

Electronic Supplementary Information (ESI)

One-pot Synthesis of Novel Ferric Cubic Mesoporous Silica (*Im3m* Symmetry) and Its High Efficient Performance of Adsorption

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Experimental section

Synthesis of FeMCM-41:

Fe/MCM-41 were prepared as follows: 3 g silica aerogel was added into 45 mL NaOH solution (0.5 M) under stirring and heating to dissolve it, then 25 mL aqueous solution containing 4.5 g CTAB was added drop-wise under stirring at room temperature. After that, ferric citrate solution was added and the molar ratio of Si: Fe was modified by control the adding amount of ferric citrate. Then, the pH value of the solution was adjusted to 11.5 by using HCl (2 M). The mixture was further stirred for an additional 6 h, and then aged at 373K for 72 h. The template was removed by calcined at 823K for 5h.

TG characterization

The thermogravimetry analysis (TGA) was carried out in air flow, with a heating rate of 5 K min⁻¹, from 308 to 1073 K.

Table S1. pH value of the solution with different molar ratio of CANa₃/HCA (x)/FeCA(y).

<i>x</i> ^a	0	0.5	0.75	1.0	1.50	2.0	2.5		
<i>y</i> ^b	0	0	0	0	0	0.05	0.1	0	0
pH	2.04	3.70	4.05	4.33	4.62	4.59	4.57	4.82	4.98

^a The molar composition of the solution is 0.2 CTAB: 1.0 HCA: *x* CANa₃: *y* FeCA: 500 H₂O.

Table S2. The textural properties of calcined composites synthesized in HCA/CANa₃/FeCA system.

<i>x</i>	<i>y</i>	Initial molar composition (<i>x</i> : <i>y</i>) ^a	S _{BET} ^b (m ² ·g ⁻¹)	V _p ^c (mL·g ⁻¹)	D _p ^d (nm)
0.5	0.05	0.5: 0.05	1012	0.48	1.9
1.0	0.075	1.0: 0.075	1156	0.88	2.9
2.5	0.15	2.5: 0.15	900	0.72	3.3

^a The initial molar composition is 1.0 TEOS: 0.2 CTAB: 1.0 HCA: *x* CANa₃: *y* FeCA: 500 H₂O ^b S_{BET}, BET surface area; ^c V_p, total pore volume; ^d D_p, BJH mesopore diameter calculated from the desorption branch.

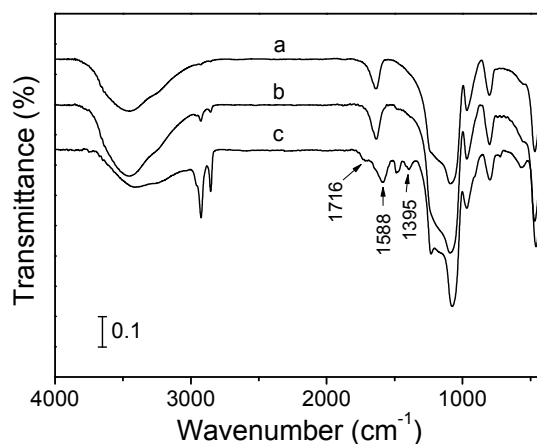


Figure S1 FTIR spectra of (a) the calcined, (b) refluxed, (c) as-synthesized CA sample.

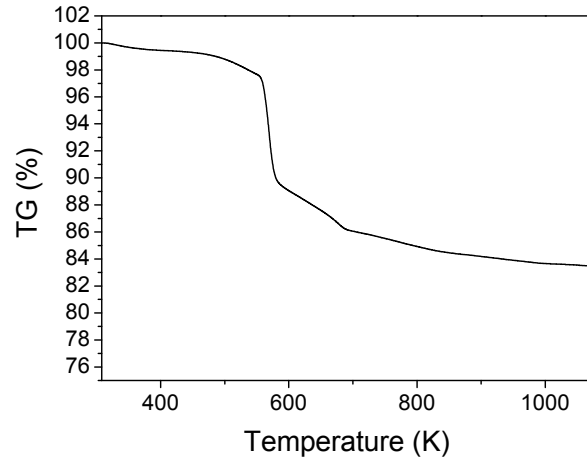


Figure S2. TG curves of as-synthesized CA sample heated from 308 to 1073 K (5K/min).

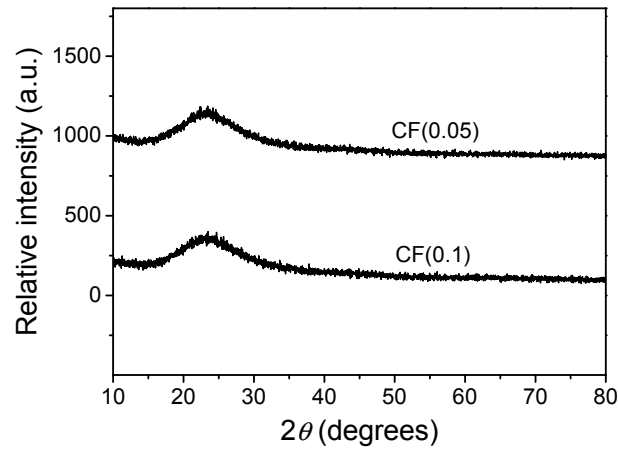


Figure S3 Wide-angle XRD patterns of different calcined samples.

