Supplementary Information

Identification of active site in CF_4 hydrolytic decomposition over γ -Al₂O₃

Hang Zhang^{‡a}; Tao Luo^{‡a}; Yan Long^{‡a,b}; Yingkang Chen^a; Junwei Fu^a; Hui Liu^c; Junhua Hu^d; Zhang Lin^c; Liyuan Chai^c; Min Liu^{a*};

^a Hunan Joint International Research Center for Carbon Dioxide Resource Utilization, School of Physics and Electronics, Central South University, Changsha 410083, China. ^bGuangdong Key Laboratory of Environmental Pollution and Health, School of Environment, Jinan University, Guangzhou 511443, China.

^cSchool of Metallurgy and Environment, Central South University, Changsha 410083, China.

^dSchool of Materials Science and Engineering, Zhengzhou University, Zhengzhou 450001, China.

* Corresponding Author

E-mail: minliu@csu.edu.cn

			1
Sample	Specific surface area (m ² /g)	Pore volume (cm ³ /g)	Average pore diameter (nm)
γ-Al ₂ O ₃ -500	285.89	1.85	25.95
γ-Al ₂ O ₃ -600	234.45	1.04	17.80
γ-Al ₂ O ₃ -700	198.82	1.43	28.81

Table S1. The BET surface area of catalysts calcined at different temperature.

sample	Strong acid	Total acid
γ-Al ₂ O ₃ -500	2.52	6.19
γ-Al ₂ O ₃ -600	6.55	10.77
γ-Al ₂ O ₃ -700	5.41	9.65

 Table S2. The amount of NH₃ desorption of the catalysts.

sample	strong desorption site
γ-Al ₂ O ₃ -500	3.42
γ -Al ₂ O ₃ -600	2.86
γ -Al ₂ O ₃ -700	1.37

Table S3. The amount of CF_4 strong desorption of the catalysts.

Sample	Specific surface	Pore volume	Average pore
	area (m ² /g)	(cm ³ /g)	diameter (nm)
spent catalyst	151.4	0.685	13.802

Table S4. The BET surface area of catalysts calcined at different temperature.



Figure S1. Local density of states (DOS) of Al site on the (100) and (110) surfaces.



Figure S2. The differential charge density of adsorbed CF_4 . The blue is the negative area and the yellow is the positive area.



Figure S3. The total density of states before and after adsorption of CF₄.



Figure S4. The XRD patterns of the precursors.



Figure S5. The TG-DSC curve of the precursors.



Figure S6. XRD patterns of catalysts under the different calcination temperatures, 800 °C (a), 900 °C (b), 1000 °C (c).



Figure S7. The high-resolution TEM of γ -Al₂O₃, the inset is the corresponding selected area electron diffraction (SAED).



Figure S8. The NH₃-TPD of the deactivated catalyst.



Figure S9. The CF_4 -TPD of the deactivated catalyst.



Figure S10. In situ FT-IR spectra of pyridine adsorbed of catalysts calcined at different temperature, 500 °C (a), 600 °C (b), 700 °C (c).



Figure S11. (a) CF_4 conversion % in the hydrolysis reaction as a function of time-onstream over γ -Al₂O₃ calcined at different temperatures. (b) CF_4 conversion % over γ -Al₂O₃ calcined at 600 °C under various reaction temperatures.



Figure S12. The XRD of the spent catalysts.



Figure S13. The TEM of the spent catalysts.



Figure S14. The XPS of the spent catalysts.



Figure S15. Potential energy diagram for the most favorable reaction pathway for CF_4 activation and decomposition on γ -Al₂O₃ active center. Free energy profiles with the corresponding structures of intermediates and transition states for CF_4 activation and decomposition on γ -Al₂O₃ active center.