Supporting Information

Mechanism of catalytic ozonation in different surface acid sites of oxides aqueous suspension

Jishuai Bing^{a, b, c, d}, Yuankai Xu^{a, b, c}, Congyu Wu^{a, b, c}, Xiufeng Lv^e, Xin Xiao^{a, b, c, *}, and Li Chen^{a, b, c,}

a. Jiangsu Key Laboratory of Marine Bioresources and Environment, Jiangsu Ocean University, 59 Cangwu Road, Haizhou, Lianyungang, 222005, China.

b. Co-Innovation Center of Jiangsu Marine Bio-industry Technology, Jiangsu Ocean University, 59

Cangwu Road, Haizhou, Lianyungang, 222005, China.

c. Jiangsu Institute of Marine Resources Development,59 Cangwu Road, Haizhou, Lianyungang, 222005, China.

d. Lianyungang Environmental Science and Technology Service Center, Lianyungang, 222005, China.

e. BaoXianLe Supply Chain Co., Ltd.

The Supporting Information contains 13 pages, 9 Figures and 1 Table.

Table S1 Main products in γ -Al₂O₃ catalytic ozonation of ibuprofen at 5 min and 20 min of reaction time.

Retention time/min	Products	Molecular structure
	Main products in the aqueous solution	1
9.71	2-oxopropanoic acid	ОН
11.53	2-hydroxy-3-methylbutanoic acid	НО ОН
26.67	propane-1,2,3-triol	ОН НООН
33.51	4-isobutylphenol	ОН
36.93	4-isobutylbenzoic acid	
42.09	ibuprofen	Он

Ibuprofen	(Reaction	5	min)
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Main products on the surface of $\gamma\text{-}Al_2O_3$

7.77	oxalic acid	о но
13.84	malonic acid	O OH OH
17.86	3-methyl-2-oxobutanoic acid	OH O
28.92	maleic acid	HOOOOH



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Retention time/min	Products	Molecular structure
	Main products in the aqueous solution	
7.77	oxalic acid	НО ОН
15.18	2-methylpropan-1-ol	ОН
16.86	2-hydroxyacetic acid	НО ОН
26.68	propane-1,2,3-triol	ОН НООН
	Main products on the surface of γ -Al ₂ O ₃	
11.53	2-hydroxy-3-methylbutanoic acid	НО ОН
28.92	maleic acid	HOOOO
29.68	2,3,4,5,6-pentahydroxycyclohexanone	HO HO HO O O HO O H
38.95	2-(3,4-dihydroxyphenyl)-2-hydroxyacetic acid	HO HO OH OH



Fig. S1 ATR-FTIR spectra of different catalyst suspensions in D_2O . (Catalyst concentration: 100 g L⁻¹, pD: 7.0).



Fig. S2 The changes of ozone concentration in bulk water (A) and the adsorbed ozone onto catalysts (B) during the decomposition of ozone in aqueous dispersions of various catalysts. (Catalyst dose: 1.5 g L⁻¹, initial ozone concentration in water: 3.82 mg L⁻¹, initial pH: 7.0).



Fig. S3 ATR-FTIR spectra of different catalysts suspended in D₂O bubbling ozone for different time.

(Gaseous ozone concentration: 30 mg L⁻¹, catalyst dose: 100 g L⁻¹, pD: 7.0).



Fig. S4 BMPO spin-trapping ESR spectra of O₃ alone (A), Fe₃O₄ (B), α -MnO₂ (C) and β -MnO₂ (D) recorded in methanol dispersion for BMPO-HO₂•/O₂•- (A1, B1, C1 and D1) and aqueous dispersion for BMPO-•OH (A2, B2, C2 and D2) with ¹⁶O₃ or ¹⁸O₃. (Initial pH: 7.0, catalyst concentration: 10 g L⁻¹, initial ozone concentration in water: 3.82 mg L⁻¹, initial BMPO concentration: 25 mM).



Fig. S5 Catalytic ozonation of humic acid (A) and acyclovir (B) in various suspensions. (Initial pH: 7.0, initial acyclovir or humic acid concentration: 10 mg L⁻¹, catalyst concentration: 1.5 g L⁻¹, gaseous ozone concentration: 30 mg L⁻¹).



Fig. S6 Comparison of IBU removal by adsorption processes in various suspensions. (Initial pH: 7.0, initial IBU concentration: 10 mg L⁻¹, catalyst concentration: 1.5 g L⁻¹).



Fig. S7 FTIR spectra for various samples: (a) fresh catalyst, (b) catalyst adsorbed IBU, (c) catalyst used for 20 min and (d) catalyst used for 60 min in the catalytic ozonation reaction with IBU. (Initial pH: 7.0, initial IBU concentration: 10 mg L⁻¹, catalyst concentration: 1.5 g L⁻¹, gaseous ozone concentration: 30 mg L⁻¹).





Fig. S8 BMPO spin trapping EPR spectra for various MCM-41 (A), α -Fe₂O₃ (B), Fe₃O₄ (C), α -MnO₂ (D) and β -MnO₂ (E) samples with O₃ recorded in methanol dispersion for BMPO-HO₂'/O₂⁻⁻ (A1, B1, C1, D1 and E1) and aqueous dispersion for BMPO-'OH (A2, B2, C2, D2 and E2). (Initial pH: 7.0, catalyst concentration: 10 g L⁻¹, initial BMPO concentration: 25 mM, recording time: 3 min).



Fig. S9 The formation of H_2O_2 during catalytic ozonation of IBU in aqueous dispersions of different catalysts. (Initial pH: 7.0, initial IBU concentration: 10 mg L⁻¹, catalyst concentration (if use): 1.5 g L⁻¹, gaseous ozone concentration: 30 mg L⁻¹).