

1 Supplementary Information

2 Modulate energy barriers and reaction pathways via dual-ligands
3 engineering for enabling efficient NO removal and hydrogen production

4

5 Kaili Wu ^{a,1}, Bin Yao ^{a,*1}, Yan Lin ^a, Yirui Qiu ^a, Lang Sun ^a, Youzhou He ^a, Yongcheng Feng ^a, Min Fu
6 ^a, Chenghua Zhang ^{b,*}, Xingyan Liu ^a, Siping Wei ^{c,*}

7

8 ^a Chongqing Key Laboratory of Environmental Catalysis, College of Environment and Resources,
9 Chongqing Technology and Business University, Chongqing 400067, China.

10 ^b School of Pharmacy, North Sichuan Medical College, Nanchong 637100, China.

11 ^c Central Nervous System Drug Key Laboratory of Sichuan Province, Department of Medicinal
12 Chemistry, School of Pharmacy, Southwest Medical University, Luzhou 646000, China.

13

14 ¹ These authors contributed equally to this work and should be considered co-first authors.

15 ^{*} Corresponding authors. E-mail addresses: yaobin@ctbu.edu.cn (B. Yao), zchua@nsmc.edu.cn (C.
16 Zhang), wei1225@swmu.edu.cn (S. Wei).

17

18 Table of content

19	Supplementary Texts.....	4
20	Text S1. Materials	4
21	Text S2. The synthesis of NM125-D-A ⁰	4
22	Text S3. Characterization of photocatalysts	4
23	Text S4. Photocatalytic water decomposition to produce hydrogen	5
24	Text S5. Photocatalytic NO purification	6
25	Text S6. <i>In-situ</i> DRIFTS spectra.....	7
26	Text S7. Electrochemical measurements.....	7
27	Text S8. Theoretical calculations	8
28	Supplementary Figures.....	9
29	Fig. S1 Pore Parameters for NM125, NM125-D and NM125-D-A.....	9
30	Fig. S2 (a) O 1s of NM125, NM125-D and NM125-D-A and (b) Au 4f of NM125-D-A	9
31	Fig. S3 TEM of (a-b) NM125-D and (c-d) NM125-D-A.	9
32	Fig. S4 TEM-EDS elemental mapping of NM125-D-A.....	10
33	Fig. S5 XRD pattern of NM125-D-A before and after NO removal.....	10
34	Fig. S6 (a) XRD pattern and (b) photocatalytic hydrogen evolution of NM125-D-A ⁰ and NM125-D-A	10
35		10
36	Fig. S7 <i>In-situ</i> infrared spectra of NO adsorption processes over (a) NM125 and (b) NM125-D-A	11
37	Fig. S8 Density of States (DOS) of NM125, NM125-D and NM125-D-A	11
38	Fig. S9 Adsorption of O ₂ and H ₂ O molecule on different Ti sites in NM125-D-A.	12
39	Fig. S10 Possible photocatalytic mechanism of NM125	12
40	Supplementary Tables	14
41	Table. S1. Au contents (wt %) of different samples characterized by ICP-OES.....	14
42	Table. S2. Specific Surface Area and Pore Parameters for NM125, NM125-D and NM125-D-A	14
43	Table. S3. Comparison of photocatalytic hydrogen evolution data of MOF-based photocatalysts	
44	reported in recent years	14
45	Table. S4. Comparison of photocatalytic NO removal data of MOF-based photocatalysts reported	

46	in recent years	16
47	Table. S5. Band structure of NM125, NM125-D and NM125-D-A	17
48	Table. S6. Substances corresponding to infrared peak values during dark adsorption and	
49	photocatalytic oxidation stages.....	17
50	Table. S7. The reaction pathway for NO removal.....	18
51	Table. S8. The reaction pathway for H ₂ production.....	19
52	References	19
53		
54		

55 **Supplementary Texts**

56 **Text S1. Materials**

57 During the experiment, 2-amino-terephthalic acid ($\text{NH}_2\text{-BDC}$, 98%, Aladdin), 2,2'-
58 bipyridine-5,5'-dicarboxylic acid (DPDC, 98%, Zhengzhou Alfa Chemical Co., Ltd),
59 Titanium tetraisopropanolate (TTIP, 99%, Adamas), N, N-dimethylformamide (DMF,
60 99%, Adamas), Methyl alcohol (MeOH, 99%, Adamas), and Tetrachloroauric acid
61 trihydrate ($\text{HAuCl}_4 \cdot 3\text{H}_2\text{O}$, 99%, Adamas) were used. All reagents are analytical grade,
62 which can be used directly without treatment.

63

64 **Text S2. The synthesis of NM125-D-A⁰**

65 NM125-D-A (80 mg) was added to deionized water (10 mL), followed by the
66 addition of glucose (100 mg). And then stirred it at room temperature for 4 h. After
67 the completion of the reaction, the resulting product was washed several times with
68 deionized water and dried overnight, named NM125-D-A⁰.

69

70 **Text S3. Characterization of photocatalysts**

71 The physical properties and chemical structure of the samples are determined
72 using X-ray diffraction (XRD, XRD-6100, SHIMADZU, Japan), Inductive coupled plasma
73 optical emission spectrometer (ICP-OES) (SPECTRO GENESIS, FES27, Germany),
74 scanning electron microscopy (SEM, SU-1510, HITACHI, Japan), transmission electron
75 microscope (TEM, JEM-F200, Japan), X-ray photoelectron spectroscopy (XPS, Thermo
76 Scientific K-Alpha+, America), and N_2 adsorption-desorption isotherms (BET, ASAP-
77 2020, USA). The optical properties are analyzed through UV-visible diffuse reflectance

78 spectroscopy (UV-vis DRS, UV-2700, SHIMADZU, Japan), Fourier transform infrared
79 (FT-IR) spectra (Nicolet Apex, Thermo Scientific, USA), synchronous thermal analyzer
80 (TGA) (STA499F3, NETZSCH, Germany), steady-state photoluminescence (PL, F-700,
81 HITACHI, Japan, and FLS-1000, Edinburgh instruments), and photoelectrochemical
82 analysis (FX-300, Perfectlight, China, and CHI660E, Chenhua, China). The mechanism
83 of the photocatalytic reaction for the samples is investigated through free radical
84 trapping experiments and the electron spin-resonance spectroscopy (ESR) (JES FA 200,
85 Japan).

