.



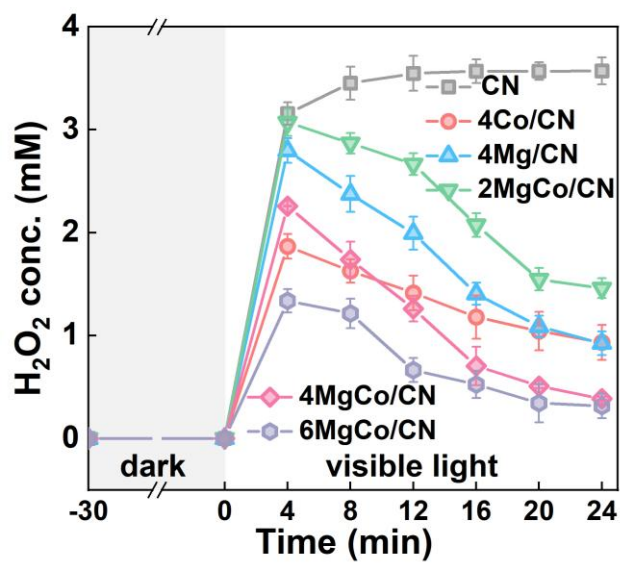
Supplementary Fig. 18. In-situ Raman of 4MgCo/CN DSACs with peroxymonosulfate(PMS)/ visible light (vis) at different reaction time. Source data are provided as a Source Data file.



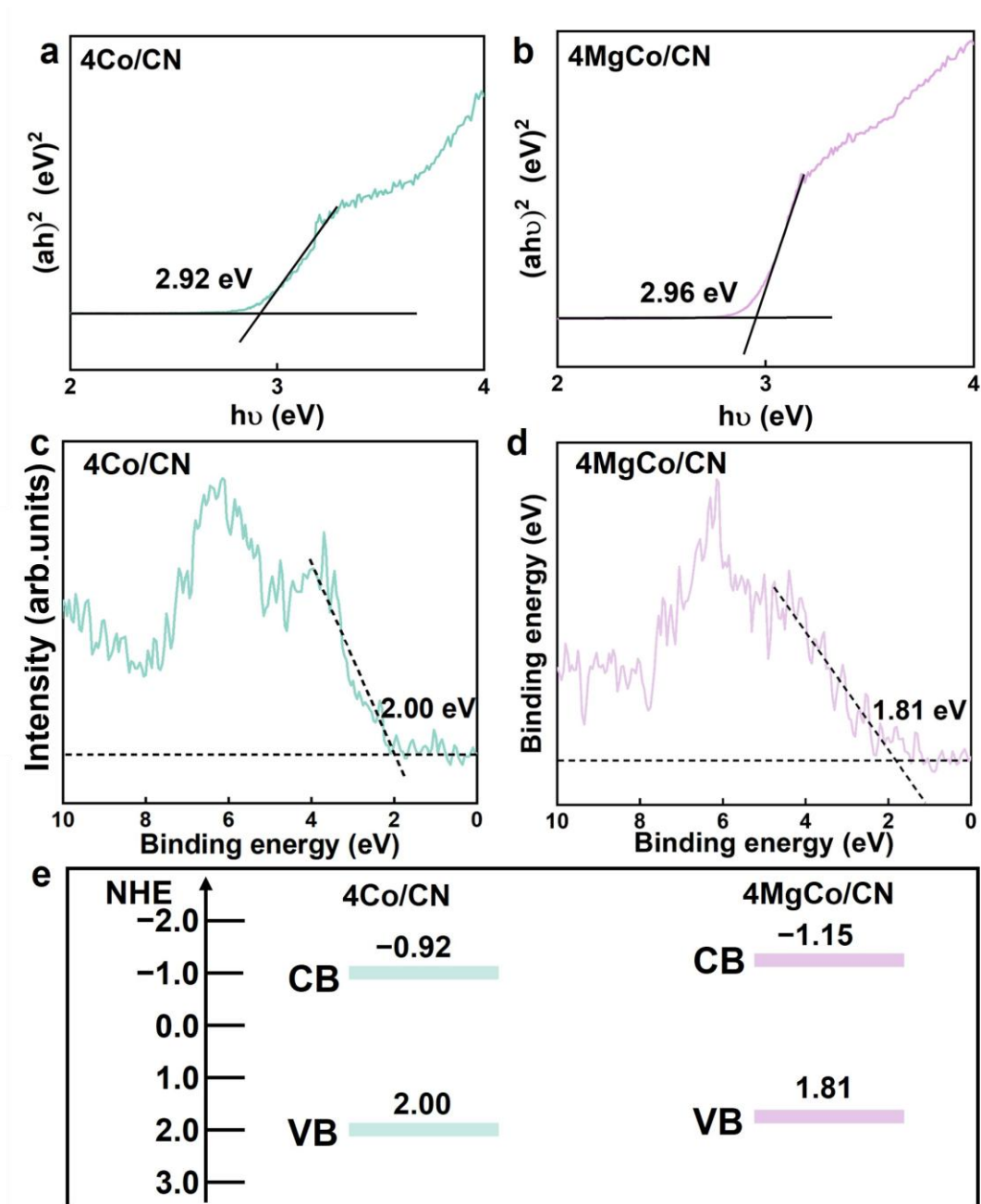
Supplementary Fig. 19. In-situ Raman of 4Co/CN SACs with peroxymonosulfate (PMS) at different reaction time. Source data are provided as a Source Data file.



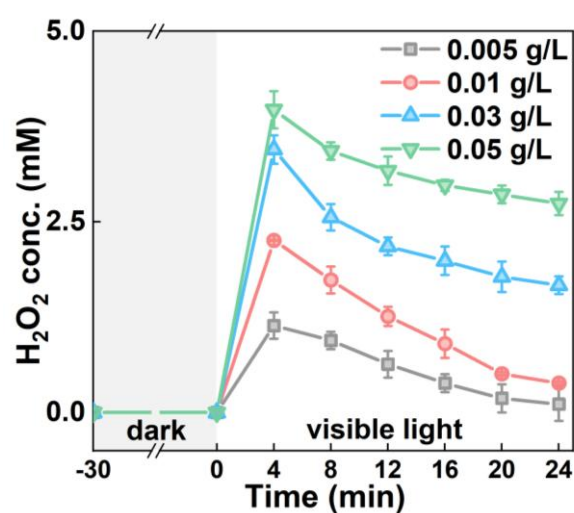
Supplementary Fig. 20. Peroxymonosulfate activation by 4MgCo/CN DSACs with different H₂O₂ dosage. Data are presented as mean values $\pm$ SD from three independent experiments (n = 3). Source data are provided as a Source Data file.



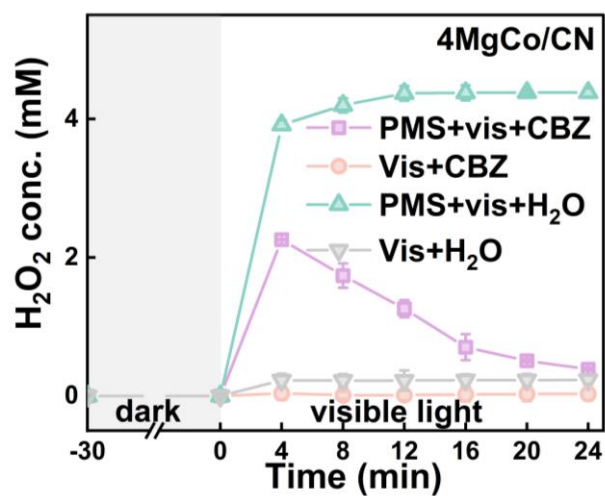
Supplementary Fig. 21. In-situ H₂O₂ production by different catalysts. Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



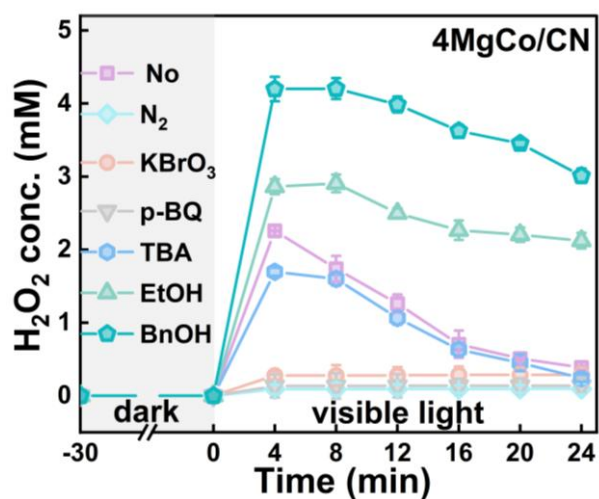
Supplementary Fig. 22. (a,b) Band gap of 4Co/CN SACs and 4MgCo/CN DSACs; (c, d) valence band (VB) spectra of 4Co/CN SACs and 4MgCo/CN DSACs; (e) energy band level structure with conduction band (CB) and valence band (VB). Source data are provided as a Source Data file.



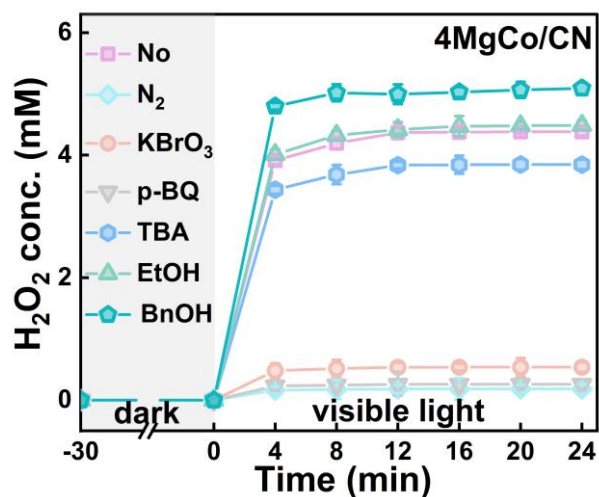
Supplementary Fig. 23. In-situ H_2O_2 production by 4MgCo/CN DSACs with different dosages. Grey represents the adsorption-desorption process under the dark condition. Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



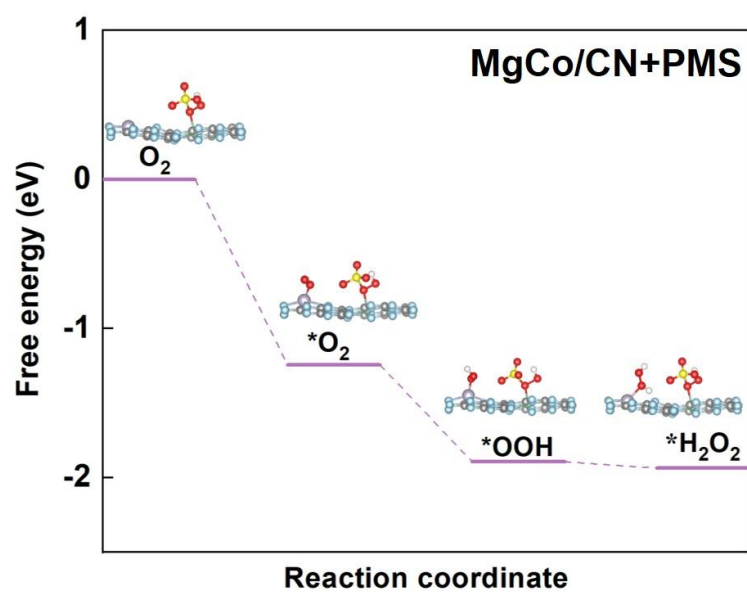
Supplementary Fig. 24. H₂O₂ generation concentration by 4MgCo/CN DSACs under different conditions, respectively. Grey represents the adsorption-desorption process under the dark condition. Data are presented as mean values $\pm$ SD from three independent experiments (n = 3). Source data are provided as a Source Data file.



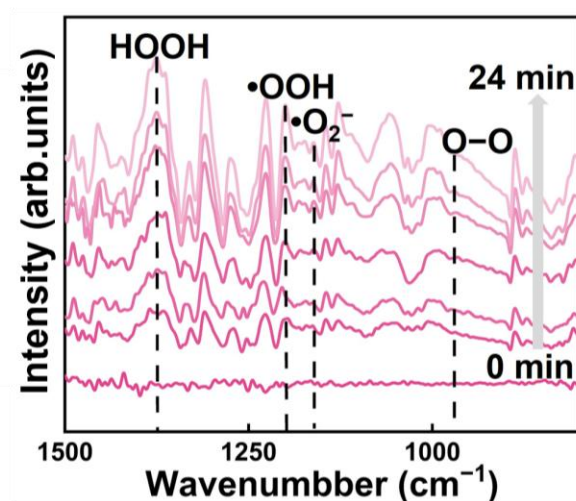
Supplementary Fig. 25. H_2O_2 generation by 4MgCo/CN DSACs in the peroxymonosulfate (PMS)/visible light (vis)/carbamazepine (CBZ) system with different scavengers. (N_2 : nitrogen, KBrO_3 : potassium bromate, p-BQ: p-benzoquinone, TBA: tert-butyl alcohol, EtOH: ethanol, BnOH: benzyl alcohol). Grey represents the adsorption-desorption process under the dark condition. Data are presented as mean values $\pm$ SD from three independent experiments ($n = 3$). Source data are provided as a Source Data file.



