Electronic Supplementary Material (ESI) for RSC Advances.

Radical-dominated reaction of CO-NO on $CaFe_2O_4$ surface in sintering flue gas recirculation

Chaoqun Li [1, 3]，Qingzhen Han [1]，Tingyu Zhu [1,2] and Wenqing Xu [1,2, *]

1 Research Center of Process Pollution Control, National Engineering Laboratory for Hydrometallurgical Cleaner Production Technology, State Key Laboratory of Multiphase Complex Systems, Institute of Process Engineering, Chinese Academy of Sciences, No. 1, 2nd North Lane, ZhongGuanCun, Beijing 100190, China

2 Center for Excellence in Regional Atmospheric Environment, Institute of Urban Environment, Chinese Academy of Sciences, Xiamen 361021, China

3 University of Chinese Academy of Sciences, Beijing 100049, China

* E-mail address: wqxu@ ipe.ac.cn.

2.2 Experimental setup and activity test

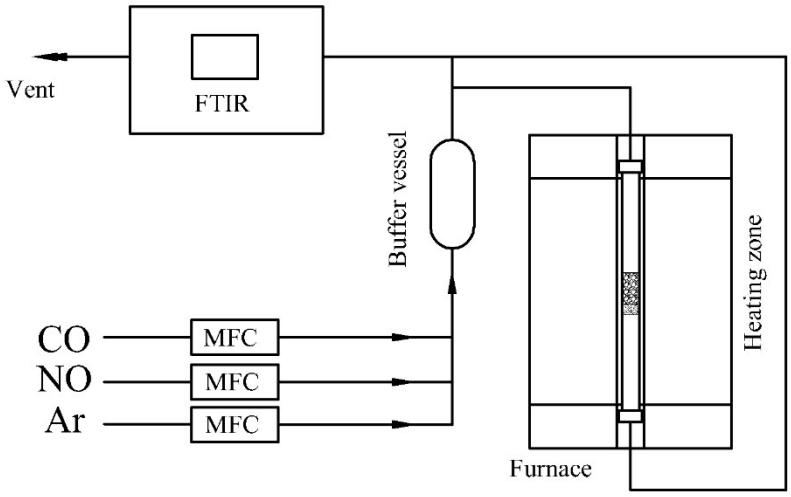

Figure S1 Schematic diagram of the experimental apparatus

The activity test was conducted on a fixed-bed experimental platform (Figure S1). All individual gas components were supplied from cylinders and were precisely controlled by mass flow controllers (MFCs). The tested materials were loaded in a quartz tube, which was placed in a temperature-programmed electric heating furnace.

3.3 Calculation results

To further clarify the mechanism of CO-NO reaction on the surface of calcium ferrite, the plane-wave ultrasoft pseudo potential method based on density functional theory (DFT) was used to calculate the molecular reaction process on the calcium ferrite surface.

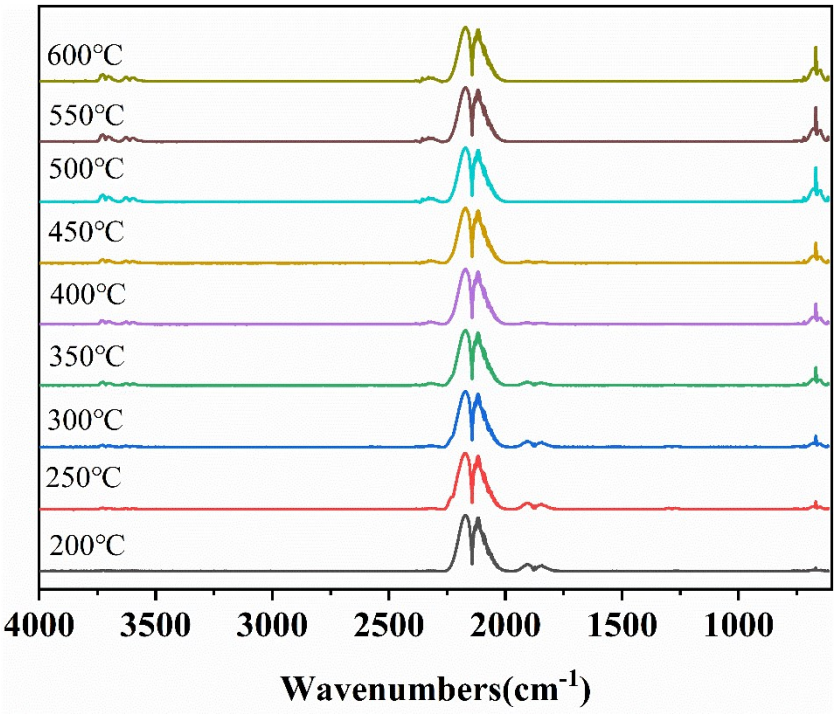

Figure S2 Product analysis after stabilization at different reaction temperatures

In the activity test, product analysis is performed on the original spectrum after the reaction at each temperature point is stable. As shown in the figure, NO_2 and N_2O were not observed throughout the reaction, indicating that no NO_2 and N_2O were produced.

