Supporting information

Boosting NH_3-SCR of NO_x performance through sustainable and economical synthesis of Cu-SAPO-34 zeolite from attapulgite

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1. Catalyst Characterization

Textural properties were measured by N_2 adsorption-desorption isotherms collected on a Micrometrics ASAP 2010 instrument. The phase compositions of all the catalysts were identified by powder X-ray diffraction (XRD). The scanning electron microscopy (SEM) images were determined with a Hitachi S-4800 instrument. Electron paramagnetic resonance (EPR) measurements of the samples were recorded using a Bruker EMX-plus model spectrometer. X-ray photoelectron spectroscopy (XPS) spectra were carried out on the electron spectrometer (VG Scientific, ESCALab220i-XL) with Mg K_α radiation. The Cu 2p binding energy was calibrated using the C 1s band at 284.8 eV. Temperature-programmed reduction of H_2 (H_2-TPR) was conducted on a Micrometrics Chemisorb 2720 analyzer. 0.1 g of the sample was first pretreated with N_2 for 1h at 300 °C, then cooled to 50 °C. Subsequently, the temperature was increased from 100 to 700 °C at a heating rate of 10 °C min^{-1} under a 10% H_2/Ar gas flow of 100 mL min^{-1}. Temperature-programmed desorption of NH_3 (NH_3-TPD) was conducted on a Micrometrics Chemisorb 2720 analyzer. 0.1 g of the sample was first pretreated at 350 °C in N_2 flow for 1 h, followed by cooling to 50°C. A 2% NH_3/N_2 gas mixture was fed for 1h. Subsequently, the catalysts were purged once again in a nitrogen flow at 50 °C for an additional 30 min. NH_3-TPD was then conducted in a nitrogen flow of 50 mL min^{-1}, ramping from 50-600 °C at a heating rate of 10°C min^{-1}.

In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) was performed on a Nicolet iS50 FTIR spectrometer. Before each experiment, the sample

was pretreated under N_2 at 400 °C for 1 h, and then the background spectrum was taken at the desired temperature. The sample spectrum was obtained by subtracting the corresponding background spectrum.

2. Computational details

Density functional theory (DFT) calculations are performed via the CASTEP module of Materials Studio software. Employing the generalized gradient approximation (GGA) and Perdew-Burke-Ernzerhof (PBE). The cutoff energy of the plane wave basis group is set to 500 eV, with a set energy threshold of 5.0×10^{-7} eV/atom and assumed convergence at a force on the atom of 0.01 eV $Å^{-1}$. An optimized 1×1 ×1 and 1×1×1 Monkhorst-Pack *k*-point grid was used for Brillouin zone sampling of AEI crystals. A vacuum layer of 20 Å was set to reduce the interaction of repeated planes.

Table S1 Physical properties of the catalysts

Sample	BET surface areas ($m^2\ g^{-1}$)	S_{ext} ($m^2\ g^{-1}$)	S_{micro} ($m^2\ g^{-1}$)	Total pore volume ($cm^3\ g^{-1}$)
$Cu_{0.05}$-SAPO-34	780	45	735	0.60
$Cu_{0.05}$-SAPO-34-ATP	825	150	674	0.57
$Cu_{0.1}$-SAPO-34-ATP	802	140	662	0.57
$Cu_{0.2}$-SAPO-34-ATP	695	26	669	0.60