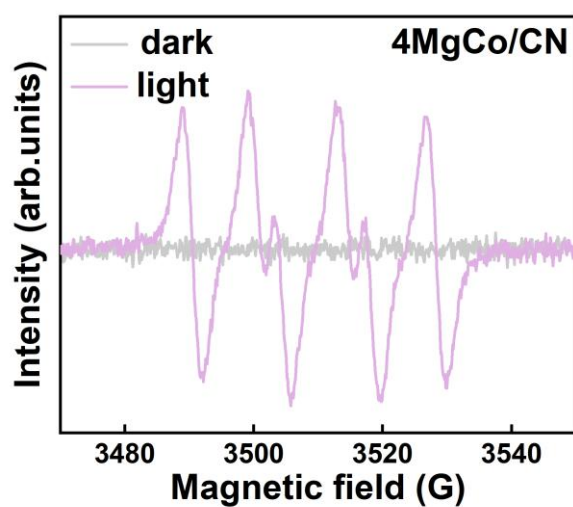
Supplementary Fig. 26. H₂O₂ generation by 4MgCo/CN DSACs in the peroxymonosulfate (PMS)/visible light (vis) system with different scavengers. (N₂: nitrogen, KBrO₃: potassium bromate, p-BQ: p-benzoquinone, TBA: tert-butyl alcohol, EtOH: ethanol, BnOH: benzyl alcohol). Data are presented as mean values $\pm$ SD from three independent experiments (n = 3). Source data are provided as a Source Data file.



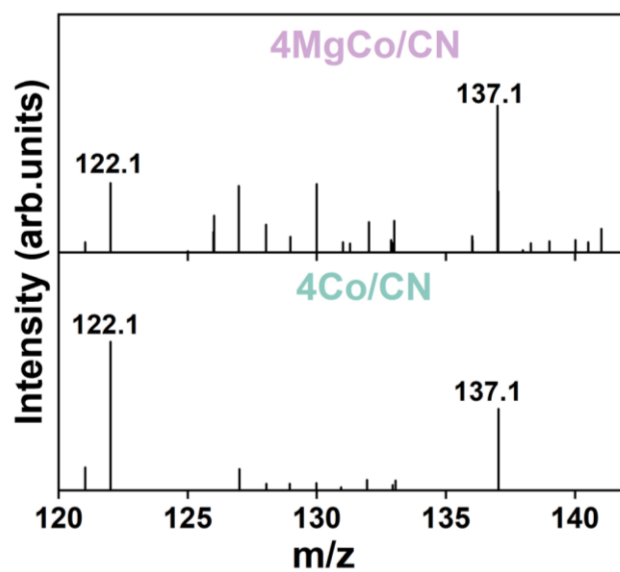
Supplementary Fig. 27. Free energy curve of oxygen reduction for H₂O₂ generation by MgCo/CN DSACs in the presence of peroxymonosulfate (PMS). Source data are provided as a Source Data file.



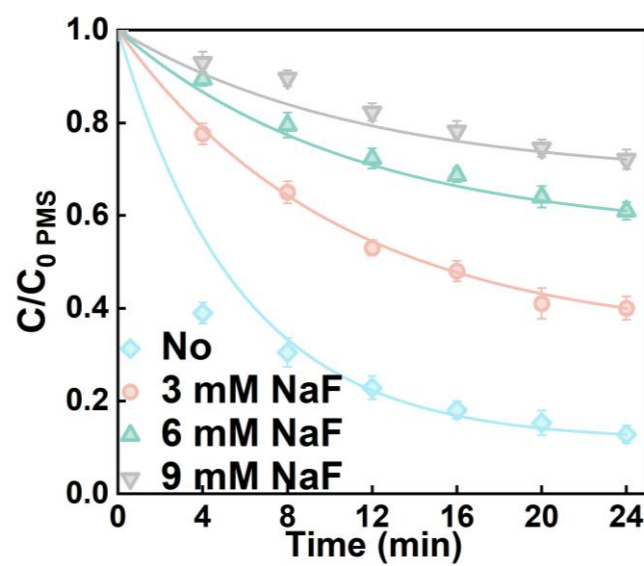
Supplementary Fig. 28. The in-situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) of 4MgCo/CN DSACs in the peroxymonosulfate (PMS)/visible light (vis) system. Source data are provided as a Source Data file.



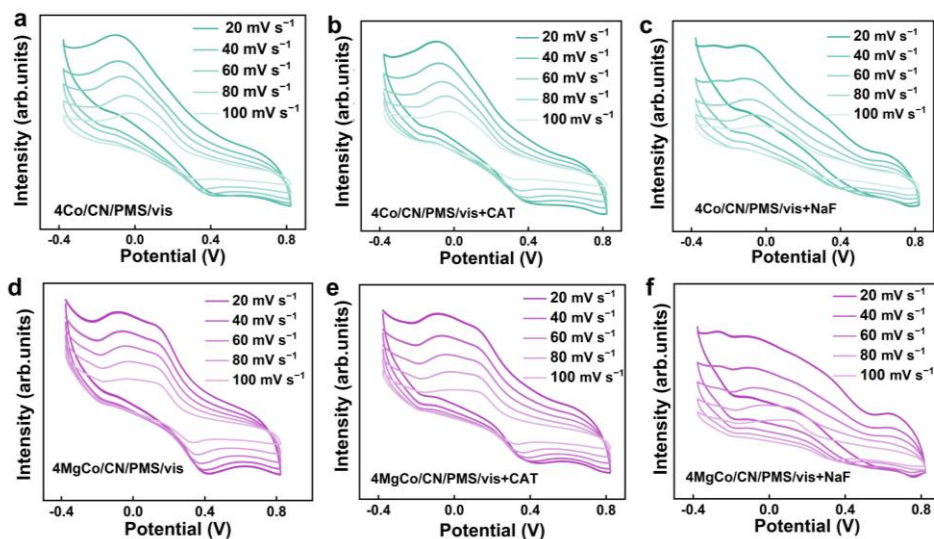
Supplementary Fig. 29. The electron spin resonance (ESR) spectra of superoxide radical ($\bullet\text{O}_2^-$) by 4MgCo/CN DSACs with/without light irradiation. Source data are provided as a Source Data file.



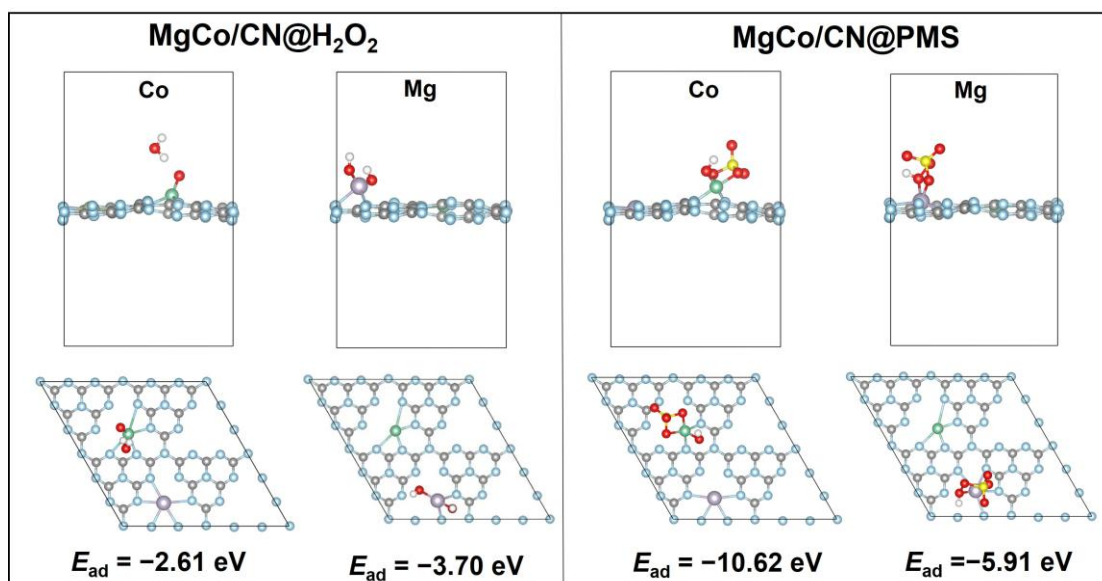
Supplementary Fig. 30. Isotopic mass spectra of surface hydroxyl radical (OH_{surf}) produced by 4MgCo/CN DSACs and 4Co/CN SACs in peroxymonosulfate (PMS)/visible light (vis) system without H_2O^{18} . Source data are provided as a Source Data file.



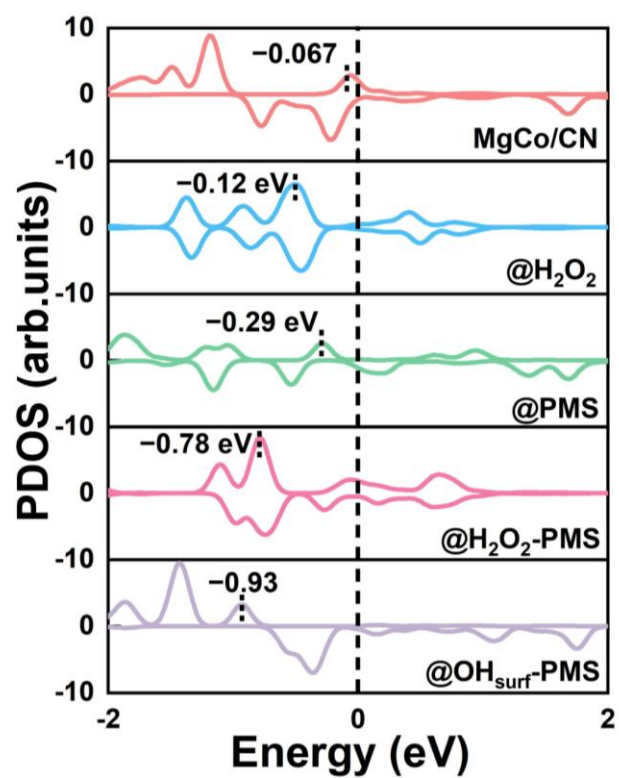
Supplementary Fig. 31. Peroxymonosulfate activation by 4MgCo/CN DSACs with different dosages of sodium fluoride (NaF). Source data are provided as a Source Data file.



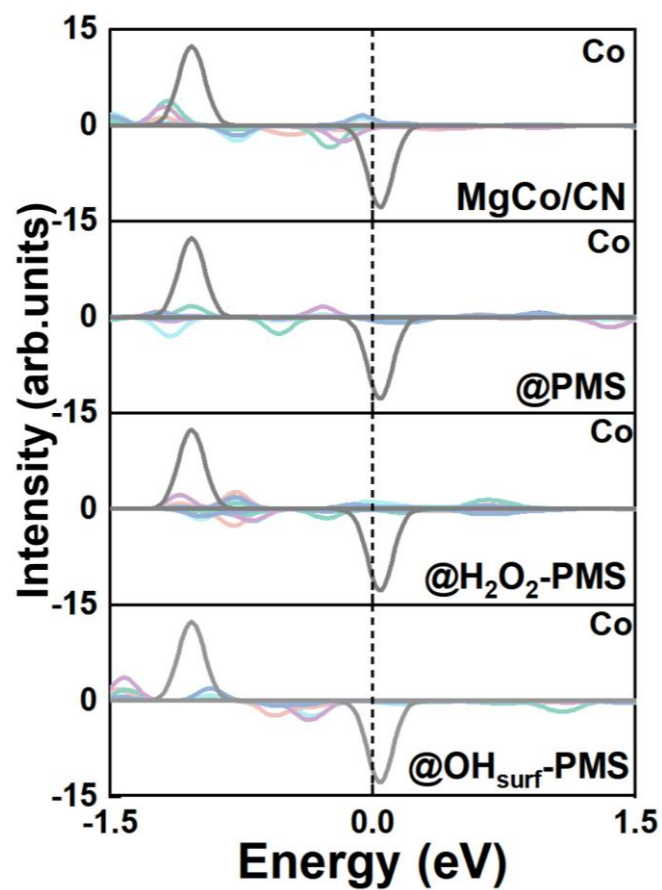
Supplementary Fig. 32. CV curves of following reaction systems with different scan rates. (a) 4Co/CN/PMS/vis system, (b) 4Co/CN/PMS/vis+CAT system, (c) 4Co/CN/PMS/vis+NaF system, (d) 4MgCo/CN/PMS/vis system, (e) 4MgCo/CN/PMS/vis+CAT system and (f) 4MgCo/CN/PMS/vis+NaF system. (CAT: catalase, NaF: sodium fluoride). Source data are provided as a Source Data file.



