

Supplementary Information for:

**Band gap matching-triggered self-sustaining photocatalytic
oxidation**

Weiwei Cheng,^a Zhiqin Yuan,^{*a} Yanjun Lin^a, and Chao Lu^{*ab}

*^a State Key Laboratory of Chemical Resource Engineering, College of Chemistry,
College of Chemical Engineering, Beijing University of Chemical Technology,
Beijing 100029, China*

*^b Green Catalysis Center, College of Chemistry, Zhengzhou University, Zhengzhou
450001, China*

***Corresponding author**

*Email: yuanzq@mail.buct.edu.cn (Z. Yuan). Tel./Fax: +86 10 64411957.

*Email: luchao@mail.buct.edu.cn (C. Lu). Tel./Fax: +86 10 64411957.

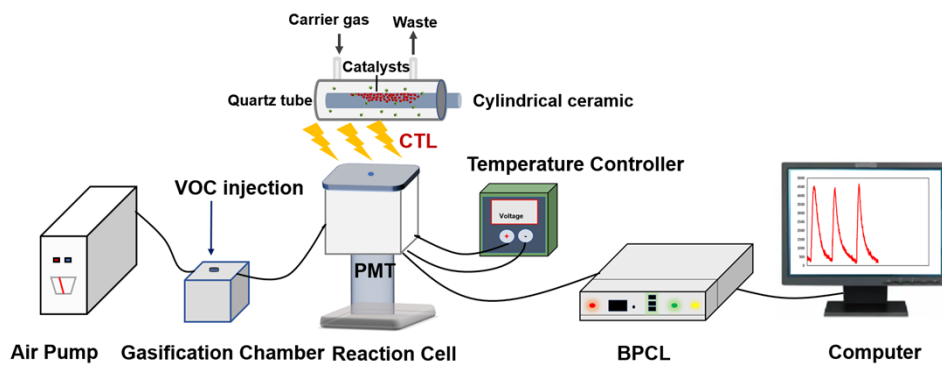


Fig. S1 Schematic diagram of the components of the CTL instrumentation.

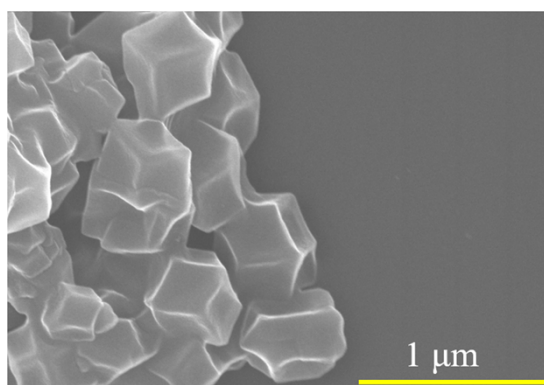


Fig. S2 SEM image of ZIF-67 synthesized without CTAB.

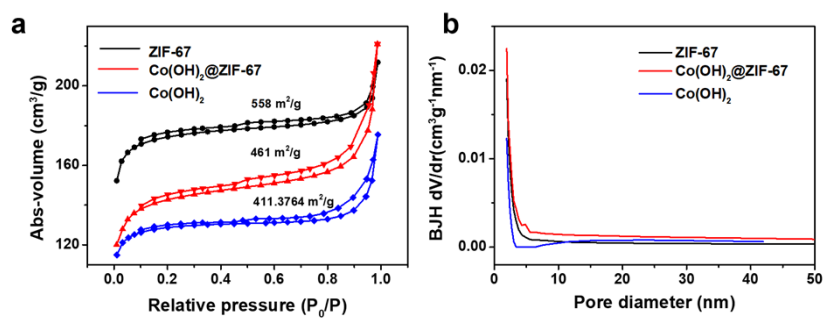


Fig. S3 N₂ isothermal adsorption and desorption curves and pore size distribution of ZIF-67, Co(OH)₂@ZIF-67 and Co(OH)₂.