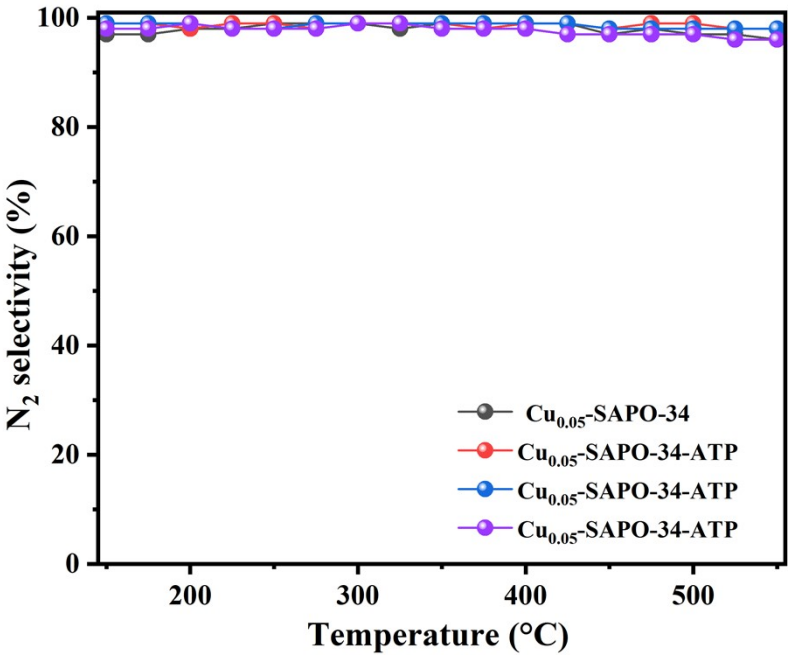

Figure S1. The N_2 selectivities of $Cu_{0.05}$-SAPO-34 and Cu_x-SAPO-34-ATP (x = 0.05, 0.1, 0.2) catalysts at 300 °C . Condition: [NO] = 500 ppm, [NH_3] = 500 ppm, [O_2] = 5%, N_2 was the balanced gas.

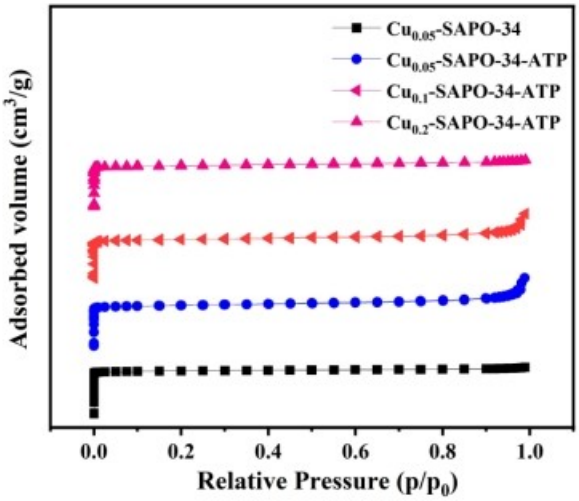

Figure S2. N_2 adsorption-desorption isotherms of the $Cu_{0.05}$-SAPO-34 and Cu_x-SAPO-34-ATP (x = 0.05, 0.1, 0.2) catalysts.