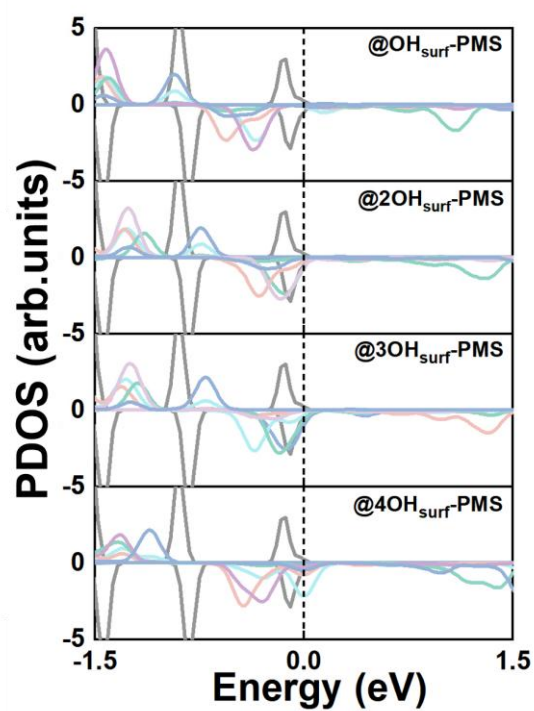
Supplementary Fig. 33. Models for H₂O₂ and peroxymonosulfate (PMS) adsorbed on MgCo/CN DSACs with different sites, respectively.



Supplementary Fig. 34. Partial density of states (PDOS) of different models. Source data are provided as a Source Data file.

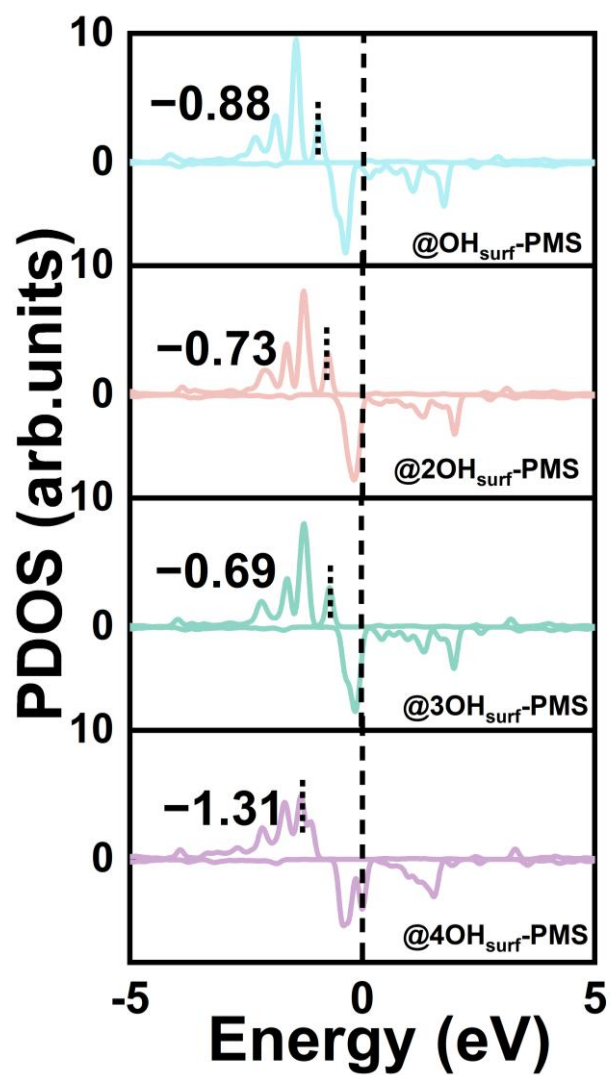


Supplementary Fig. 35. Partial density of states (PDOS) of MgCo/CN DSACs under different conditions. Source data are provided as a Source Data file.

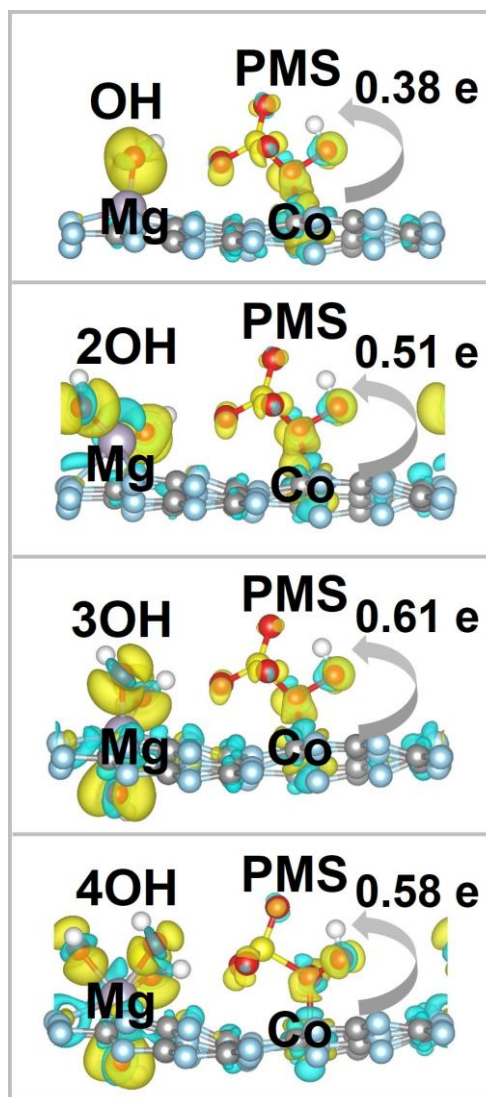


Supplementary Fig. 36. Partial density of states (PDOS) of MgCo/CN DSACs after the adsorption of PMS and surface hydroxyl radical (OH_{surf}) with different numbers.

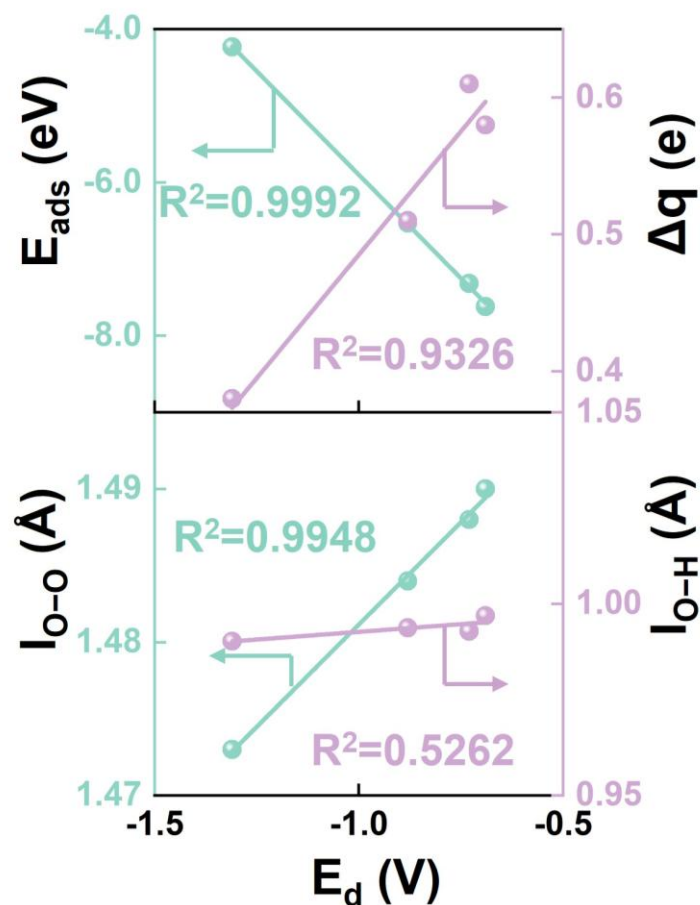
Source data are provided as a Source Data file.



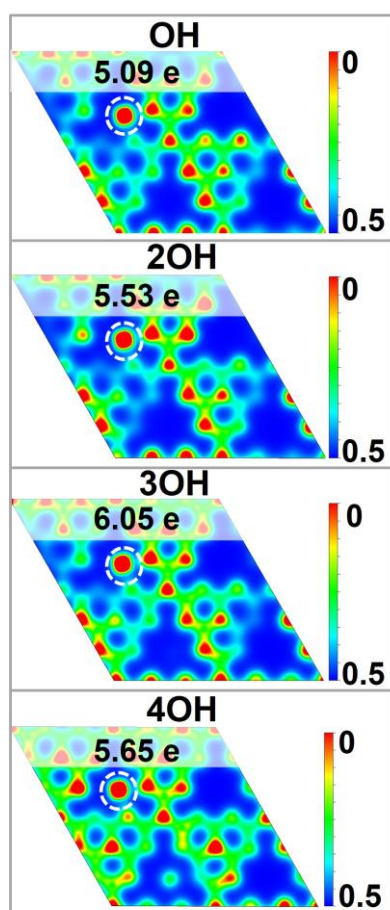
Supplementary Fig. 37. The d-band center of Co site in MgCo/CN DSACs with different amounts of surface hydroxyl radical (OH_{surf}). Source data are provided as a Source Data file.



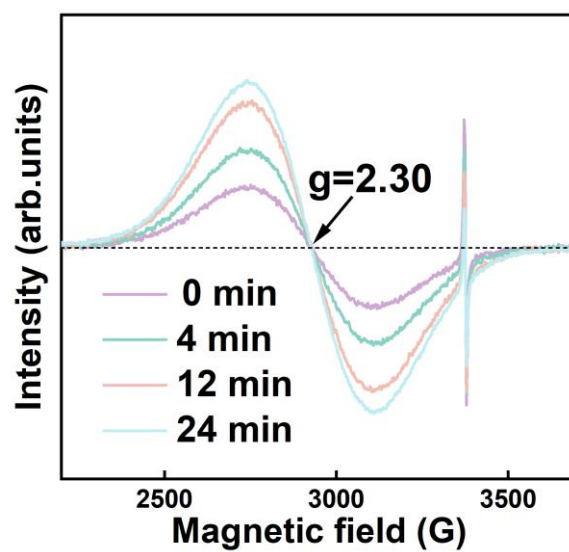
Supplementary Fig. 38. The differential charge of the MgCo/CN DSACs with different amounts of surface hydroxyl radical (OH_{surf})..



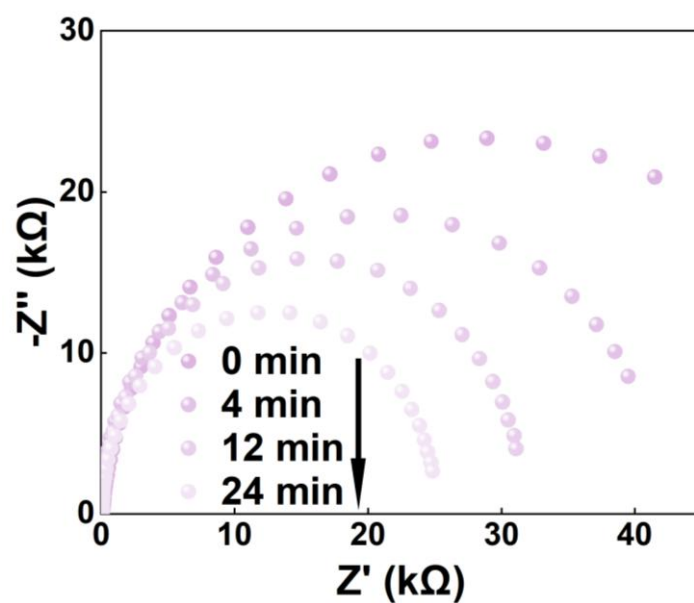
Supplementary Fig. 39. Relationship among adsorption energy (E_{ads}), transferred electron amount between the catalyst and PMS (Δq) and O–O bond length (I_{O-O}) and O–O bond O–O bond (I_{O-H}) with Co d-band center of MgCo/CN DSACs with different amounts of surface hydroxyl radical (OH_{surf}). Source data are provided as a Source Data file.



Supplementary Fig. 40. Valence electron densities of Co sites in MgCo/CN DSACs with different amounts of surface hydroxyl radical (OH_{surf}).