86

87 **Text S4. Photocatalytic water decomposition to produce hydrogen**

88 Typically, 18 mL acetonitrile, 2 mL triethanolamine, 0.2 mL deionized water, and
89 1 mL chloroplatinate acetonitrile solution (1 mg/mL) are added to the quartz reactor,
90 respectively. Among them, acetonitrile is used as a solvent, triethanolamine is used as
91 an electron sacrifice agent, deionized water is used as a proton source, and
92 chloroplatinic acid is used as a cocatalyst. Then, 10 mg sample is added, the mixture is
93 ultrasonically dispersed, and nitrogen is then injected into the mixture for 20 min to
94 remove the air in the solution. Finally, a 300 W Xenon lamp is placed above the reactor
95 and a 420 nm cut-off filter was installed to drive the photocatalytic hydrogen evolution
96 reaction. In order to keep the reaction at a constant temperature, a constant
97 temperature cooling circulation pump is equipped to keep the temperature of the
98 reactor at 5 °C, and then the hydrogen generation is measured online by gas
99 chromatography (GC 7920, Ceaulight, Beijing).

100 In addition, the apparent quantum yield (AQY) and energy conversion efficiency
 101 (STH) corresponding to hydrogen production are measured for the prepared samples
 102 under continuous illumination at 380, 420 and 500 nm.

$$103 \quad AQY (\%) = \frac{N_e}{N_p} \times 100\% = \frac{2N_A R}{E\lambda/hc}$$

104 In this equation, N_e represents the total number of transferred electrons in the
 105 reaction and N_p represents the number of incident photons. R represents hydrogen
 106 production (mol), N_A represents Avogadro constant, E represents optical power (W),
 107 λ represents incident optical wavelength (nm), h represents Planck constant (J·s) and
 108 c represents the speed of light (m/s).

$$109 \quad STH (\%) = \frac{\alpha \times \Delta G}{P_{light} \times S} \times 100\%$$

110 In this equation, α represents the hydrogen production efficiency (mmol/s), ΔG
 111 represents the Gibbs free energy (J/mol), P_{light} represents the energy flux of the
 112 incident light (mW/cm²), and S represents the area of the reactor (cm²).

113

114 **Text S5. Photocatalytic NO purification**

115 Initially, the sample (0.1 g) is sonicated in an ethanol solution to ensure
 116 homogenous dispersion. It is then evenly distributed in two Petri dishes with a
 117 diameter of 12 cm. After drying, the sample is placed in a rectangular glass reactor
 118 measuring 30 cm × 15 cm × 10 cm. Above the reactor, a Xenon lamp with a power of
 119 300 W is placed and equipped with a 420 nm cut-off filter. The air flow (2.4 L/min) and
 120 NO gas flow (24 mL/min) are activated. Once the NO_x analyzer (Thermo Environmental

121 Instruments Inc., Model 42i-TL) detected a stable NO concentration of 550 ppb, the
122 Xenon lamp is switched on for a duration of 30 min. After the designated time, the
123 lamp is turned off.

$$124 \quad \eta (\%) = \left(1 - \frac{C_t}{C_0}\right) \times 100\%$$

125 In this equation, C_t and C_0 represent the NO concentrations in the inlet and outlet
126 air, respectively.

127

128 **Text S6. *In-situ* DRIFTS spectra**

129 For in-situ analysis of the intermediate species involved in the degradation of NO,
130 the Rruker70v spectrometer (Harrick) equipped with an MCT detector is employed.
131 The catalyst prepared is placed onto the surface of a diamond ATR crystal, followed
132 by a 30 min vacuum treatment to eliminate adsorbed water molecules. Subsequently,
133 a mixture of NO and O₂ is introduced into the gas pipeline, and after a 30 min
134 adsorption of NO, the system is exposed to simulated visible light for 30 min to initiate
135 photocatalytic oxidation. Infrared spectra are recorded every 2 min during the
136 process, allowing for real-time monitoring of the changing molecular species.

137

138 **Text S7. Electrochemical measurements**

139 An electrochemical instrument with a three-electrode system was used to analyze
140 electrochemical measurements. The working electrode was prepared as follows: add
141 50 μ L H₂O, 450 μ L ethanol, 10 μ L Nafion, the sample (1 mg) and ultrasonic dispersion
142 for 30 min, and then transferred 100 μ L suspension to coat the ITO. The electrode was

143 dried in air at room temperature. The reference electrode was calomel electrode and
144 the counter electrode was platinum electrode. Electrochemical impedance
145 spectroscopy (EIS) and transient photocurrent tests were conducted in Na₂SO₄ (0.2
146 M). A xenon lamp (300 W) was treated as the light irradiation for photocurrent test.

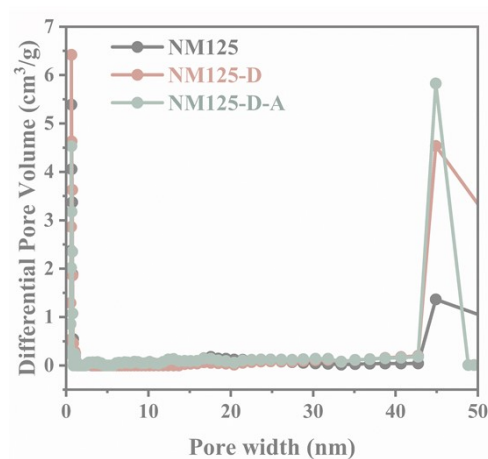
147

148 **Text S8. Theoretical calculations**

149 The Vienna Ab Initio Package (VASP) is employed to perform all the density
150 functional theory (DFT) calculations within the generalized gradient approximation
151 (GGA) using the Perdew, Burke, and Enzerhof (PBE) formulation ^{1, 2}. The projected
152 augmented wave (PAW) potentials are applied to describe the ionic cores and take
153 valence electrons into account using a plane wave basis set with a kinetic energy cutoff
154 of 450 eV ^{3, 4}. Partial occupancies of the Kohn–Sham orbitals are allowed using the
155 Gaussian smearing method and a width of 0.05 eV. The 3×3×1 Monkhorst-Pack grid is
156 used to sample the Brillouin region.