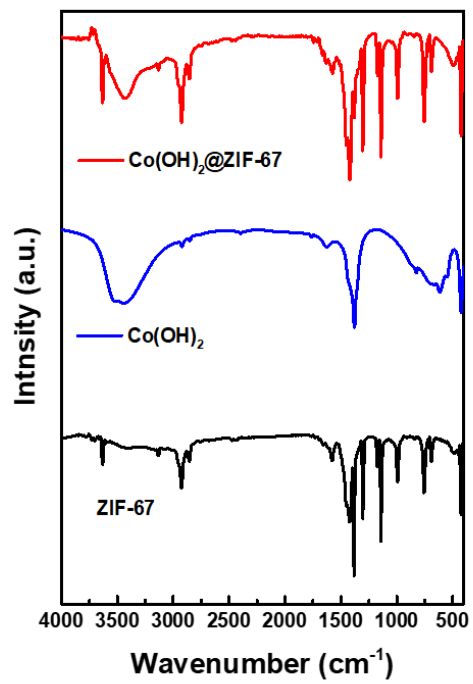


Fig. S4 FT-IR spectra of ZIF-67, Co(OH)₂, and Co(OH)₂@ZIF-67.

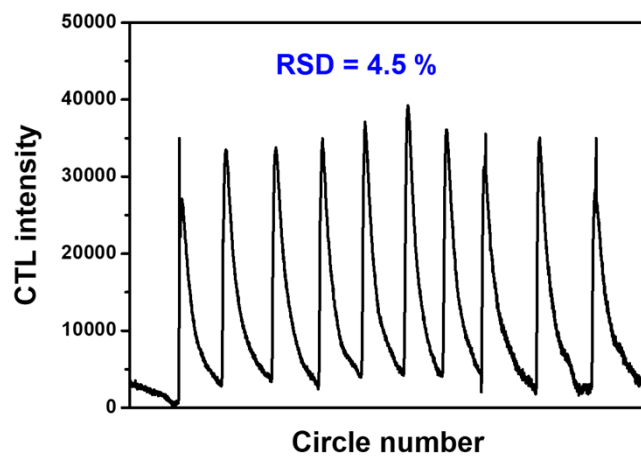


Fig. S5 Cycling experiments of photocatalytic oxidation of acetone on $\text{Co(OH)}_2\text{@ZIF-67}$ the catalyst surface. CTL measurement conditions: air flow rate 200 mL min^{-1} , reaction temperature $150 \text{ }^\circ\text{C}$, negative pressure -1000 V , acquisition interval 0.1 s .

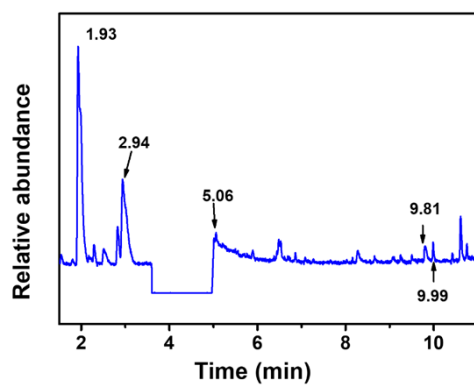


Fig. S6 Gas chromatography-mass spectrometry (GC-MS) analysis of the products collected in acetonitrile following CTL catalyzed by acetone over catalyst $\text{Co}(\text{OH})_2@$ ZIF-67.

Table S1 Conversion rates of acetone on clean ceramic rod surfaces, ZIF-67, Co(OH)₂@ZIF-67 and Co(OH)₂ surfaces. The conversion efficiency (CE) of acetone was calculated through $1-(c_1/c_0)\times 100\%$ equation.

Catalysts	c_0 (ppm)		c_1 (ppm)		CE (%)
clean ceramic rod	2000	1264	1427	1345	32.7 ± 4.1
	1000	725	757	735	26.1 ± 1.6
	500	471	460	465	6.9 ± 1.1
ZIF-67	2000	544	526	535	73.3 ± 0.5
	1000	240	260	231	75.6 ± 1.5
	500	68	70	92	84.7 ± 2.7
Co(OH) ₂ @ZIF-67	2000	238	268	257	87.3 ± 0.8
	1000	24	41	32	96.8 ± 0.9
	500	13	7	12	97.9 ± 0.6
Co(OH) ₂	2000	271	298	252	86.3 ± 1.2
	1000	132	117	125	87.5 ± 0.8
	500	45	30	32	92.9 ± 1.6

Table S2 Comparison of acetone catalytic oxidation performances with proposed $\text{Co(OH)}_2@\text{ZIF-67}$ and other reported catalysts.