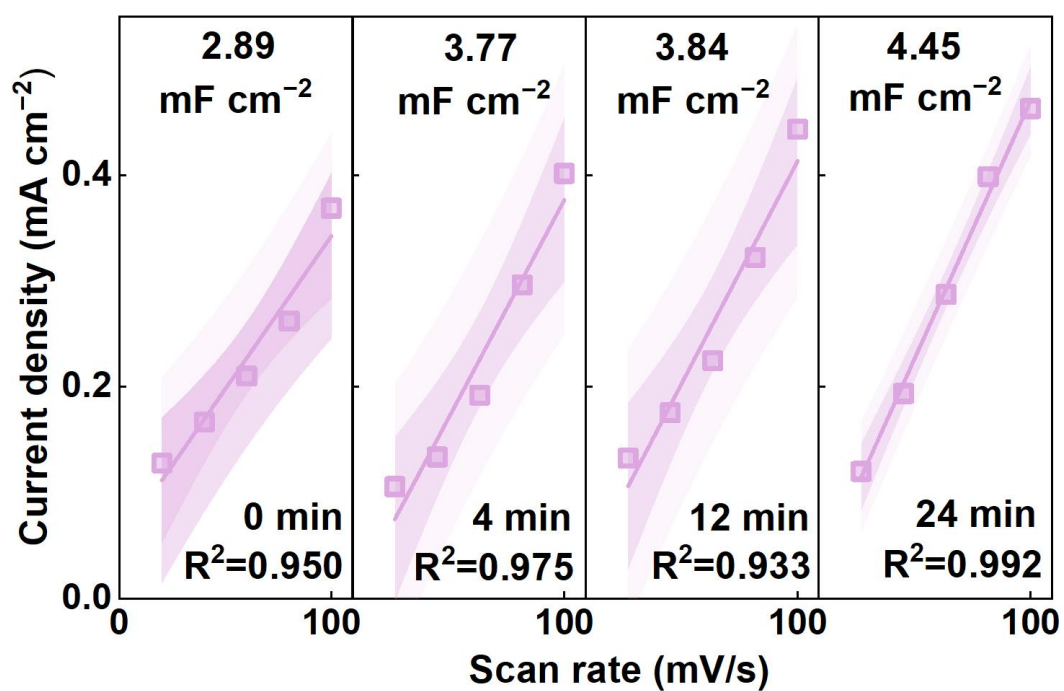


Supplementary Fig. 41. Electron paramagnetic resonance (EPR) spectroscopy of MgCo/CN DSACs after different reaction time. Source data are provided as a Source Data file.



Supplementary Fig. 42. Electrochemical impedance spectroscopy (EIS) of MgCo/CN

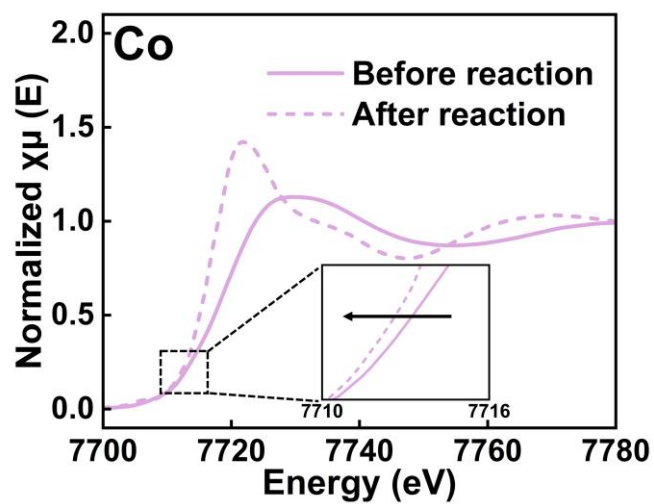
DSACs after different reaction time. Source data are provided as a Source Data file.



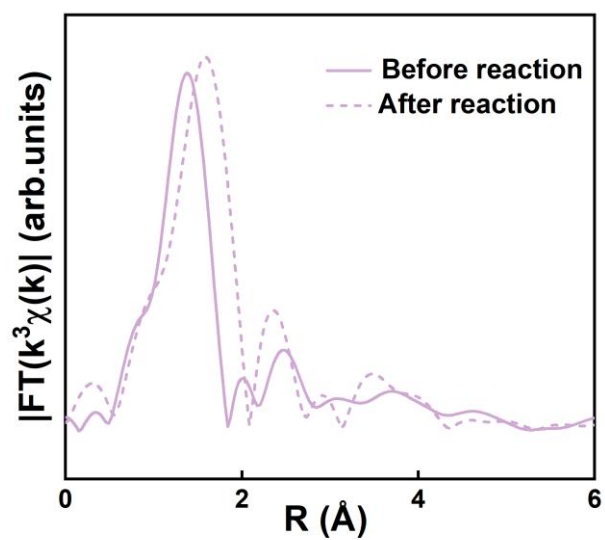
Supplementary Fig. 43. Electrochemical active surface area (ECSA) of 4MgCo/CN

DSACs after different reaction time. Source data are provided as a Source Data file.

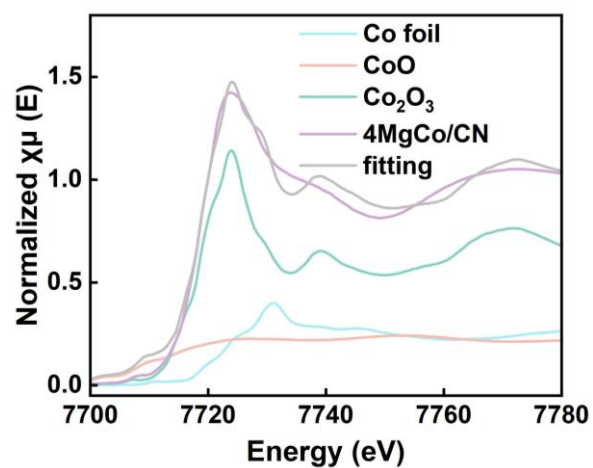
The functional form and fitting parameters are shown in Supplementary Table 10.



Supplementary Fig. 44. The Co K-edge X-ray absorption near-edge structure (XANES) spectra, of 4MgCo/CN DSACs before and after reaction. Source data are provided as a Source Data file.

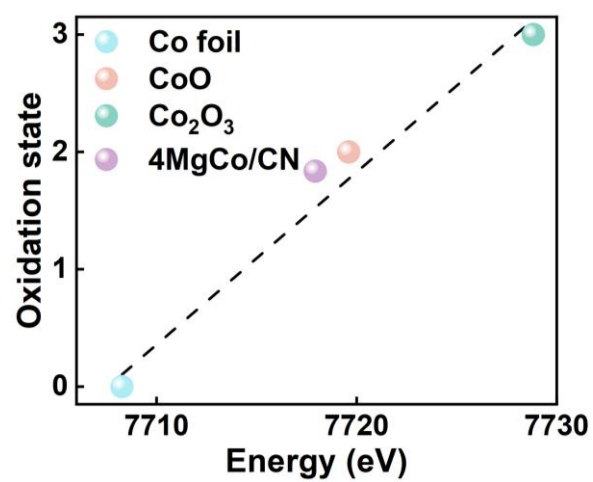


Supplementary Fig. 45. FT k^3 -weighted Co K-edge extended X-ray absorption fine structure (EXAFS) spectra of 4MgCo/CN DSACs before and after reaction. Source data are provided as a Source Data file.

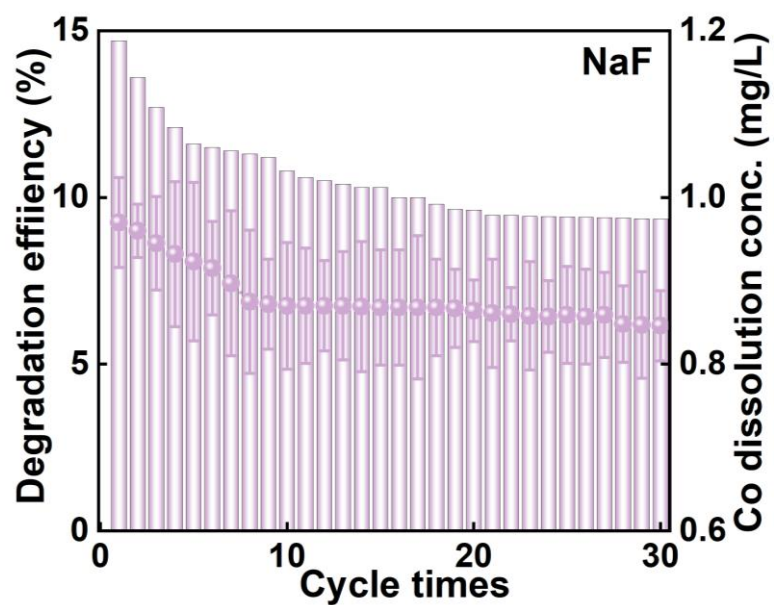


Supplementary Fig. 46. The linear combination fitting result for 4MgCo/CN DSACs

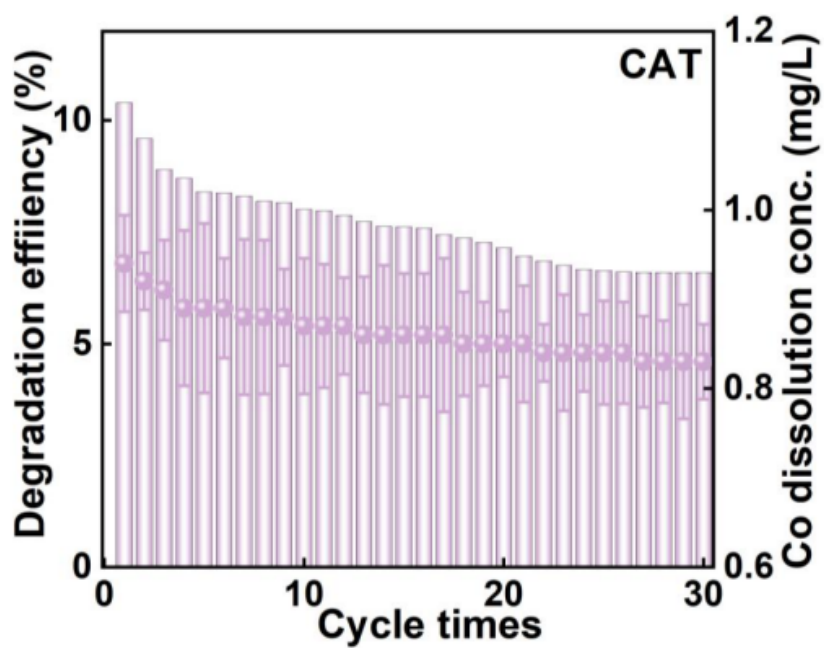
after reaction. Source data are provided as a Source Data file.



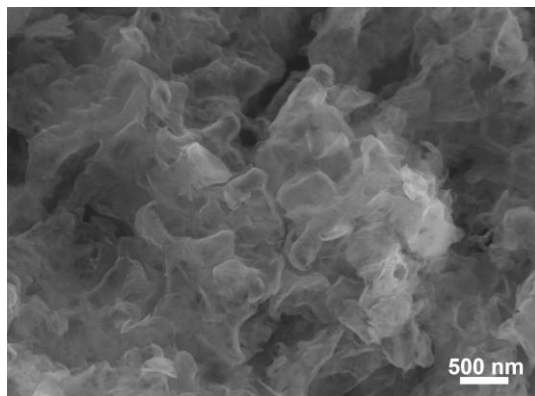
Supplementary Fig. 47. The oxidation state of Co species in 4MgCo/CN DSACs after reaction. The functional form and fitting parameters are shown in note of Supplementary Table 11. Source data are provided as a Source Data file.