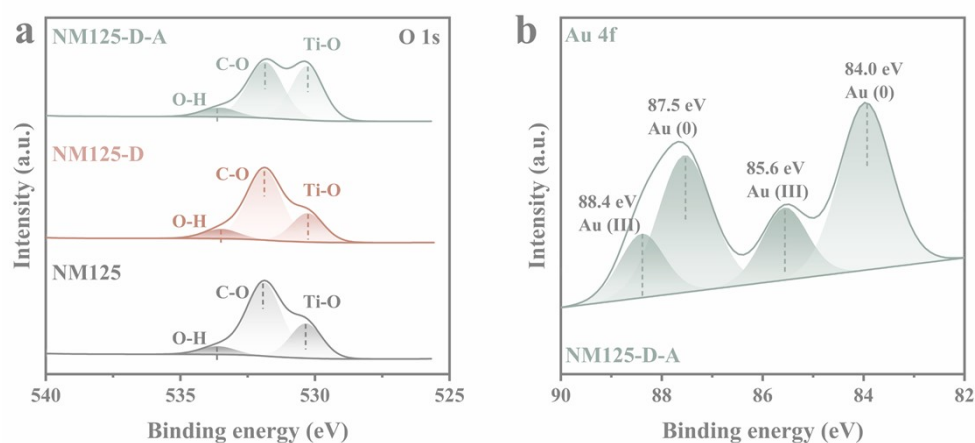
157

158 Supplementary Figures



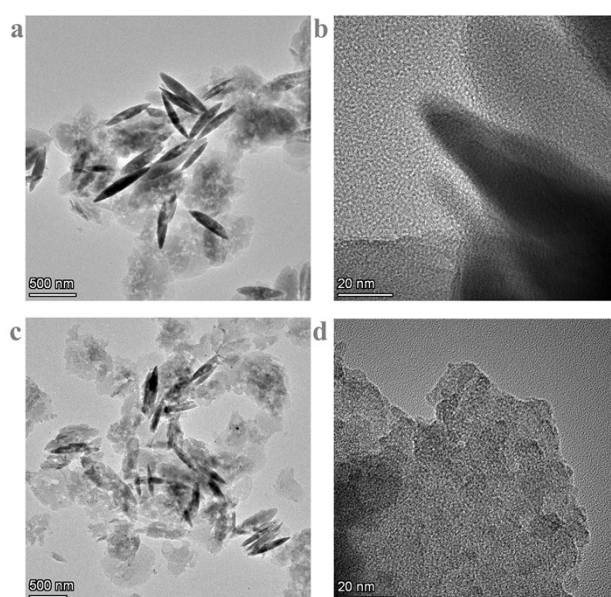
159

160 **Fig. S1** Pore Parameters for NM125, NM125-D and NM125-D-A



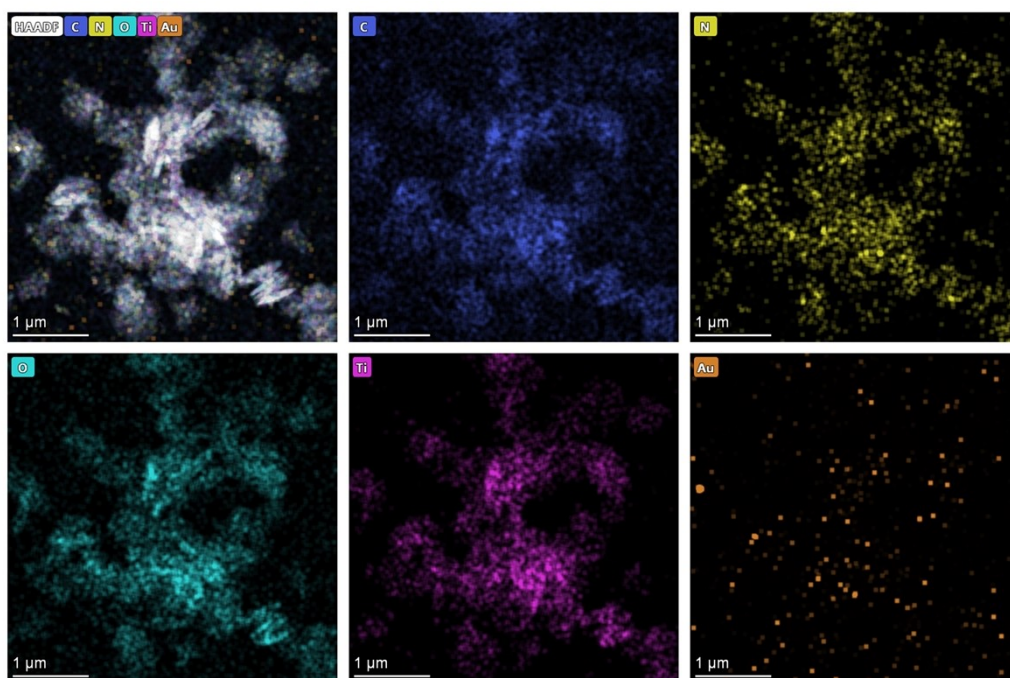
161

162 **Fig. S2** (a) O 1s of NM125, NM125-D and NM125-D-A and (b) Au 4f of NM125-D-A



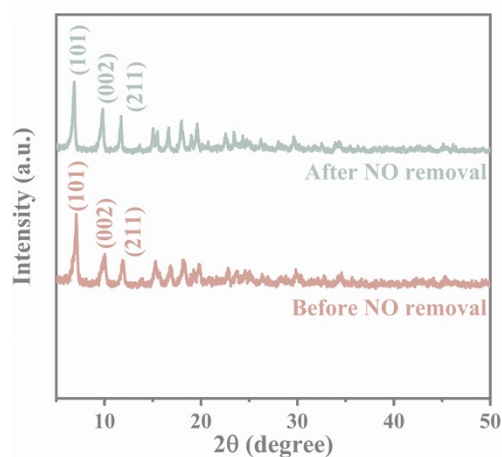
163

164 **Fig. S3** TEM of (a-b) NM125-D and (c-d) NM125-D-A.