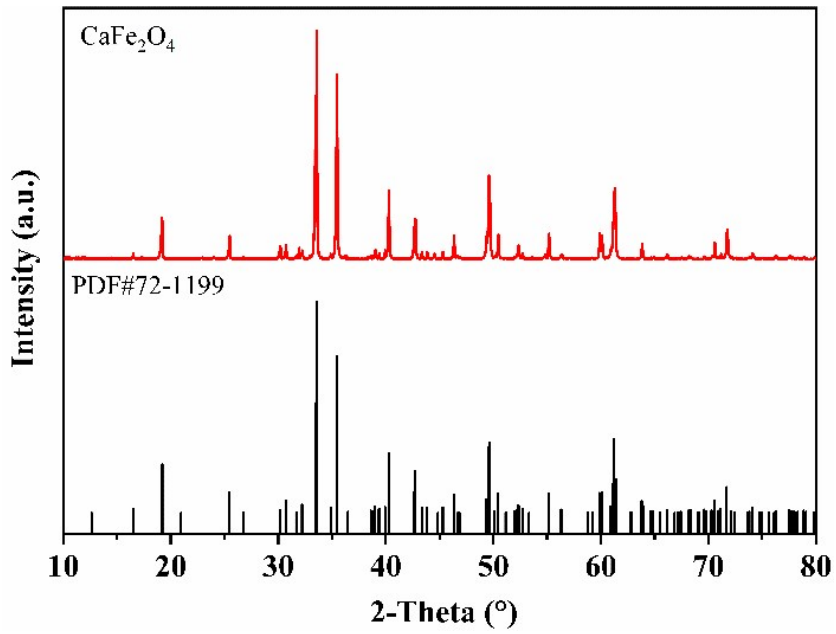

Figure S3 XRD pattern of $CaFe_2O_4$

First, XRD (Figure S3) measurements were performed to confirm the $CaFe_2O_4$ crystallographic structures. As shown in Figure S3, the XRD spectrum of $CaFe_2O_4$ shows a distinct spinel structure of $CaFe_2O_4$.

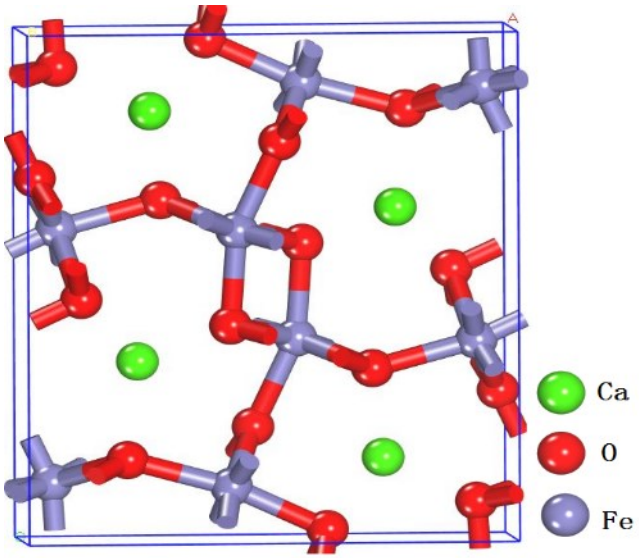

Figure S4 Calculation model of the $CaFe_2O_4$ (optimized) crystal structure

According to the XRD crystal data (Figure S3), the calculation model of the $CaFe_2O_4$ crystal structure is constructed and optimized (Figure S4).

Table S1. Optimized lattice parameters a, b, c, and space group of the $CaFe_2O_4$ unit cell

	$CaFe_2O_4$ (optimized)	PDF#72-1199
a (Å)	9.23	9.23
b (Å)	10.705	10.705
c (Å)	3.024	3.024
Space group	PNAM	PNAM

The optimized lattice parameters a, b, c, and space group (Table S1)

are in good agreement with the former experimental measurements from XRD data in this work and the literature.

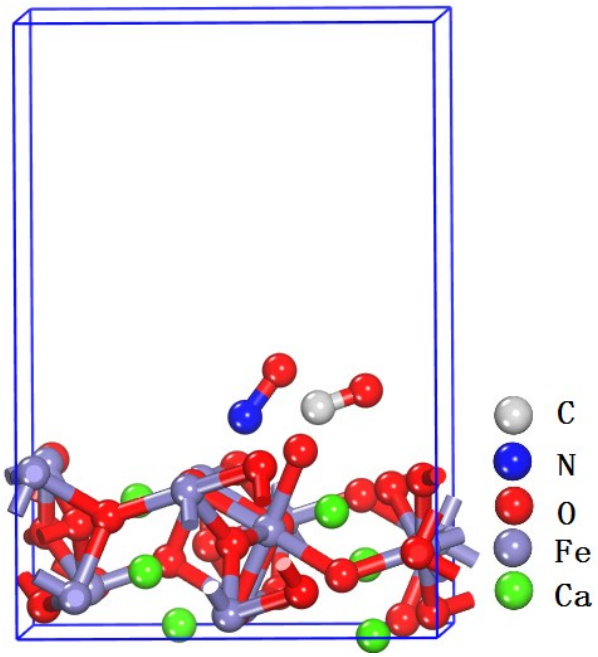

Figure S5 The optimized structure of $CaFe_2O_4$ (110) adsorbed the NO and CO.

Then the 10-layer-atoms periodic structure of $CaFe_2O_4$ (110) adsorbed the NO and CO molecules (Figure S5) was adopted as the best adsorption method. The initial adsorption distance was set at 2.5 Å.

Table S2. Adsorption energy and work function of reactant and product adsorption on the $CaFe_2O_4$ (110).

	CO	NO	N_2	CO_2	$CaFe_2O_4$ (110)
Adsorption energy (eV)	-0.57	-2.54	-1.84	-9.48	0
Work function (eV)	4.831	4.727	4.915	4.918	4.271

The adsorption methods for all reactants (NO and CO) and products (CO_2 and N_2) were optimized and analysed on $CaFe_2O_4$ (110). The

adsorption energy E_a and the work function of the reaction gases CO, NO, CO_2, and N_2 on the $CaFe_2O_4$ (110) surface are listed in Table S2.