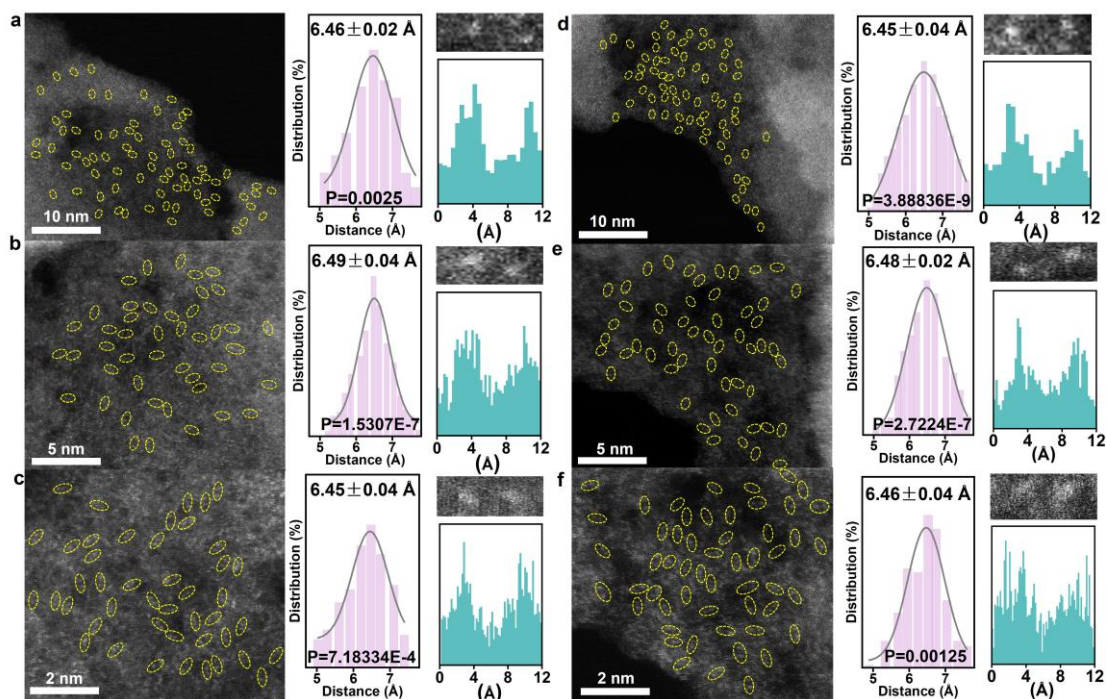
Supplementary Fig. 48. Degradation of carbamazepine (CBZ) by 4MgCo/CN DSACs after the addition of sodium fluoride (NaF) over 30-time cycles in the peroxymonosulfate (PMS)/visible light (vis) system. Source data are provided as a Source Data file.



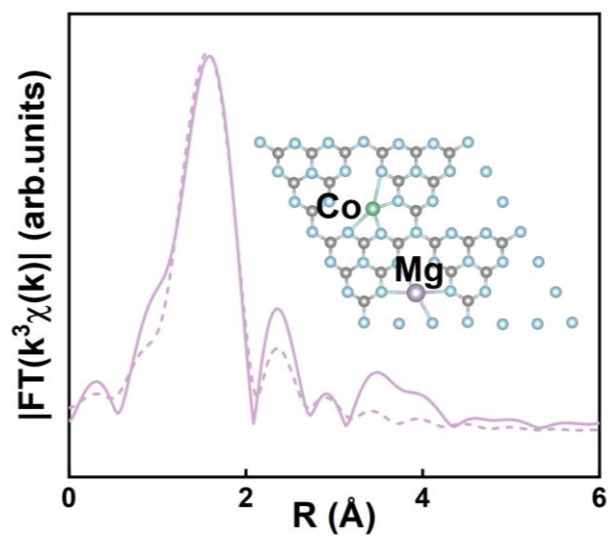
Supplementary Fig. 49. Degradation of carbamazepine (CBZ) by 4MgCo/CN DSACs after the addition of catalase (CAT) over 30-time cycles in the peroxymonosulfate (PMS)/visible light (vis) system. Source data are provided as a Source Data file.



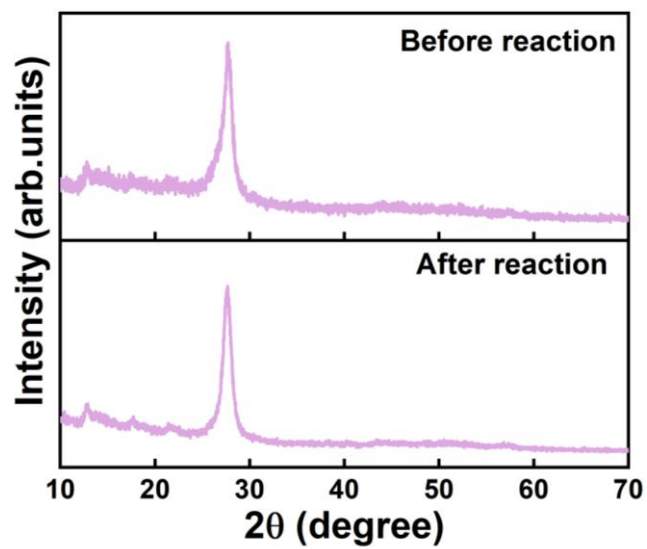
Supplementary Fig. 50. Scanning electron microscope (SEM) image of 4MgCo/CN DSACs after reaction. Image is representative of three independent measurements with similar results. Scale bar: 500 nm.



Supplementary Fig. 51. The aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (AC-HAADF-STEM) images of 4MgCo/CN DSACs after reaction with different magnifications at different regions and corresponding atomic distance distribution, respectively. Image are representative of three independent measurements with similar results. Scale bar is 10 nm (a,d), 5 nm (b,e) and 2 nm (c,f), respectively.

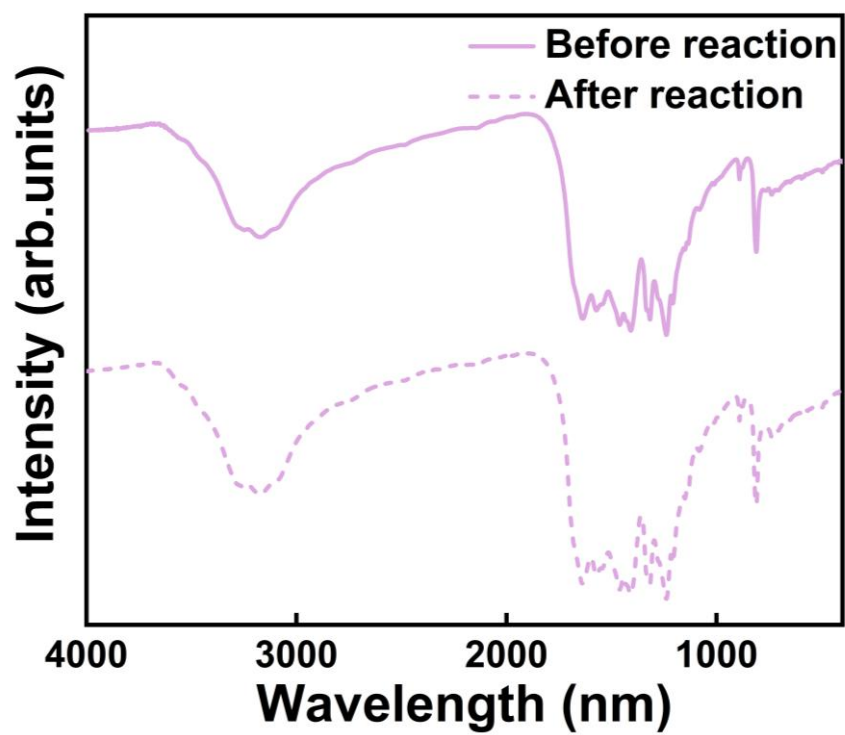


Supplementary Fig. 52. Fourier transformed (FT) k^3 -weighted Co K-edge extended X-ray absorption fine structure (EXAFS) spectra of 4MgCo/CN DSACs after reaction. Source data are provided as a Source Data file.



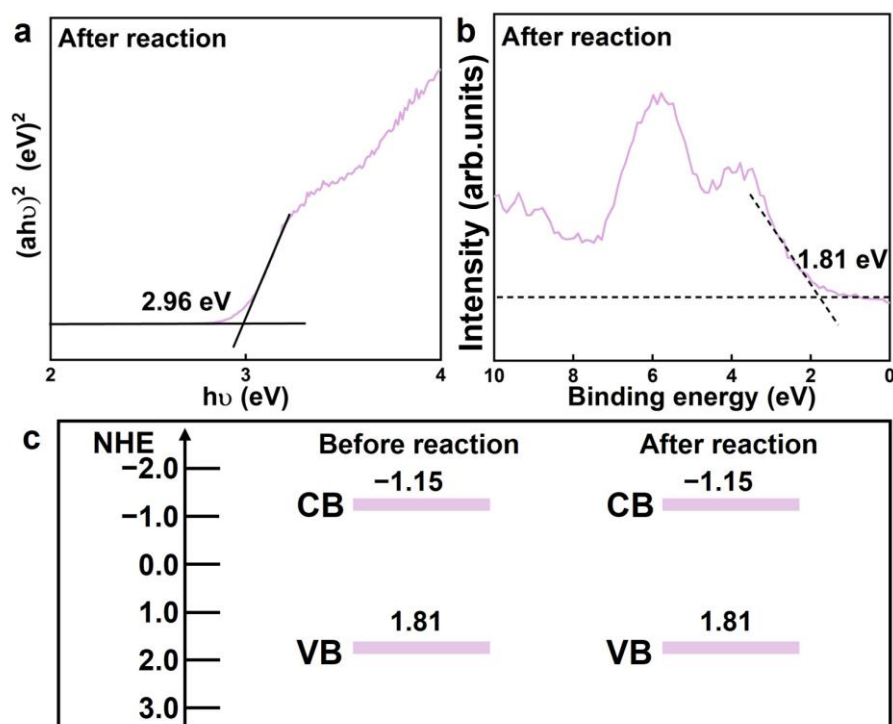
Supplementary Fig. 53. X-ray diffraction (XRD) patterns of 4MgCo/CN DSACs

before and after reaction. Source data are provided as a Source Data file.

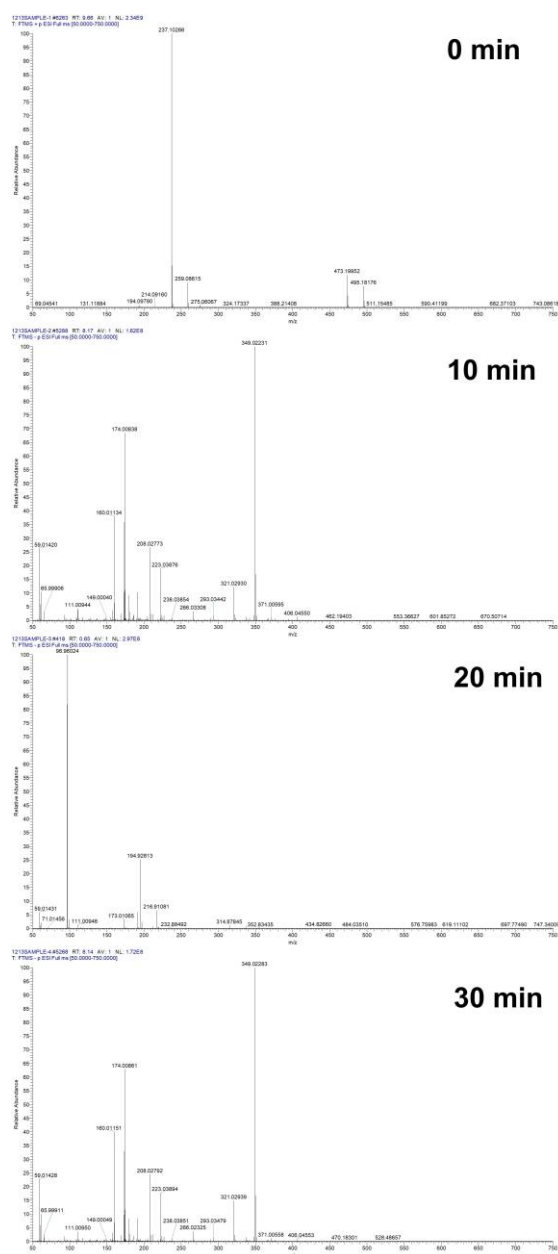


Supplementary Fig. 54. Fourier transform infrared (FT-IR) spectra of 4MgCo/CN

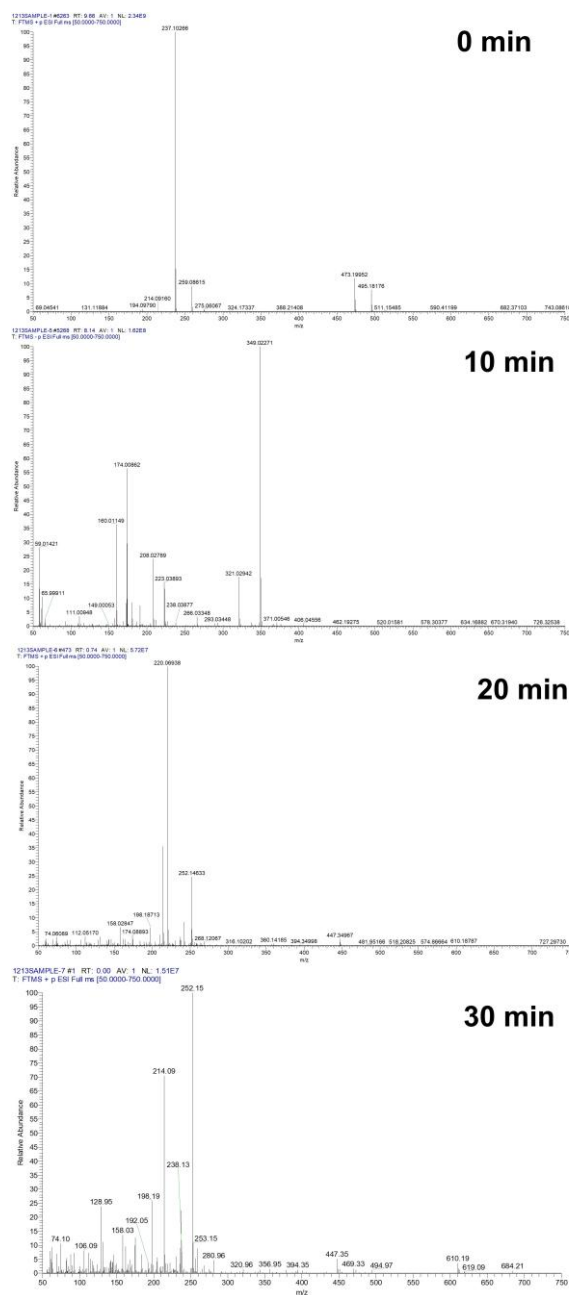
DSACs before and after reaction. Source data are provided as a Source Data file.