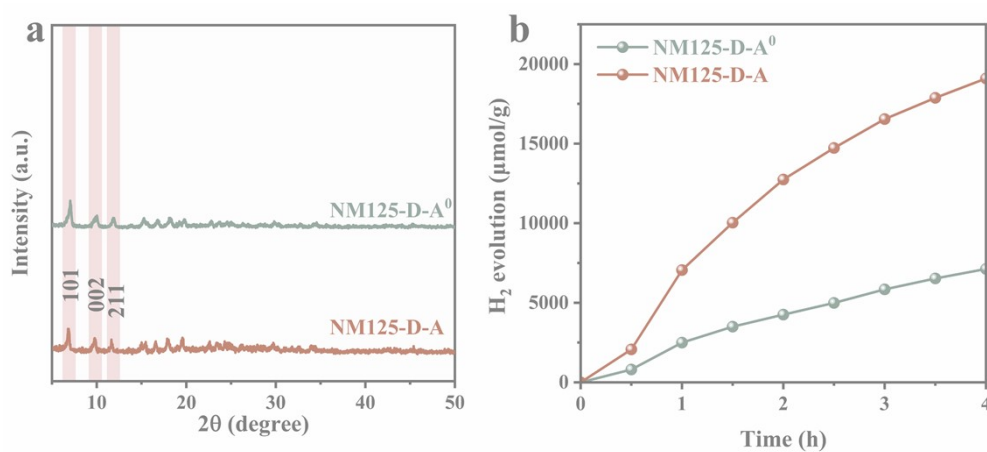
165

166 **Fig. S4** TEM-EDS elemental mapping of NM125-D-A



167

168 **Fig. S5** XRD pattern of NM125-D-A before and after NO removal

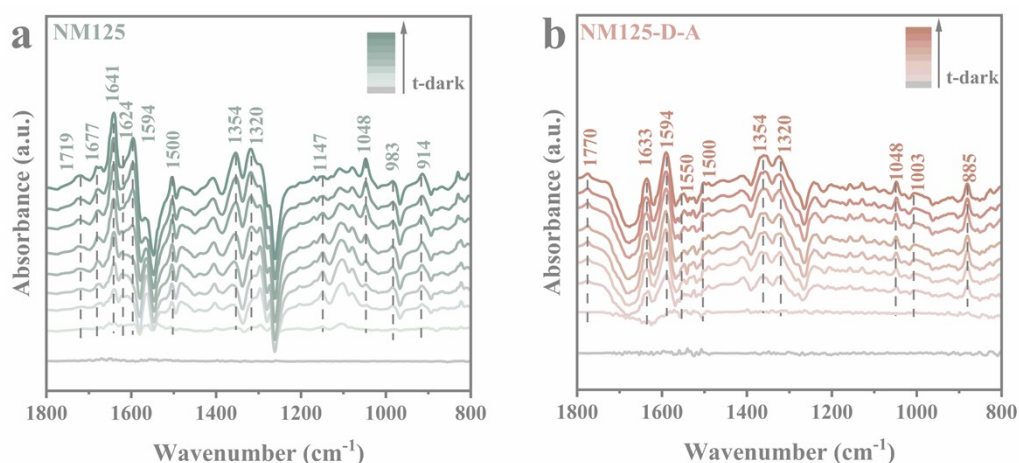


169

170 **Fig. S6** (a) XRD pattern and (b) photocatalytic hydrogen evolution of NM125-D-A⁰ and

171 NM125-D-A

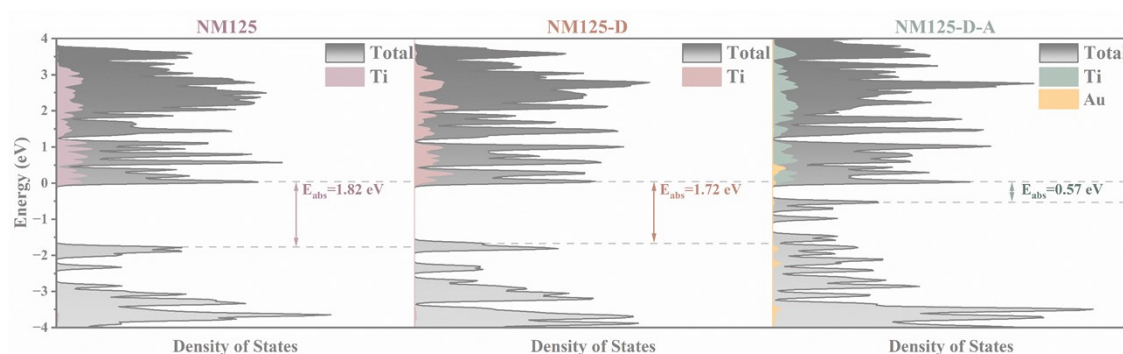
172 We reduced the Au ions in NM125-D-A to the metallic state using glucose
 173 (denoted as NM125-D-A⁰)⁵. XRD results (Fig. S6a) showed that the patterns of NM125-
 174 D-A⁰ and NM125-D-A were highly consistent, indicating that the reduction process did
 175 not cause the collapse of the MOF framework. The results (Fig. S6b) showed that the
 176 hydrogen production rate of NM125-D-A⁰ sharply decreased to 1780.90 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$,
 177 which was much lower than that of NM125-D-A (4773.50 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$).