Ref	Catalyst	Concentration ppm	Conversion rate	Conditions
1	$\text{SnO}_2\text{-Zn}_2\text{SnO}_4$	300 ppm	11% (140 min)	25 °C, 3 W LED ($\lambda = 420 \pm 10 \text{ nm}$)
2	$\text{Zr}_{0.4}\text{Co}_{0.6}\text{O}_x$	40000 $\text{mL}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	90%	208 °C
3	$\text{MnAl}_{0.5}$ oxides	1000 ppm	90%	165 °C
4	$\text{Pd}_{0.01}\text{Mn}_{0.1}/\text{Ti}$	1000 ppm	95%	259 °C
5	TiO_2	300 ppm	100% (120 min)	15W@365 nm, 0.41 W/cm ² ,
6	TiO_2	650 ppm	100% (30 min)	10.2 mW/cm ² $\lambda_{\text{max}} \sim 373 \text{ nm}$
This work	$\text{Co(OH)}_2@\text{ZIF-67}$	1000 ppm	96%	150 °C, $\lambda = 400\text{-}600 \text{ nm}$ without external lamp

- [1] Y. Li, X. Wu, W. Ho, K. Lv, Q. Li, M. Li, S. C. Lee, *Chem. Eng. J.*, 2018, **336**, 200–210.
 [2] X. Zhang, M. Li, X. Cui, X. Niu, Y. Zhu, *Chem. Eng. J.*, 2023, 465, 142857.
 [3] J.-R. Li, W.-P. Zhang, J. Zhao, M. Tian, K. Wu, H. Xiao, C. He, *ACS Appl. Mater. Interfaces*, 2022, **14**, 36536–36550.
 [4] Q. Zhao, Y. Ge, K. Fu, Y. Zheng, Q. Liu, C. Song, N. Ji, D. Ma, *Appl. Surf. Sci.*, 2019, **496**, 143579.
 [5] T. Shi, Y. Duan, K. Lv, Z. Hu, Q. Li, M. Li, X. Li, *Front. Chem.*, 2018, **6**, 175.
 [6] D.S. Selishchev, N.S. Kolobov, A.A. Pershin, D.V. Kozlov, *Appl. Catal., B*, 2017, **200**, 503–513.

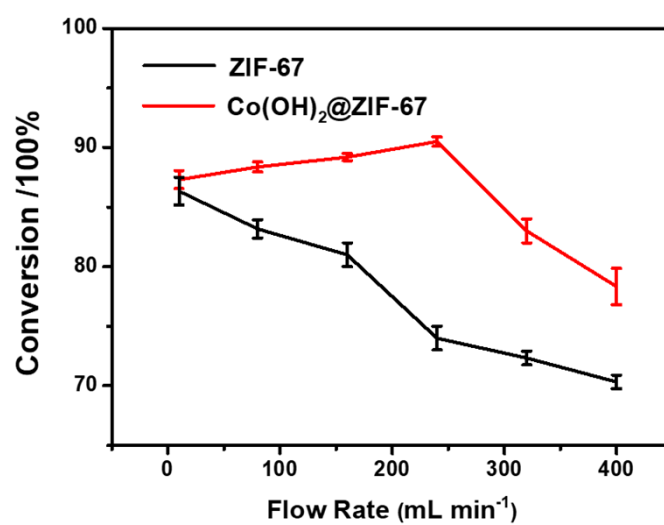


Fig. S7 Conversion of acetone at different carrier gas flow rates, $c_0=2000$ ppm.