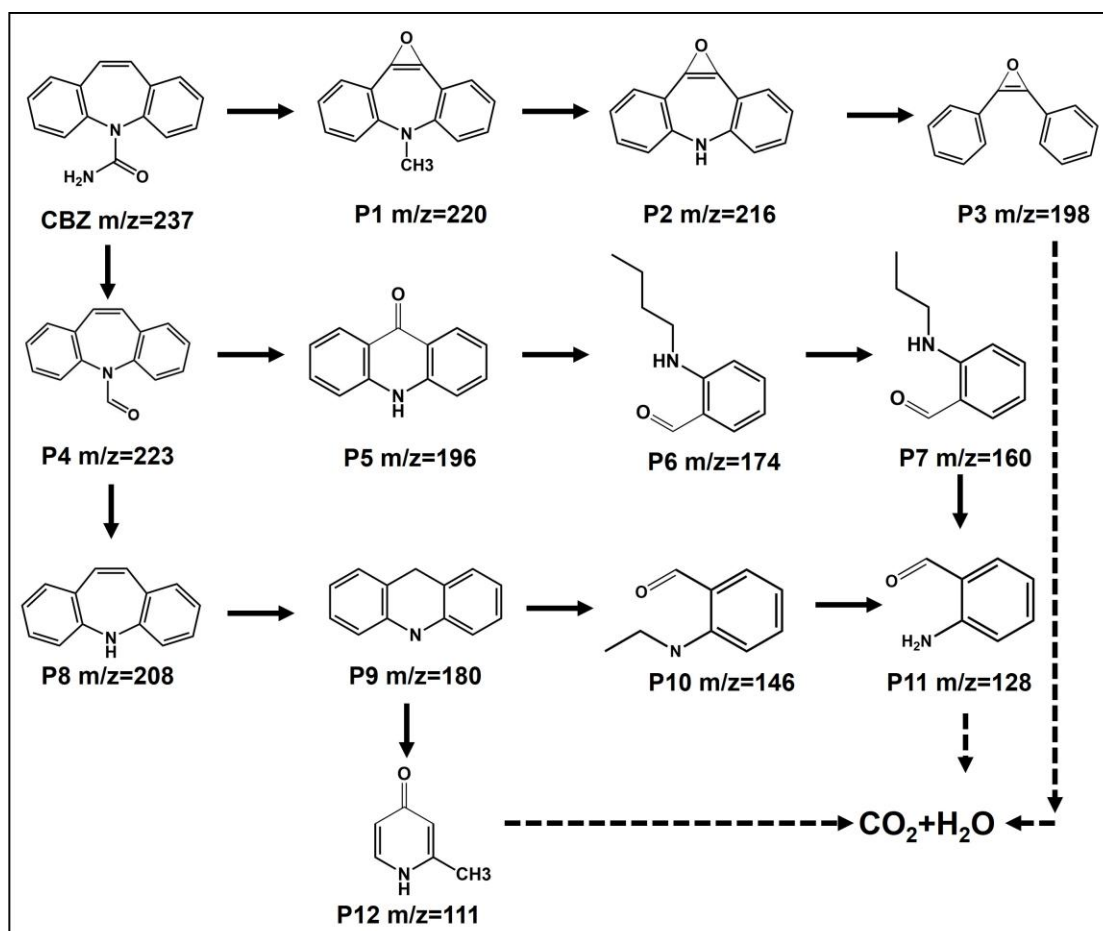
Supplementary Fig. 55. (a) Band gap and (b) valence band (VB) spectra of 4MgCo/CN DSACs after reaction; (c) Energy band level structures of 4MgCo/CN DSACs before and after reaction with conduction band (CB) and valence band (VB). Source data are provided as a Source Data file.



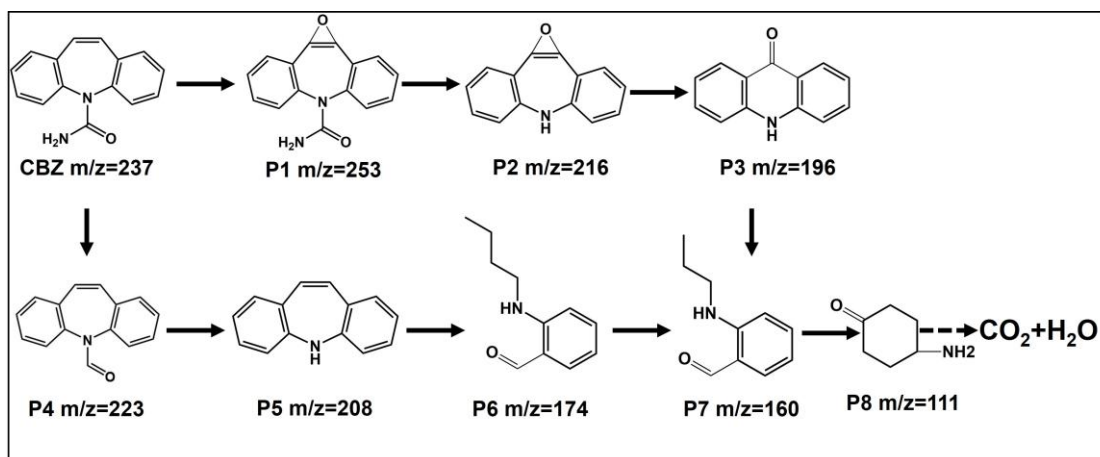
Supplementary Fig. 56. Mass spectra of carbamazepine (CBZ) and its degradation products in the 4MgCo/CN DSACs/peroxymonosulfate (PMS)/visible light (vis) system.



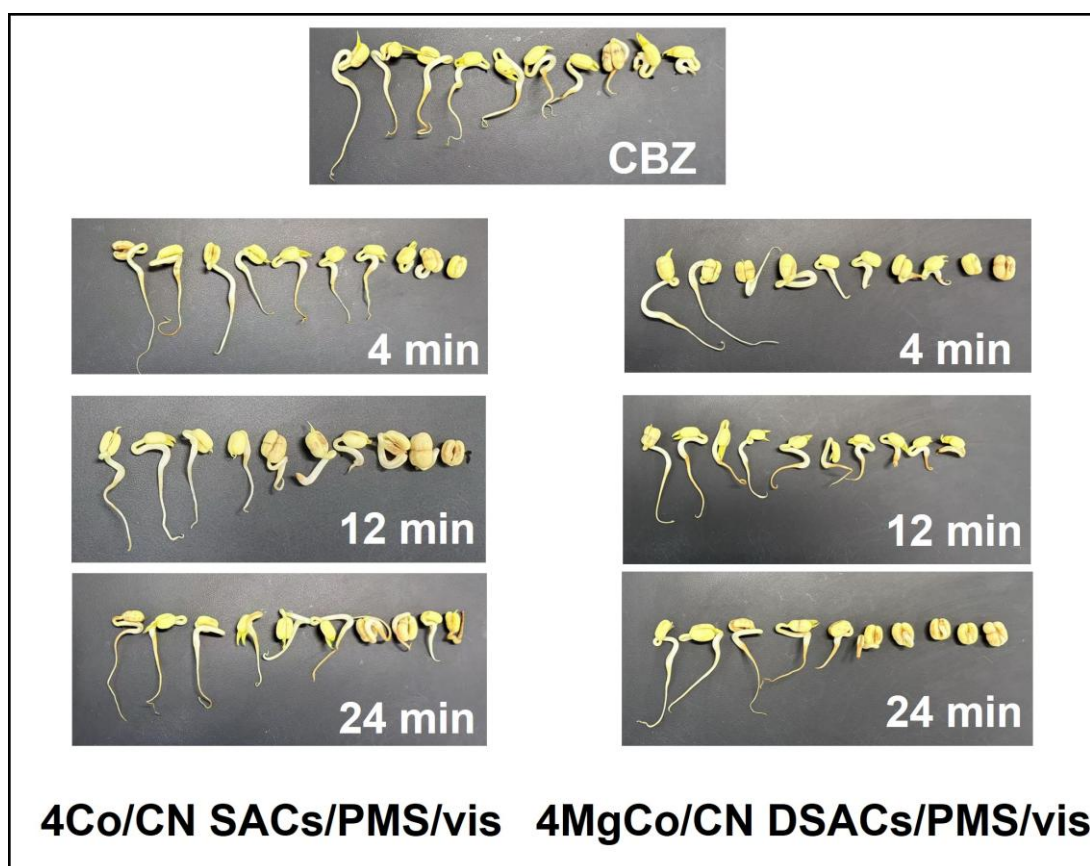
Supplementary Fig. 57. Mass spectra of carbamazepine (CBZ) and its degradation products in the 4Co/CN SACs/peroxymonosulfate (PMS)/visible light (vis) system.



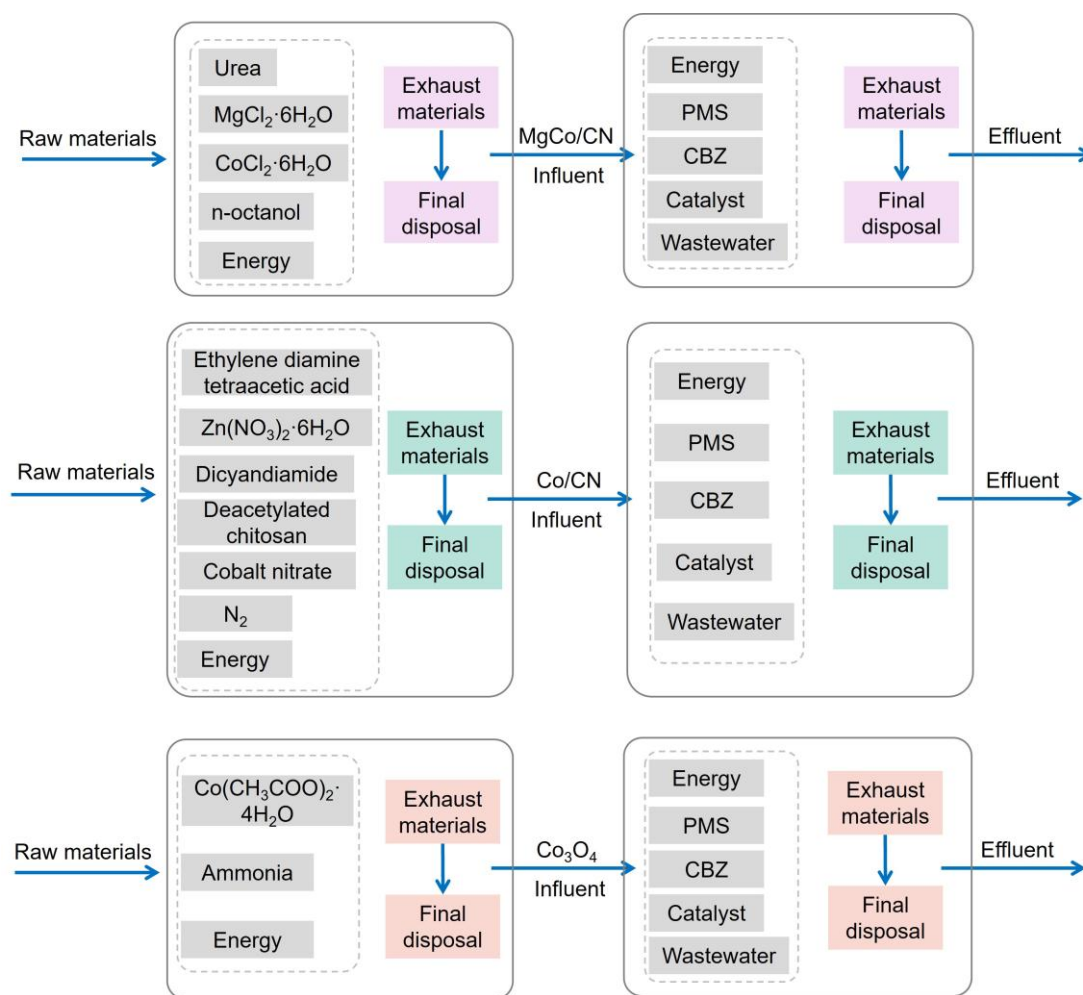
Supplementary Fig. 58. Degradation pathway of carbamazepine (CBZ) in the 4Co/CN SACs/peroxymonosulfate (PMS)/visible light (vis) system. The notation P1–P12 refer to degradation products 1 to 12 of carbamazepine, where each number corresponds to a distinct product structure observed during the degradation process.