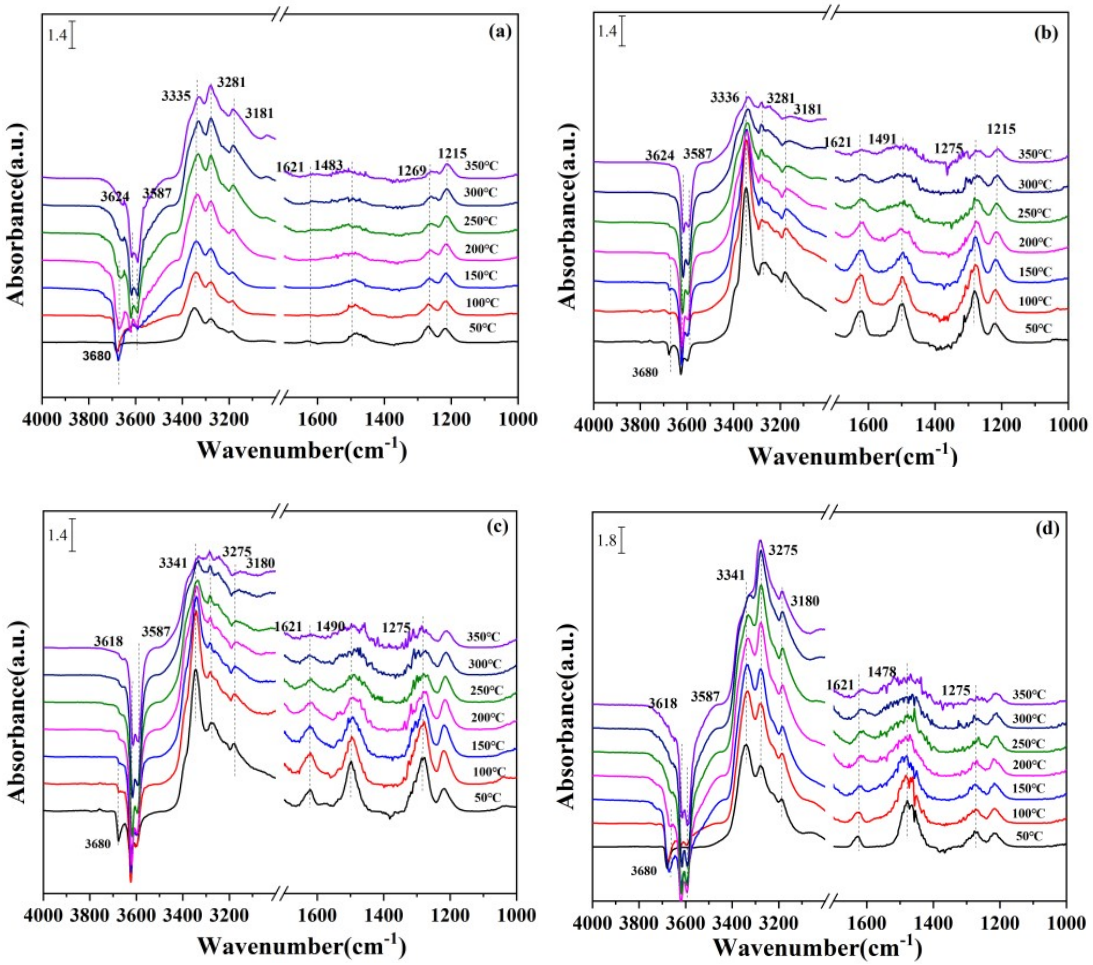

Figure S3. *In situ* DRIFT spectra of NH_3 adsorption on $Cu_{0.05}$-SAPO-34 (a), $Cu_{0.05}$-SAPO-34 -ATP(b), $Cu_{0.1}$SAPO-34 -ATP (c) and $Cu_{0.2}$SAPO-34 -ATP (d) catalysts at different temperatures.

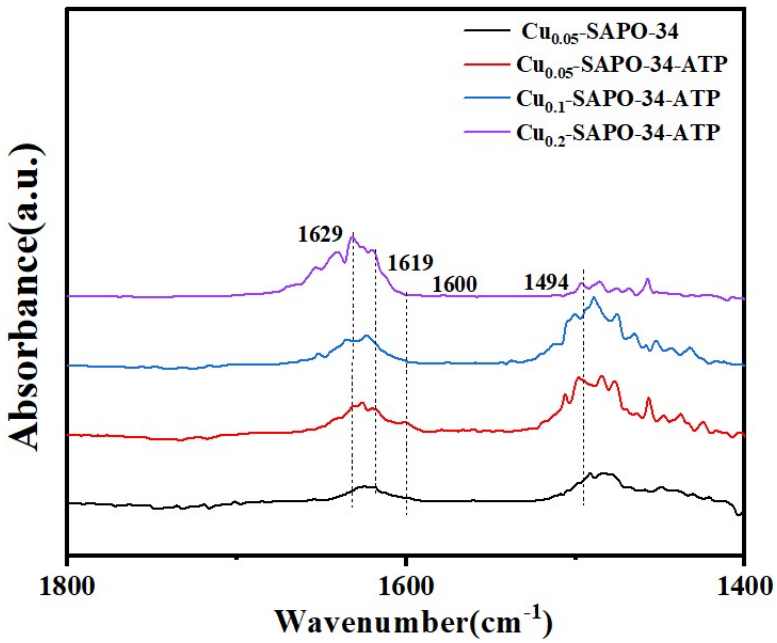

Figure S4. The DRIFT spectra of the NO+O_2 adsorption over the $Cu_{0.05}$-SAPO-34 and Cu_x-SAPO-34-ATP (x = 0.05, 0.1, 0.2) catalysts at 50 °C.