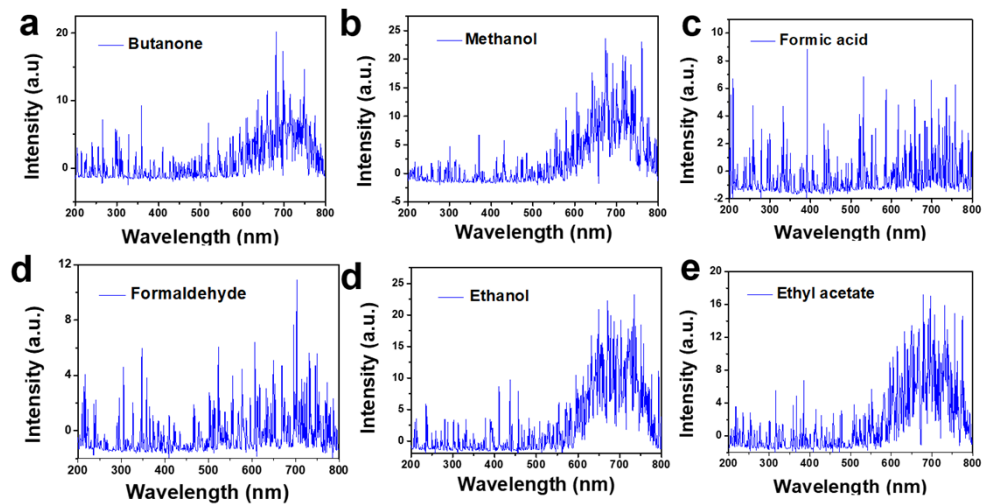


Fig. S8 CTL emission spectra of various VOCs on the surface of $\text{Co}(\text{OH})_2@\text{ZIF-67}$.

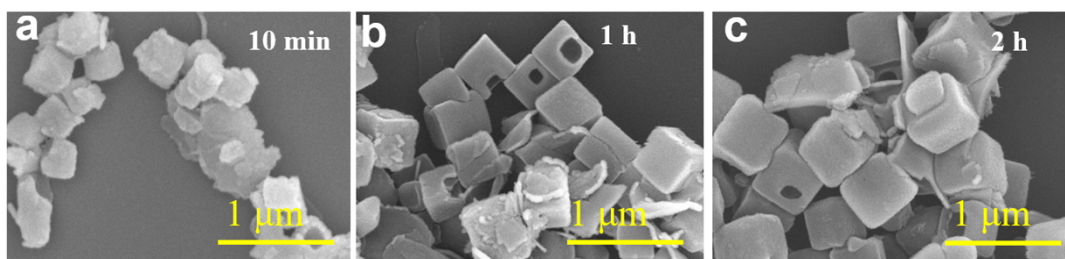


Fig. S9 SEM images of $\text{Co(OH)}_2@\text{ZIF}$ 67-10min, $\text{Co(OH)}_2@\text{ZIF}$ 67-1h, $\text{Co(OH)}_2@\text{ZIF}$ 67-2h.

Table S3 Conversion efficiency (CE) of ethanol, butanone, ethyl acetate, acetaldehyde and formic acid on Co(OH)₂@ZIF-67 surfaces.

VOC	c_0 (ppm)	c_1 (ppm)	CE in dark (%)	c_1 (ppm)	CE with LED (%)
Ethanol	2000	1790	10.5	1286	35.7
Butanone	2000	1330	33.5	1076	46.2
Ethyl acetate	2000	1540	23.0	1172	41.4
Acetaldehyde	2000	1572	21.7	1504	24.8
Formic acid	2000	1856	7.2	1800	10.0