Supplementary Fig. 59. Degradation pathway of carbamazepine (CBZ) in the 4MgCo/CN DSACs/peroxymonosulfate (PMS)/visible light (vis) system. The notation P1–P8 refer to degradation products 1 to 8 of carbamazepine, where each number corresponds to a distinct product structure observed during the degradation process.



Supplementary Fig. 60. Bean sprouts cultured with aqueous solutions of carbamazepine (CBZ) and its degradation products in the 4Co/CN SACs/peroxymonosulfate (PMS)/visible light (vis) system and 4MgCo/CN DSACs/peroxymonosulfate (PMS)/visible light (vis) system.



Supplementary Fig. 61. System boundaries for the processes studied in this work in

LCA. The different colors represent the different systems.

Supplementary Table 1. Linear combination fitting for Co in 4MgCo/CN

Standard	Weight	E ₀
Co foil	0.251 (0.039)	0.000 (0.000)
CoO	0.324 (0.024)	0.000 (0.000)
Co ₂ O ₃	0.425 (0.046)	0.000 (0.000)

R-factor = 0.0078

Chi-square = 0.0818

Reduced chi-square = 0.0015

Co in 4MgCo/CN=0*0.251+2*0.324+3*0.425=1.923

Note: Functional form: $y=a+b*x$, Fitting parameters: $a=-1133.47144 \pm 149.75284$,
 $b=0.14706 \pm 0.01940$. The x represents the energy. The y represents Co oxidation state.

Supplementary Table 2. Linear combination fitting for Mg in 4MgCo/CN

Standard	Weight	E ₀
Mg foil	0.776 (0.012)	0.000 (0.000)
MgO	0.224 (0.054)	0.000 (0.000)

R-factor = 0.0185

Chi-square = 0.7127

Reduced chi-square = 0.0043

Mg in 4MgCo/CN=0*0.776+2*0.224=0.448

Note: Functional form: $y=a+b*x$, Fitting parameters: $a=-1108.76962$ $b=0.84667$. he x represents the energy. The y represents Mg oxidation state.

Supplementary Table 3. Extended X-ray absorption fine structure (EXAFS) spectra fitting parameters at the Co K-edge for various samples.

Sample	shell	CN	R(Å)	ΔE_0	σ^2 (10^{-3}Å^2)	R factor
Co foil	Co-Co	12 (fix)	2.49±0.003	2.08±0.45	5.78±0.32	0.002
CoO	Co-O	6 (fix)	2.10±0.011	-1.27±0.85	8.59±1.33	0.019
	Co-Co	12 (fix)	3.01±0.006	-1.27±0.85	7.47±0.34	
	Co-O	6 (fix)	1.92±0.006	-7.52±0.89	4.72±0.61	
	Co-O	6 (fix)	1.92±0.006	-7.52±0.89	4.72±0.61	
Co ₃ O ₄	Co-Co	6 (fix)	2.86±0.007	-7.52±0.89	6.02±0.45	0.015
	Co-Co	6 (fix)	3.37±0.008	-7.52±0.89	4.73±0.52	
Co ₂ O ₃	Co-O	6 (fix)	1.92±0.008	-5.83±1.69	4.22±1.57	0.005
	Co-Co	8 (fix)	2.89±0.018	-5.83±1.69	7.95±0.69	
	Co-Co	2 (fix)	3.38±0.011	-5.83±1.69	4.07±3.28	
	Co-Co	2 (fix)	3.38±0.011	-5.83±1.69	4.07±3.28	
4MgCo/CN before reaction	Co-N	3.53± 0.48	1.89±0.012	-5.68±1.92	8.90±1.90	0.015
4MgCo/CN after reaction	Co-N	4.02±0. 84	2.09±0.015	2.12±0.13	7.24±2.58	0.018

Note: CN: Coordination Number; R: Bond Distance; σ^2 : Debye-Waller Factor; ΔE_0 :

Inner Potential Correction; R Factors: Goodness of Fitting.

Supplementary Table 4. Extended X-ray absorption fine structure (EXAFS) spectra fitting parameters at the Mg K-edge for various samples.

Sample	shell	CN	R(Å)	ΔE_0	$\sigma^2 (10^{-3} \text{Å}^2)$	R factor
Mg foil	Mg–Mg	12 (fix)	3.02±0.024	−7.35±2.36	6.38±2.63	0.021
MgO	Mg–O	6 (fix)	1.94±0.041	8.68±1.88	3.01±1.11	0.017
	Mg–Mg	12 (fix)	3.07±0.023	8.68±1.88	5.31±1.62	
4MgCo/CN	Mg–N	3.59± 0.26	2.12±0.024	6.364±1.57	3.0±4.57	0.013

Note: CN: Coordination Number; R: Bond Distance; σ^2 : Debye-Waller Factor; ΔE_0 :

Inner Potential Correction; R Factors: Goodness of Fitting.

Supplementary Table 5. Comparison of the kinetics of organic contaminant degradation in recently reported photo-Fenton-like processes.

Catalyst (g L ⁻¹)	PMS (mM)	Pollutant (mg L ⁻¹)	Removal efficiency	<i>k</i> _{obs} (min ⁻¹)	<i>k</i> -value (min ⁻¹ ·M ⁻¹)	Ref.
MgCo/CN (0.01)	0.1	SMX (20.0)	100%	0.5961	596.1	This work
MgCo/CN (0.01)	0.1	CBZ (20 mg/L)	99.5%	0.5953	595.3	This work
MgCo/CN (0.01)	0.1	TCH (20.0)	92.7%	0.234	234	This work
MgCo/CN (0.01)	0.1	4-CP (20.0)	86.8%	0.1487	148.7	This work
MgCo/CN (0.01)	0.1	BPA (20.0)	99.0%	0.3434	343.4	This work
Fe-CN-650 (0.1)	1.0	SMX (10.0)	80.0%	0.472	47.2	1
MoSO-Co-C (0.05)	0.4	SMX (10.0)	98.0%	0.723	361.5	2
Co _{0.70} Fe _{0.30} WO ₄ (0.1)	0.065	SMX (10.0)	100.0%	0.243	373.8	3
C-ZIF-67- CN/PMS (0.4)	0.4	SMX (20.0)	95.0%	0.870	108.7	4
CuFeO ₂ @C R (0.3)	0.13	CBZ (20.0)	91.3 %	0.152	77.95	5
CoMgFe-LDO (0.02)	0.2	CBZ (5.0)	78.1%	0.391	488.75	6
Co-N ₃ (0.1)	0.5	CBZ (10.0)	100.0%	0.640	128	7
S _{0.3} -Co@P ₂ C (0.16)	0.325	CBZ (20.0)	80.0%	0.596	229.23	8
ABF-5(0.3)	1.0	CBZ (10.0)	99.07 %	0.0083	277.78	9
Ag ₂ O/NCDs@P TCN (0.3)	0.45	CBZ (2.0)	84.2 %	0.0320	474.07	10
α-MnO ₂ (0.17)	0.88	CBZ (5.0)	99.7%	0.0083	277.41	11
CoMnHCF (2.0)	0.13	TCH (20.0)	100.0%	0.592	45.5	12
boron, nitrogen co-doped porous carbon (0.03)	0.13	TCH (20.0)	80.0%	0.057	292.3	13
ZnAl-LDO/ Ag ₂ S (0.05)	6.0	TCH (20.0)	96.5%	0.096	6.4	14
NiFe ₂ O ₄ /g-C ₃ N ₄ (0.25)	0.2	TCH (20.0)	80.0%	2.60	240	15

CuFe ₂ O ₄ /CuO (0.1)	0.4	TCH (20.0)	69.3 %	0.006	3	16
NBC (0.5)	3.25	4-CP (100.0)	90.9%	0.054	3.32	17
Mn ₃ O ₄ /CNNS (0.3)	1.0	4-CP (50.0)	100.0%	0.082	13.7	18
1%Cu- 2%Co@ZnO (0.2)	2.0	4-CP (40.0)	96.0%	0.036	3.6	19
LCO (0.7)	2.0	BPA (11.4)	96.7 %	0.057	0.464	20
NOPC (0.2)	0.15	BPA (10.0)	100.0%	0.30	100	21
CNS/CN (0.3)	0.48	BPA (50.0)	80.0%	0.013	1.81	22
FeOCl (0.5)	12 .0	BPA (50.0)	100.0%	1.667	5.56	23
Mn-MGO (0.5)	5.0	BPA (91.4)	95.0%	0.113	4.13	24

Note:

$$k - value = (k_{obs} \times c[pollutant]) / (c[catalyst]) \times c[PMS]$$

Supplementary Table 6. The fitting information for the removal efficiency with addition dosages of different scavengers.

		Functional form	Fitting parameters
4MgCo/CN	CAT	$y=a+b*x$	$a=-66.54897 \pm 24.66761$ $b=64.82071 \pm 17.20344$
	NaF	$y=a+b*x$	$a=-7.34644 \pm 2.87352$ $b=66.02806 \pm 16.20312$
	MeOH	$y=a+b*x$	$a=-0.10465 \pm 0.0049$ $b=98.0343 \pm 3.75721$
4Co/CN	CAT	$y=a+b*x$	$a=-54.95577 \pm 18.38852$ $b=56.88501 \pm 11.10988$
	NaF	$y=a+b*x$	$a=-3.39635 \pm 1.7548$ $b=52.80476 \pm 10.95301$
	MeOH	$y=a+b*x$	$a=-0.05296 \pm 0.01534$ $b=58.23799 \pm 9.92235$

Note: The x represents the addition dosage of catalase (CAT), sodium fluoride (NaF) and methanol (MeOH), respectively. The y represents the removal efficiency of carbamazepine (CBZ) by 4MgCo/CN and 4Co/CN after the addition of corresponding scavenger in the peroxymonosulfate (PMS)/visible light (vis) system, respectively.

Supplementary Table 7. Active species contribution under different reaction systems mediated by typical DSACs and SACs.

Systems	$\bullet\text{SO}_4^-$	OH_{surf}	Others
Fe/CN/PMS/vis	23.8	11.2	65.05
Mn/CN/PMS/vis	19.2	21.9	58.9
Fe/CN/PMS	20.1	17.9	62
Mn/CN/PMS	11.4	19.7	68.9
MgFe/CN/PMS/vis	49.7	44.8	5.5
MgMn/CN/PMS/vis	45.8	40.6	13.6
MgFe/CN/PMS	23.9	24.9	51.2
MgMn/CN/PMS	14.2	15.9	69.9

Supplementary Table 8. The fitting information for electrochemical active surface area (ECSA) of 4MgCo/CN DSACs and 4Co/CN SACs under different conditions, respectively.

		Functional form	Fitting parameters
4Co/CN	No	$y=a+b*x$	$a=0.00134\pm2.04556E-4$ $b=0.06709\pm0.01357$
	CAT	$y=a+b*x$	$a=8.4725E-4\pm1.8354E-4$ $b=0.0908\pm0.01217$
	NaF	$y=a+b*x$	$a=0.00203\pm4.35692E-4$ $b=0.11152\pm0.0289$
4MgCo/CN	No	$y=a+b*x$	$a=0.00289\pm3.82342E-4$ $b=0.05381\pm0.02536$
	CAT	$y=a+b*x$	$a=0.00134\pm8.94687E-5$ $b=0.06145\pm0.00593$
	NaF	$y=a+b*x$	$a=9.07953E-4\pm7.65804E-5$ $b=0.05512\pm0.00508$

Note: The x represents the scan rate. The y represents current density by 4MgCo/CN and 4Co/CN without and with scavengers, respectively.

Supplementary Table 9. The energy level of different samples.

Energy level	MgCo/CN	MgCo/CN@ PMS	MgCo/CN@H ₂ O ₂ -PMS	MgCo/CN@OH _{surf} -PMS
d_{xy}	-0.06	-0.27	-0.0265	-0.94
$d_x^2-y^2$	-0.07	-0.27	-0.112	-0.946
d_z^2	-1.16	-0.28	-0.775	-1.399
d_{xz}	-1.19	-0.283	-1.110	-1.419
d_{yz}	-1.2	-0.27	-0.781	-1.49
PMS-O _p			-0.138	
SO ₄ -O _p			-1.032	

Supplementary Table 10. The fitting information for electrochemical active surface area (ECSA) of 4MgCo/CN DSACs after different reaction time.