178

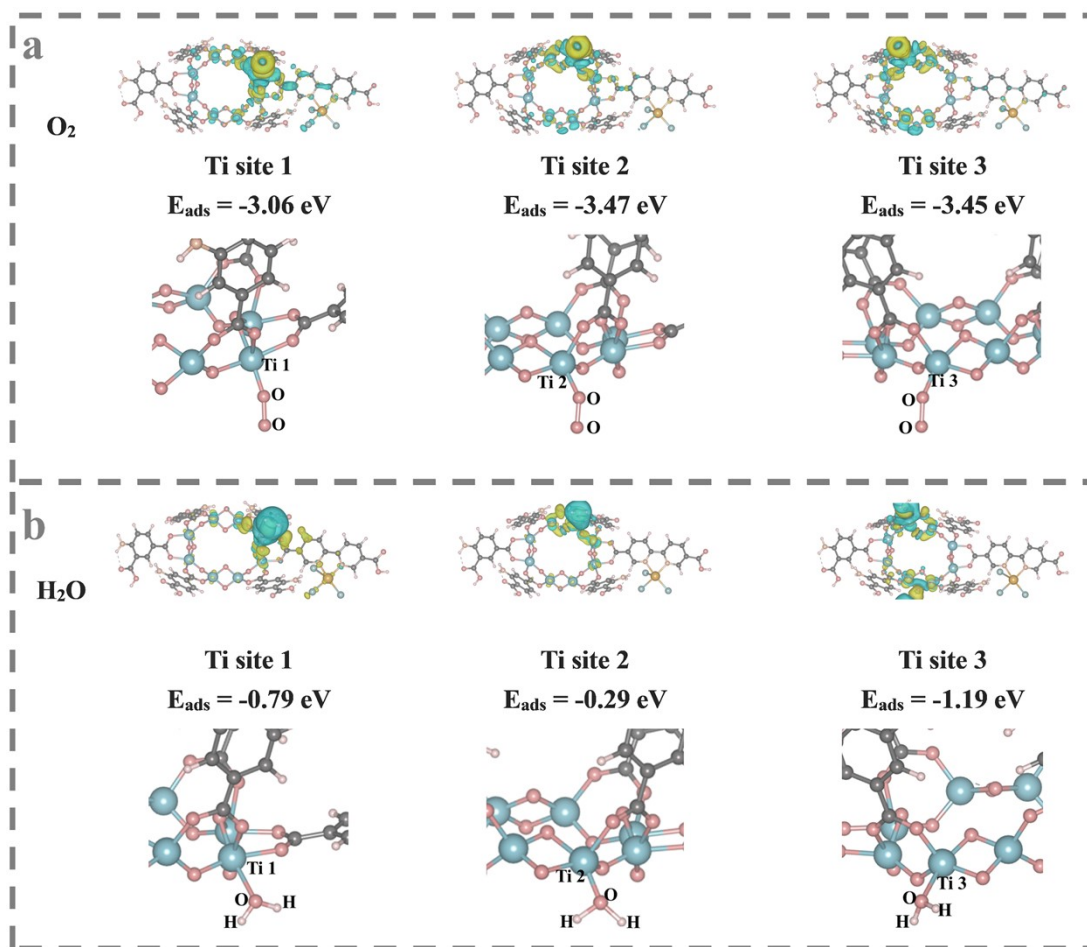
179 **Fig. S7** *In-situ* infrared spectra of NO adsorption processes over (a) NM125 and (b)

180 NM125-D-A



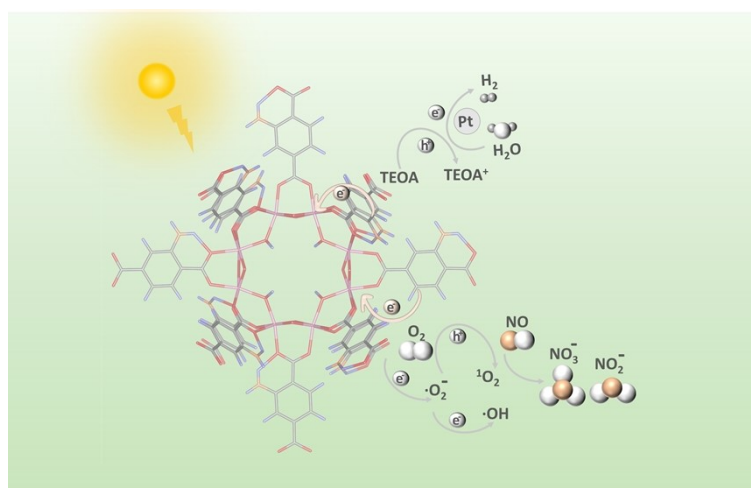
181

182 **Fig. S8** Density of States (DOS) of NM125, NM125-D and NM125-D-A



183

184 **Fig. S9** Adsorption of O₂ and H₂O molecule on different Ti sites in NM125-D-A.



185

186 **Fig. S10** Possible photocatalytic mechanism of NM125

187 For the parent NM125 (Fig. S10), the ligand 2-Aminoterephthalic acid (NH₂-BDC)

188 acted as a light-harvesting antenna. Following photoexcitation, the generated charge

189 carriers were transferred to the Ti-oxo cluster, representing a conventional ligand-to-
190 metal charge transfer (LMCT) process. The Ti-oxo site then served as the active center
191 for the subsequent catalytic reactions.

192

Supplementary Tables

Table. S1. Au contents (wt %) of different samples characterized by ICP-OES

Sample	Au contents (wt %)
NM125-D-A	0.65

Table. S2. Specific Surface Area and Pore Parameters for NM125, NM125-D and

NM125-D-A

Sample	BET surface area (m ² /g)	Total pore volume (cm ³ /g)	Mesoporous pore volume (cm ³ /g)	Average pore diameter (nm)
NM125	1165.43	0.627	0.178	2.15
NM125-D	1306.29	0.749	0.243	2.29
NM125-D-A	905.00	0.610	0.284	2.70

Table. S3. Comparison of photocatalytic hydrogen evolution data of MOF-based photocatalysts reported in recent years