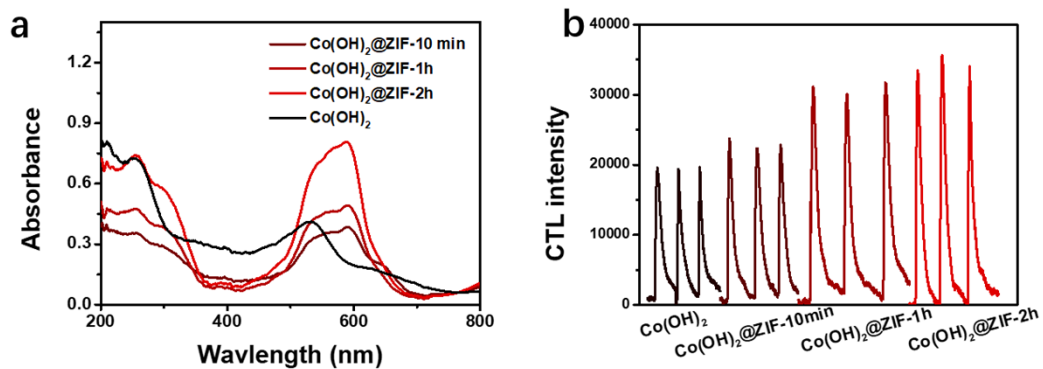


Fig. S10 (a) UV-vis absorbance of Co(OH)_2 , $\text{Co(OH)}_2@ZIF-67-10\text{min}$, $\text{Co(OH)}_2@ZIF-67-1\text{h}$ and $\text{Co(OH)}_2@ZIF-67-2\text{h}$; (b) CTL signals of acetone on the surfaces of Co(OH)_2 , $\text{Co(OH)}_2@ZIF-67-10\text{min}$, $\text{Co(OH)}_2@ZIF-67-1\text{h}$ and $\text{Co(OH)}_2@ZIF-67-2\text{h}$.

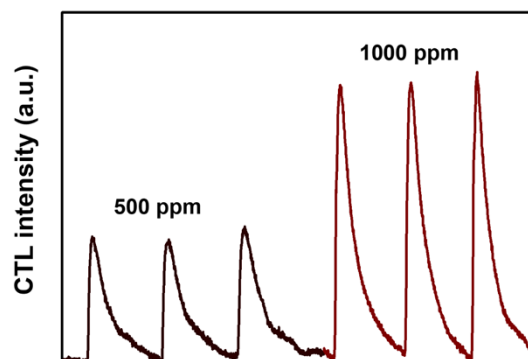


Fig. S11 CTL signals of acetone at 500 and 1000 ppm on Co(OH)₂@ZIF-67 surface.

CTL measurement conditions: air flow rate 200 mL/min, reaction temperature 150 °C,

negative pressure -1000 V, acquisition interval 0.1s.

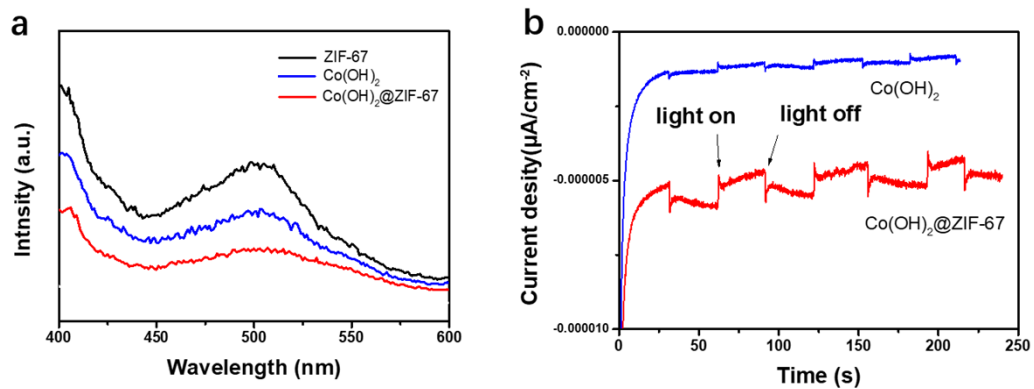


Fig. S12 (a) Fluorescence spectra of ZIF-67, $\text{Co(OH)}_2@ZIF-67$ and Co(OH)_2 .

Experimental conditions: excitation wavelength 380 nm, slit 5 nm, solvent methanol.

(b) Photogenerated current plots of Co(OH)_2 and $\text{Co(OH)}_2@ZIF-67$.