	Functional form	Fitting parameters
0 min	$y=a+b*x$	$a=0.00289\pm3.82342E-4$ $b=0.05381\pm 0.02536$
4 min	$y=a+b*x$	$a=0.00377\pm4.99578E-4$ $b=-4.8E-4\pm0.03314$
12 min	$y=a+b*x$	$a=0.00384\pm5.0672E-4$ $b=0.02905\pm0.03361$
24 min	$y=a+b*x$	$a=0.00445\pm2.0555E-4$ $b=0.02522\pm0.01363$

Note: The x represents the scan rate. The y represents current density by 4MgCo/CN , after different reaction time.

Supplementary Table 11. Linear combination fitting for Co in 4MgCo/CN after reaction

Standard	Weight	E ₀
Co foil	0.172 (0.023)	0.000 (0.000)
CoO	0.648 (0.021)	0.000 (0.000)
Co ₂ O ₃	0.180 (0.041)	0.000 (0.000)

R-factor = 0.0142

Chi-square = 0.4662

Reduced chi-square = 0.0025

Co in 4MgCo/CN=0*0.172+2*0.648+3*0.180=1.836

Note: Functional form: $y=a+b*x$, Fitting parameters: $a=-1133.47144\pm149.75284$

$b=0.14706\pm0.01940$. The x represents the energy. The y represents Co oxidation state.

Supplementary Table 12. Water properties of actual wastewater.

Samples	TOC	pH	Cl ⁻	NO ₃ ⁻	SO ₄ ²⁻
TW	26.21	8.01	23.5	10.54	24.65
SE	23.4	8.13	53.25	59.64	29.50

Supplementary Table 13. The predicted toxicity of carbamazepine (CBZ) and its degradation products were obtained using a structure-activity relationship system in the 4Co/CN SACs/peroxymonosulfate (PMS)/visible light (vis) system.

Possible products	Daphnia magna	Oral rat	Developmental toxicity	Mutagenicity
CBZ	0.31	2.17	0.76	0.57
P1	0.57	2.92	0.61	0.45
P2	0.98	2.96	0.61	0.72
P3	0.8	1.86	0.48	0.46
P4	0.64	2.21	0.57	0.62
P5	1.1	1.84	0.43	0.64
P6	1.02	1.78	0.53	0.16
P7	0.76	1.97	0.46	0.35
P8	0.31	2.27	0.37	0.08
P9	0.94	2.15	0.29	0.35
P10	1.22	2.03	0.6	-0.06
P11	0.72	2.09	0.28	0.08
P12	1.22	2.08	0.86	0.1

Supplementary Table 14. The predicted toxicity of carbamazepine (CBZ) and its degradation products were obtained using a structure-activity relationship system in the 4MgCo/CN SACs/peroxymonosulfate (PMS)/visible light (vis) system.

Possible products	Daphnia magna	Oral rat	Developmental toxicity	Mutagenicity
CBZ	5.06	2.17	0.76	0.57
P1	4.56	3.07	0.8	0.86
P2	4.33	2.96	0.61	0.72
P3	4.19	1.84	0.43	0.64
P4	4.71	2.21	0.57	0.62
P5	4.98	2.27	0.37	0.08
P6	4.22	1.78	0.53	0.16
P7	4.46	1.97	0.46	0.35
P8	3.83	2.08	0.86	0.1

Supplementary Table 15. Comparison of electrical energy per order (EE/O) across different catalytic system.

Catalytic	k_{obs} (min^{-1})	V (L)	P (kwh)	EE/O (kWhL^{-1})	Ref.
Fe-CN/PMS/Vis	0.070	0.05	0.3	3.289	22
BiOCl/I/Vis	0.426	0.05	0.3	0.541	23
KCN/I/Vis	0.076	0.05	0.3	3.049	23
AC-TiO ₂ /Cl/Uv	0.093	0.70	0.01	0.006	24
LFCO@CFC/PMS/Vis	/	/	/	0.46	25
ZIF-g-C ₃ N ₄ /PMS/Vis	0.051	0.05	0.05	4.515	26
g-C ₃ N ₄ -BiOCl/Vis	0.225	0.05	0.5	1.706	27
TiO ₂ /I/Vis	0.132	0.132	0.3	1.747	28
Fe-CN-Nv/PAA/Vis	0.330	0.330	0.3	0.698	29
g-C ₃ N ₄ /PDS/Vis	0.068	0.10	0.3	1.693	30
CdS/I/Vis	0.029	0.05	0.3	7.940	28
GCN/H ₂ O ₂ /Vis	0.060	0.060	0.3	3.838	31
Cl/Uv	0.267	0.10	0.3	0.431	32
ZG/Vis	0.064	0.05	0.036	0.432	33
MgCo/CN/PMS/vis	0.5953	2.0	0.286	0.143	This work

Supplementary Table 16. Input materials and energy required in the catalyst production stage to degrade 1 kg carbamazepine (CBZ) through MgCo/CN DSACs, Co/CN SACs and Co₃O₄ in advanced oxidation process.

Catalyst production stage	Input	Amount	Unit	Output	Amount	Unit
Stage 1 (MgCo/CN DSACs)	Heat for preparation	30	kw·h	Intermediates (Catalyst)	5	kg
	Urea	10	kg	Exhausted volatile substance	1.5	kg
	MgCl ₂ ·6H ₂ O	0.5	kg	Exhausted materials	4.5	kg
	CoCl ₂ ·6H ₂ O	0.5	kg	Butanol	3.0	L
	n-octanol	3.0	L			
Stage 1 (Co/CN SACs)	deacetylated chitosan	20	kg	Intermediates (Catalyst precursors)	20	kg
	ethylene diamine tetraacetic acid	6	kg	Exhausted materials	23.169	kg
	cobalt nitrate	8.149	kg	Exhausted water	1	L
	Zn(NO ₃) ₂ ·6H ₂ O	9.02	kg			
	Water	1	L			
Stage 2 (Co/CN SACs)	Heat for preparation	5	kw·h			
	Catalyst precursors	20	kg	Intermediates (Catalyst)	10	kg
	Dicyandiamide	200	kg	Exhausted volatile substance	14	kg
	Heat for preparation	480	kw·h			
	N ₂	14400	L			
Stage 1 (Co ₃ O ₄)	Co(CH ₃ COO) ₂ ·4H ₂ O	40	kg	Intermediates (Catalyst precursors)	20	kg
	water	2	L	Exhausted materials	18	kg
	Ammonia	0.2	L	Exhausted volatile substance	2.2	kg
Stage 2 (Co ₃ O ₄)	Heat for preparation	10	kw·h			
	Catalyst precursors	20	kg	Intermediates (Catalyst)	10	kg

Heat for preparation	360	kw·h	Exhausted volatile substance	10	kg
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Calculations based on catalytic activity showed that 10 kg of MgCo/CN DSACs or 10 kg of Co/CN SACs or 10 kg of Co₃O₄ were required to treat 1 kg carbamazepine (CBZ), respectively.

Supplementary Table 17. Input materials and energy required in the catalyst application stage to degrade 1 kg carbamazepine (CBZ) through MgCo/CN DSACs, Co/CN SACs and Co₃O₄ in advanced oxidation process.

Catalyst application stage	Input	Amount	Unit	Output	Amount	Unit
MgCo/CN DSACs	Catalyst	10	kg	Exhausted catalyst	10	kg
	Power supply	140	kw·h	Byproducts	7.147	kg
	Peroxymonosulfate	6.147	kg	Effluent	200000	L
	Carbamazepine	1	kg			
Co/CN SACs	Wastewater (influent)	200000	L			
	Catalyst	10	kg	Exhausted catalyst	10	kg
	Power supply	240	kw·h	Byproducts	31.735	kg
	Peroxymonosulfate	30.735	kg	Effluent	200000	L
Co ₃ O ₄	Carbamazepine	1	kg			
	Wastewater (influent)	200000	L			
	Catalyst	10	kg	Exhausted catalyst	10	kg
	Power supply	640	kw·h	Byproducts	62.47	kg
	Peroxymonosulfate	61.47	kg	Effluent	200000	L
	Carbamazepine	1	kg			
	Wastewater (influent)	200000	L			

Calculations based on catalytic activity showed that 10 kg of MgCo/CN DSACs or 10 kg of Co/CN SACs or 10 kg of Co₃O₄ were required to treat 1 kg carbamazepine (CBZ), respectively.

Supplementary Table 18. Description and calculation formulas for LCA

Impact Category	Description	Formula
Global warming (GW, kg CO ₂ -eq)	Measures the potential contribution to global warming over a specific time frame.	$I_{GW} = \sum (EF_i \times CF_{i,GW})$
Stratospheric ozone depletion (SOD, kg CFC-11-eq)	Assesses the impact on stratospheric ozone layer depletion.	$I_{SOD} = \sum (EF_i \times CF_{i,SOD})$
Ionizing radiation (IR, kg U235 eq)	Evaluates the impact on human health and ecosystems due to exposure to ionizing radiation from nuclear fuel cycle or other sources.	$I_{IR} = \sum (EF_i \times CF_{i,IR})$
Ozone formation for human health (OFHH, kg NO _x eq)	Evaluates the impact on human health due to ground-level ozone formation	$I_{OFHH} = \sum (EF_i \times CF_{i,OFHH})$
Fine particulate matter formation (FPMF, kg PM2.5 eq)	Measures the formation of fine particulate matter and its impact on air quality.	$I_{FPMF} = \sum (EF_i \times CF_{i,FPMF})$
Ozone formation for Terrestrial ecosystems (OFTE, kg NO _x eq)	Assesses the impact on terrestrial ecosystems due to ground-level ozone formation.	$I_{OFTE} = \sum (EF_i \times CF_{i,OFTE})$
Terrestrial acidification (TA, kg SO ₂ eq)	Measures the potential for acidification of terrestrial ecosystems.	$I_{TA} = \sum (EF_i \times CF_{i,TA})$
Freshwater eutrophication (FE, kg P eq)	Evaluates the impact on freshwater ecosystems due to nutrient enrichment.	$I_{FE} = \sum (EF_i \times CF_{i,FE})$
Marine eutrophication (ME, kg N eq)	Assesses the impact on marine ecosystems due to nutrient enrichment.	$I_{ME} = \sum (EF_i \times CF_{i,ME})$
Terrestrial ecotoxicity (TE, kg 1,4-DCB)	Quantifies the potential toxic impact on terrestrial ecosystems.	$I_{TE} = \sum (EF_i \times CF_{i,TE})$
Freshwater ecotoxicity (FE, kg 1,4-DCB)	Measures the potential toxic impact on Freshwater ecosystems.	$I_{FE} = \sum (EF_i \times CF_{i,FE})$
Marine ecotoxicity (ME, kg 1,4-DCB)	Assesses the potential toxic impact on marine ecosystems.	$I_{ME} = \sum (EF_i \times CF_{i,ME})$
Human carcinogenic toxicity (HCT, kg 1,4-DCB)	Quantifies the potential carcinogenic impact on human health.	$I_{HCT} = \sum (EF_i \times CF_{i,HCT})$

Human non-carcinogenic toxicity (HNT, kg 1,4-DCB)	Measures the potential Noncarcinogenic impact on human health.	$I_{\text{HNT}} = \Sigma (EF_i \times CF_{i,\text{HNT}})$
Land use (LU, m ² a crop eq)	Assesses the land area required, considering the equivalent productivity of crops.	$I_{\text{LU}} = \Sigma (EF_i \times CF_{i,\text{LU}})$
Mineral resource scarcity (MRS, kg Cu eq)	Evaluates the impact on resource depletion due to the extraction and use of finite mineral resources, affecting future availability and economic accessibility.	$I_{\text{MRS}} = \Sigma (EF_i \times CF_{i,\text{MRS}})$
Fossil resource scarcity (FRS, kg oil eq)	Measures the scarcity of fossil resources, considering oil as an equivalent.	$I_{\text{FRS}} = \Sigma (EF_i \times CF_{i,\text{FRS}})$
Water consumption (WC, m ³)	Quantifies the Freshwater consumption during the life cycle of a product or process.	$I_{\text{WC}} = \Sigma (EF_i \times CF_{i,\text{WC}})$

Supplementary Table 19. HPLC condition for concentration analysis.

Compounds	ultrapure water	acetonitrile	methanol	flow rate (mL/min)	wavelength (nm)
SMX	30%	70%	/	1.0	265
CBZ	40%	60%	/	1.0	286
TCH	30%	70%	/	1.0	357
4-CP	70%	30%	/	1.0	220
BPA	30%	70%	/	1.0	230

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