Photocatalysts	Mass of photocatalyst	Light source	Sacrificial agents	Cocatalyst	H ₂ Production rate	Ref.
NM125-D-A	10 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	Pt	4773.50 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	This work ¹
M-125-45-N	10 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	Pt	3700 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	⁶
C/TiO ₂ /MIL-125	10 mg	132.6 mW LED lamp, $\lambda \geq 400$ nm	Methanol	—	314 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	⁷
W-MIL-125	25 mg	300 W Xe lamp, $\lambda \geq 300$ nm	TEOA	Pt	1110.7 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	⁸

		nm				
MIL-125(Ti)/ZnIn ₂ S ₄	100 mg	—	Na ₂ S/Na ₂ SO ₃	—	873.4 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	⁹
g-C ₃ N ₄ /TiO ₂ /MIL-125	25 mg	300 W Xe lamp	Glycerol	NiS	1330 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁰
MIL-125-NH ₂ @TiO ₂	5 mg	300 W Xe lamp, $\lambda \geq 380$ nm	TEOA	—	496 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹¹
Pd/PdTCPP/NH ₂ -MIL-125	10 mg	300 W Xe lamp $\lambda \geq 420$ nm	TEOA	—	603 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹²
Co-CDs/NH ₂ -MIL-125	30 mg	300 W Xe lamp $\lambda \geq 380$ nm	TEOA	Pt	2261 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹³
Yb-NH ₂ -MIL-125	10 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	Pt	1884 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁴
1 % PCN-222(Pd)/g-C ₃ N ₄ -AA	50 mg	300 W xenon lamp	TEOA	Pt	2338.17 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁵
Ti-MOF@P-Pt ₁ SACs	10 mg	300 W xenon lamp, $\lambda \geq 400$ nm	TEOA	—	4193 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁶
TiO ₂ @NM/Ni10%	10 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	—	1659.9 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁷
ENHM-2	10 mg	300 W Xe lamp	TEOA	Pt	2150 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁸
Ti ₃ C ₂ @MIL-NH ₂	70 mg	300 W Xe arc lamp with an AM- 1.5 filter	TEOA	—	4383.1 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	¹⁹
Au@NH ₂ -UiO-66/CdS	5 mg	300 W Xe lamp, $\lambda \geq 420$ nm	lactic acid	—	664.9 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	²⁰

CdS/MIL-53(Fe)	5 mg	300 W Xe lamp, $\lambda \geq 420$ nm	benzyl alcohol	—	2334 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	21
CP@U6N	50 mg	300 W Xe lamp, $\lambda \geq 400$ nm	H_3PO_2	—	141.87 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	22
UNiMOF	50 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	—	572 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	23
UiO-66@ZnIn ₂ S ₄	40 mg	300 W Xe lamp, $\lambda \geq 400$ nm	TEOA	—	3061.61 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	24
					1	
Ni-BDC/Ni-TCPP-3	10 mg	300 W Xe lamp	TEOA	—	428.0 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	25
PdS@MIL-125-NH ₂ @ZnS	10 mg	225 W Xe lamp	TEOA	—	1164.2 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	26
CdS/Ni-MOF	30 mg	300 W Xe lamp, $\lambda \geq 420$ nm	lactic acid	—	2508 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	27
MOF-5/CuO@ZnIn ₂ S ₄	100 mg	300 W Xe lamp	Methanol	—	1938.3 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	28
NH ₂ -MIL-125/Co(dmgH) ₂	10 mg	300 W Xe lamp, $\lambda \geq 420$ nm	TEOA	—	2195 $\mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$	29

199 **Table. S4. Comparison of photocatalytic NO removal data of MOF-based**
200 **photocatalysts reported in recent years**

Photocatalysts	Mass of photocatalyst	Light source	NO removal rate	Ref.
NM125-D-A	100 mg	300 W Xe lamp, $\lambda \geq 420$ nm	65.04%	This work
N/C/MIL-125(Ti)	100 mg	300 W Xe lamp, $\lambda \geq 420$ nm	49%	30
Co-CDs-NH ₂ -MIL-125	100 mg	12 W LED lamp	67.6%	31

Au/MIL-125-NH ₂ (Ti)/PdTCPP	100 mg	150 W tungsten halogen lamp	63.72%	32
TiO ₂ /NH ₂ -MIL-125(Ti)	200 mg	150 W tungsten halogen lamp, $\lambda \geq 420$ nm	68.08%	33
Defect-NH ₂ -MIL-125/Eosin Y	200 mg	150 W tungsten halogen lamp, $\lambda \geq 420$ nm	62.05%	34
Au@NH ₂ -MIL-125(Cu/Ti)	100 mg	12 W LED lamp	43%	5
STO/GQDs/NU6	100 mg	300 W Xe lamp, $\lambda \geq 400$ nm	69.0%	35
CN/NU6	100 mg	300 W Xe lamp, $\lambda \geq 400$ nm	65.4%	36
GO/NH ₂ -MIL-125(Ti)	50 mg	two 150 W tungsten halogen lamp, $\lambda \geq 420$ nm	50%	37
65-NH ₂ -MIL-125	100 mg	12 W LED lamp	65.49%	38
Protonated NH ₂ -MIL-125	100 mg	12 W LED lamp	49.17%	39

201 **Table. S5.** Band structure of NM125, NM125-D and NM125-D-A

Material	Band gap (E_g , eV)	Conduction band (E_{CB} , V)	Valence band (E_{VB} , V)
NM125	2.66	-0.61	2.05
NM125-D	2.62	-0.76	1.86
NM125-D-A	2.57	-0.83	1.74

202 **Table. S6.** Substances corresponding to infrared peak values during dark adsorption

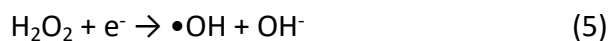
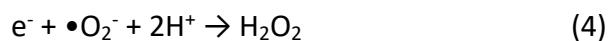
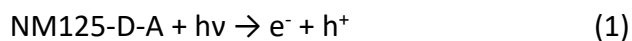
203 and photocatalytic oxidation stages

	NM125			NM125-D-A		
	Wavenumber	Band attribution	Ref	Wavenumber	Band attribution	Ref
	r			r		
	(cm ⁻¹)			(cm ⁻¹)		
Adsorption process	914, 1677	N ₂ O ₄	40, 41	885, 1320	NO ₂	42, 43