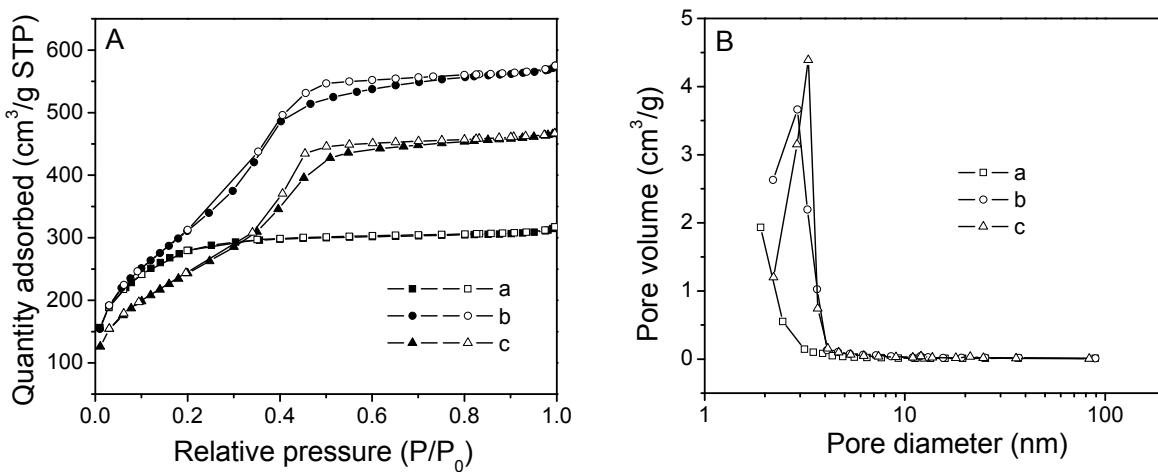


Figure S4. A) Nitrogen sorption isotherms and B) pore size distribution of ferric containing mesoporous silica composites that were synthesized with the molar ratio of 0.2 CTAB: 1 HCA: x CANa_3 : 500 H_2O : y FeCA , in which x and y denote the molar ratio of CANa_3 and FeCA to CA respectively. a, $x = 0.5$, $y = 0.05$; b, $x = 1.0$, $y = 0.075$; c, $x = 1.0$, $y = 0.15$.

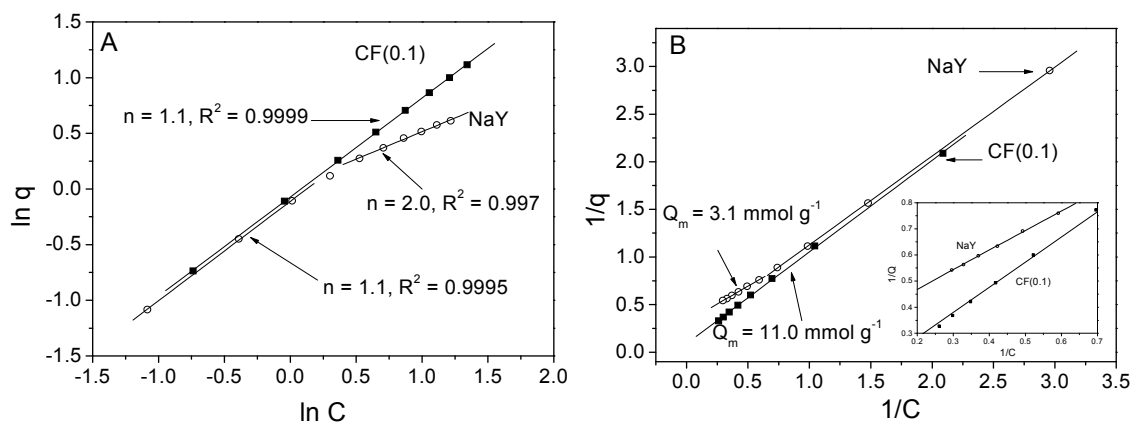


Figure S5 The isotherm fitted with A) Freundlich equation: $\ln q = \ln K_F + (1/n) \ln C$ and B) Langmuir equation: $1/q = 1/K_L/q_m/C + 1/q_m$, in which q and C is the amount of nitrosamine captured or passed by per gram adsorbent respectively. The isotherm of CF(0.1) accords throughout the whole C range but the one of NaY fits in separate C range.

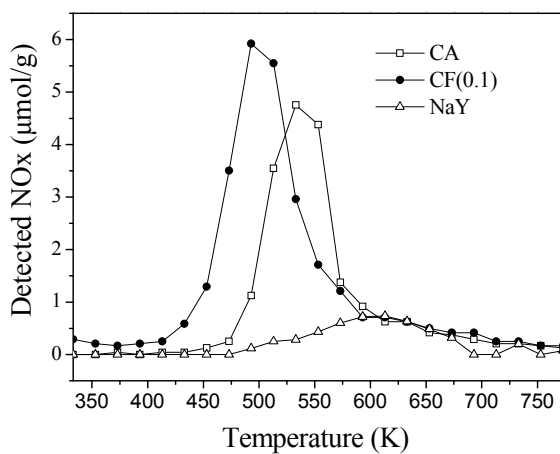


Figure S6 The profiles of NO_x released in the TPSR process of NNN.