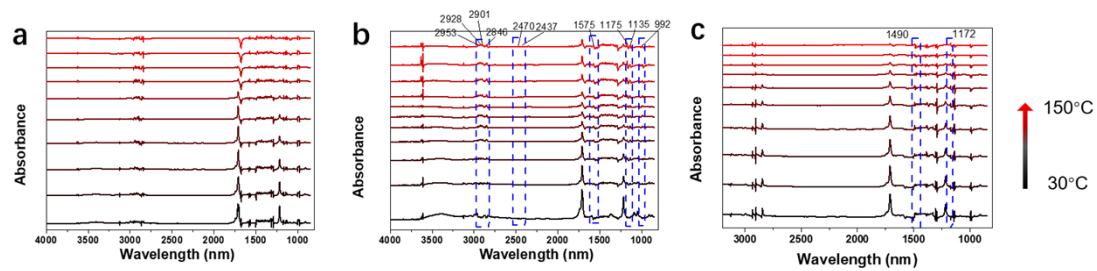


Fig. S13 In situ-IR spectra of CTL intermediates from acetone on the surface of ZIF-67 (a), $\text{Co(OH)}_2@ZIF-67$ (b), and Co(OH)_2 (c) catalysts. Acetone was added by the bubbling method at a rate of $10\text{ }^\circ\text{C}/\text{min}$ and the test range was $30\text{-}150\text{ }^\circ\text{C}$.

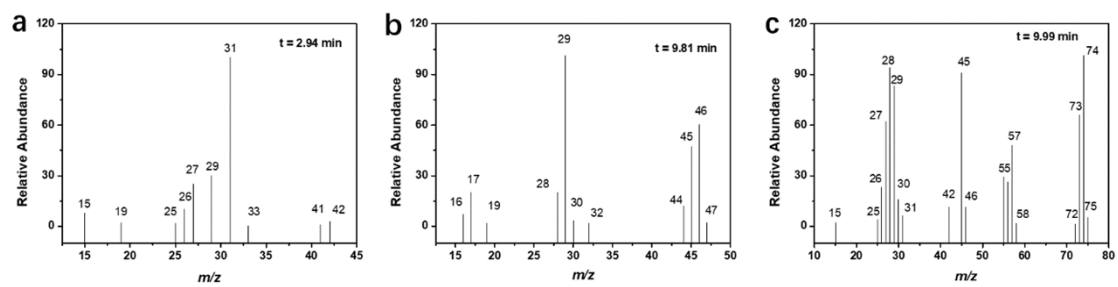


Fig. S14 MS spectra of the main products from exhaust gas.

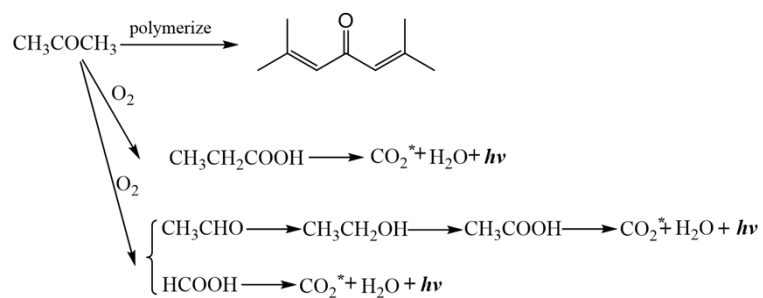


Fig. S15 Inference diagram of the oxidation process of acetone on the $\text{Co}(\text{OH})_2@ZIF-67$ surface reaction.

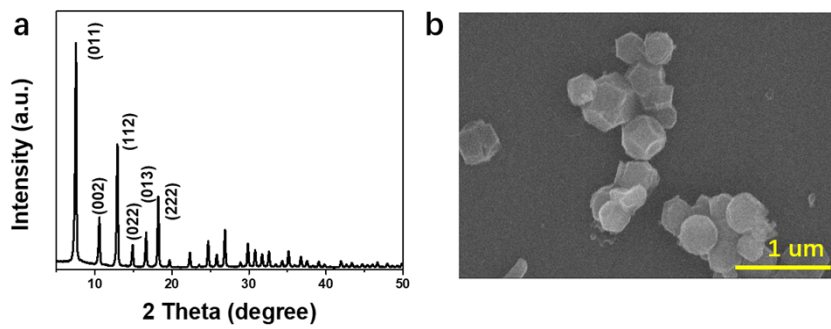


Fig. S16 XRD and SEM image diagram of ZIF-8.