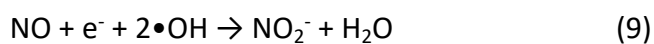
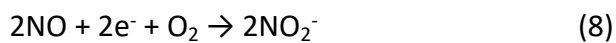
Photocatalytic process	983, 1354, 1594, 1719	NO_2^-	44-46	1003, 1048, 1500, 1550, 1770	NO_3^-	30, 46-48
	1048, 1500	NO_3^-	48	1354, 1594, 1633	NO_2^-	45, 46
	1147, 1641	NO	49, 50	885, 1320	NO_2	42, 43
	1320, 1624	NO_2	43	914, 1677	N_2O_4	40, 41
				983, 1354, 1594, 1719	NO_2^-	44-46
				871, 1048, 1122, 1500	NO_3^-	48, 51, 52
				1147, 1641	NO	49, 50
				1320	NO_2	43

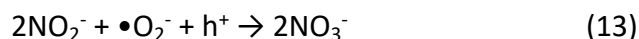
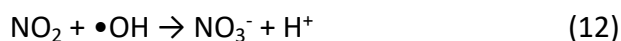
204 **Table. S7.** The reaction pathway for NO removal

Generation of reactive species of NM125-D-A



Photocatalytic removal of NO reaction of NM125-D-A





205 **Table. S8.** The reaction pathway for H₂ production



206

207 References

- 208 1. G. Kresse and D. Joubert, *Phys. Rev. B*, 1999, **59**, 1758.
- 209 2. J. P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.*, 1996, **77**, 3865-3868.
- 210 3. G. Kresse and J. Furthmüller, *Phys. Rev. B Condens. Matter*, 1996, **54**, 11169-
211 11186.
- 212 4. S. Grimme, J. Antony, S. Ehrlich and H. Krieg, *J. Chem. Phys.*, 2010, **132**, 154104.
- 213 5. Y. He, H. Li, J. Wu, Z. Liu, Y. Chen, W. Guo, Y. Wu, M. Fu and X. Liu, *Appl. Surf. Sci.*,
214 2022, **604**, 154641.
- 215 6. X. Liu, K. Wu, C. Jia, Y. He, Y. Qiu, Y. Fang, H. Ma, S. Wang, S. Wei and F. Dong, *J.*
216 *Colloid Interface Sci.*, 2025, **680**, 948-964.
- 217 7. Y. Zhao, N. Yang, T. Zhou, W. Zhan, J. Zhao, M. Chen, T. He, J. Zhang, Y. Zhang, G.
218 Zhang and Q. Liu, *Int. J. Hydrogen Energy*, 2024, **65**, 151-157.
- 219 8. Y. Zhang, F. Mao, Y. Liu, X. Wu, C. Wen, S. Dai, P. Liu and H. Yang, *Sci. China*
220 *Mater.*, 2022, **65**, 1237-1244.
- 221 9. T. Liu, B. Wang, M. Wang, J. Gu, W. Wang, H. Shen and J. Zhang, *J. Mater. Sci.*,
222 2024, **59**, 1253-1264.
- 223 10. B. Tatykayev, B. Chouchene, L. Balan, T. Gries, G. Medjahdi, E. Girot, B.
224 Uralbekov and R. Schneider, *Nanomaterials*, 2020, **10**, 1387.
- 225 11. B. Zhang, J. Zhang, X. Tan, D. Shao, J. Shi, L. Zheng, J. Zhang, G. Yang and B. Han,
226 *ACS Appl. Mater. Interfaces*, 2018, **10**, 16418-16423.
- 227 12. C. Jia, Y. Wang, R. Zeng, X. Liu, Y. You, Y. Feng, S. Wang, Y. He, S. Li and S. Wei,
228 *Mol. Catal.*, 2024, **556**, 113925.
- 229 13. Y. He, S. Luo, Y. Tan, M. Chen, H. Zhou, J. Yu, L. Pu, Y. Huang, M. Fu and X. Liu, *J.*
230 *Alloys Compd.*, 2022, **913**, 165226.
- 231 14. H. Li, X. Liu, H. Feng, J. Zhao, P. Lu, M. Fu, W. Guo, Y. Zhao and Y. He, *Catal. Sci.*
232 *Technol.*, 2021, **11**, 6225-6233.
- 233 15. Y. Li, W. Qin, X. Li, Q. Zhu, F.-q. Bai and T. Tian, *Chem. Eng. J.*, 2025, 168119.
- 234 16. Y. Zhu, N. Song, S. Liu, K. Zhang, B. Liu and Y. Wang, *Green Chem.*, 2025, **27**,

- 235 7973-7981.
- 236 17. J. Li, H. Chang, S. Feng, H. Jian, Q. Shen, X. Liu, H. Jia and J. Xue, *Chem. Eng. J.*,
237 2024, **498**, 155542.
- 238 18. Y. Liu, X. Xin, Y. Shi, Z. Zhao, J. Tan, D. Yang and Z. Jiang, *Chem. Eng. J.*, 2024, **482**,
239 149193.
- 240 19. Y. Li, Y. Liu, Z. Wang, P. Wang, Z. Zheng, H. Cheng, Y. Dai and B. Huang, *Chem.*
241 *Eng. J.*, 2021, **411**, 128446.
- 242 20. Z. Li, J. Zi, X. Luan, Y. Zhong, M. Qu, Y. Wang and Z. Lian, *Adv. Funct. Mater.*,
243 2023, **33**, 2303069.
- 244 21. P. Li, X. Yan, S. Gao and R. Cao, *Chem. Eng. J.*, 2021, **421**, 129870.
- 245 22. Y.-Y. Wang, X.-Y. Ji, M. Yu and J. Tao, *Mater. Chem. Front.*, 2021, **5**, 7796-7807.
- 246 23. A. Cao, M. Zhang, X. Su, V. Romanovski and S. Chu, *ACS Appl. Nano Mater.*,
247 2022, **5**, 5416-5424.
- 248 24. X. Peng, L. Ye, Y. Ding, L. Yi, C. Zhang and Z. Wen, *Appl. Catal. B: Environ.*, 2020,
249 **260**, 118152.
- 250 25. Y. Ma, H.-X. Fang, R. Chen, Q. Chen, S.-J. Liu, K. Zhang and H.-J. Li, *Rare Met.*,
251 2023, **42**, 3993-4004.
- 252 26. Z. Tai, G. Sun, T. Wang, Z. Li and J. Tai, *J. Mater. Sci. Technol.*, 2023, **145**, 116-
253 124.
- 254 27. J. Guo, Y. Liang, L. Liu, J. Hu, H. Wang, W. An and W. Cui, *Appl. Surf. Sci.*, 2020,
255 **522**, 146356.
- 256 28. Y. Yang, Z. Xing, W. Kong, C. Wu, H. Peng, Z. Li and W. Zhou, *Nanoscale*, 2022,
257 **14**, 14741-14749.
- 258 29. S. Luo, X. Liu, X. Wei, M. Fu, P. Lu, X. Li, Y. Jia, Q. Ren and Y. He, *J. Hazard. Mater.*,
259 2020, **399**, 122824.
- 260 30. M. Chen, X. Wei, L. Zhao, Y. Huang, S.-c. Lee, W. Ho and K. Chen, *Ind. Eng. Chem.*
261 *Res*, 2020, **59**, 6470-6478.
- 262 31. S. Luo, Y. Zheng, W. Xia, M. Mao, Y. He, X. Liu and J. Wang, *Sep. Purif. Technol.*,
263 2025, **355**, 129737.
- 264 32. Y. Li, J. Zhou, X. He, Y. He, J. Jing, X. Liu, S. Li and S. Wei, *J. Alloys Compd.*, 2024,
265 **1002**, 175428.
- 266 33. M. Xu, P. Zhu, Q. Cai, M. Bu, C. Zhang, H. Wu, Y. He, M. Fu, S. Li and X. Liu, *Chin.*
267 *Chem. Lett.*, 2024, **35**, 109524.
- 268 34. M. Xu, Y. Xu, C. Zhang, S. Chen, X. Liu, H. Wu, S. Li, Y. He and F. Dong, *Sep. Purif.*
269 *Technol.*, 2023, **322**, 124374.
- 270 35. Z. Zhou, D. Chen, S. Dong, N. Li, Q. Xu, H. Li, J. He and J. Lu, *Ind. Eng. Chem. Res.*,
271 2022, **61**, 3550-3560.
- 272 36. Z. Zhou, D. Chen, N. Li, Q. Xu, H. Li, J. He and J. Lu, *Chem. Eng. J.*, 2021, **418**,
273 129117.
- 274 37. X. Li, Z. Le, X. Chen, Z. Li, W. Wang, X. Liu, A. Wu, P. Xu and D. Zhang, *Appl. Catal.*
275 *B: Environ.*, 2018, **236**, 501-508.
- 276 38. Y. He, Y. Tan, M. Song, Q. Tu, M. Fu, L. Long, J. Wu, M. Xu and X. Liu, *J. Hazard.*
277 *Mater.*, 2022, **430**, 128468.
- 278 39. S. Luo, C. Zhang, X. Liu, Y. Li, L. Tang, M. Fu, S. Wang, J. Wu, M. Xu, X. Wang and

279 Y. He, *Chem. Eng. J.*, 2022, **432**, 134244.

280 40. C. Wang, M. Fu, J. Cao, X. Wu, X. Hu and F. Dong, *Chem. Eng. J.*, 2020, **385**,
281 123833.

282 41. W. Huo, W. Xu, T. Cao, Z. Guo, X. Liu, G. Ge, N. Li, T. Lan, H.-C. Yao, Y. Zhang and
283 F. Dong, *J. Colloid Interface Sci.*, 2019, **557**, 816-824.

284 42. F. Zhong, C. Yuan, Y. He, Y. Sun, J. Sheng and F. Dong, *J. Hazard. Mater.*, 2022,
285 **438**, 129463.

286 43. W. Yang, Q. Ren, F. Zhong, Y. Wang, J. Wang, R. Chen, J. Li and F. Dong,
287 *Nanoscale*, 2021, **13**, 20601-20608.

288 44. Y. Liu, S. Yu, Z. Zhao, F. Dong, X. A. Dong and Y. Zhou, *J. Phys. Chem. C*, 2017, **121**,
289 12168-12177.

290 45. R. Chen, H. Wang, H. Wu, J. Sheng, J. Li, W. Cui and F. Dong, *Chin. J. Catal.*, 2020,
291 **41**, 710-718.

292 46. X. Li, Q. Dong, F. Li, Q. Zhu, Q. Tian, L. Tian, Y. Zhu, B. Pan, M. Padervand and C.
293 Wang, *Appl. Catal. B Environ.*, 2024, **340**, 123238.

294 47. R. Li, X. Liu, Y. Tang, J. Yu, Y. Chen, M. Fu, S. Li and Y. He, *Sep. Purif. Technol.*,
295 2023, **306**, 122598.

296 48. J. Li, X. a. Dong, Y. Sun, G. Jiang, Y. Chu, S. C. Lee and F. Dong, *App. Catal. B:*
297 *Environ.*, 2018, **239**, 187-195.

298 49. K. Li, H. Wang, L. Chen, J. Li and F. Dong, *App. Catal. B: Environ.*, 2022, **312**,
299 121423.

300 50. R. Li, Z. Wu, Y. Chen, X. Liu, W. Guo, Y. Huang, M. Fu and Y. He, *Fuel*, 2023, **336**,
301 126766.

302 51. K. Li, W. Cui, J. Li, Y. Sun, Y. Chu, G. Jiang, Y. Zhou, Y. Zhang and F. Dong, *Chem.*
303 *Eng. J.*, 2019, **378**, 122184.

304 52. G. Jiang, X. Li, M. Lan, T. Shen, X. Lv, F. Dong and S. Zhang, *App. Catal. B:*
305 *Environ.*, 2017, **205**, 532-540.

306 53. M. Sun, W. Zhang, Y. Sun, Y. Zhang and F. Dong, *Chin. J. Catal.*, 2019, **40**, 826-
307 836.

308