Supporting Information:

Iron-containing TS-1 zeolite with controllable mesopores by desilication and its application in the phenol hydroxylation

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Table S1 Notation of the samples and conditions of the treatments in this study

Samples	Si/Fe[a]	Si/Ti[b]	Si/metal[c]	HA[d](M)	SD[e](M)
FTS-50	50	40	22	-	-
FTS-100	100	40	29	-	-
FTS-150	150	40	32	-	-
FTS-50-H	50	40	22	0.1	-
FTS-50-D	50	40	29	-	0.1
FTS-100-D	100	40	32	-	0.1
FTS-150-D	150	40	22	-	0.1
FTS-50-H-D	50	40	29	0.1	0.1
TS-40	-	40	40	-	-
TS-40-D	-	40	40	-	0.1
TS-40-H-D	-	40	40	0.1	0.1
FS-25	25	-	25	-	-
TS-25	-	25	25	-	-
FS-25-D	25	-	25	-	0.1
TS-25-D	-	25	25	-	0.1

[a]Si/Fe: the molar ratio of Si/Fe in the precursor solution

[b]Si/Ti: the molar ratio of Si/Ti in the precursor solution

[c]Si/metal: the molar ratio of Si/metal (=Si/Ti+Fe) in the precursor solution

[d]HA: treatment in hydrochloric acid solution with corresponding concentration

[e]SD: desilication treatment in sodium hydroxide solution with corresponding concentration

Table S2 Relative crystallinity of FTS-50-H, FTS-50-D, FTS-100-D, FTS-150-D, FTS-50-H-D, TS-40-D and TS-40-H-D

Samples	Relative crystallinity (%)
FTS-50	100
FTS-50-H	96.7
FTS-50-D	57.6
FTS-100-D	52.7
FTS-150-D	50.4
FTS-50-H-D	56.8
TS-40	100
TS-40-D	48.9
TS-40-H-D	48.1

The relative crystallinity was calculated as follows:

$$C_s = \frac{A_s}{A_r} \times 100\%$$

Where C_s represents for the relative crystallinity of the chosen sample. A_s and A_r are the sum of the five typical MFI diffraction peak areas of the chosen sample and reference sample, respectively.

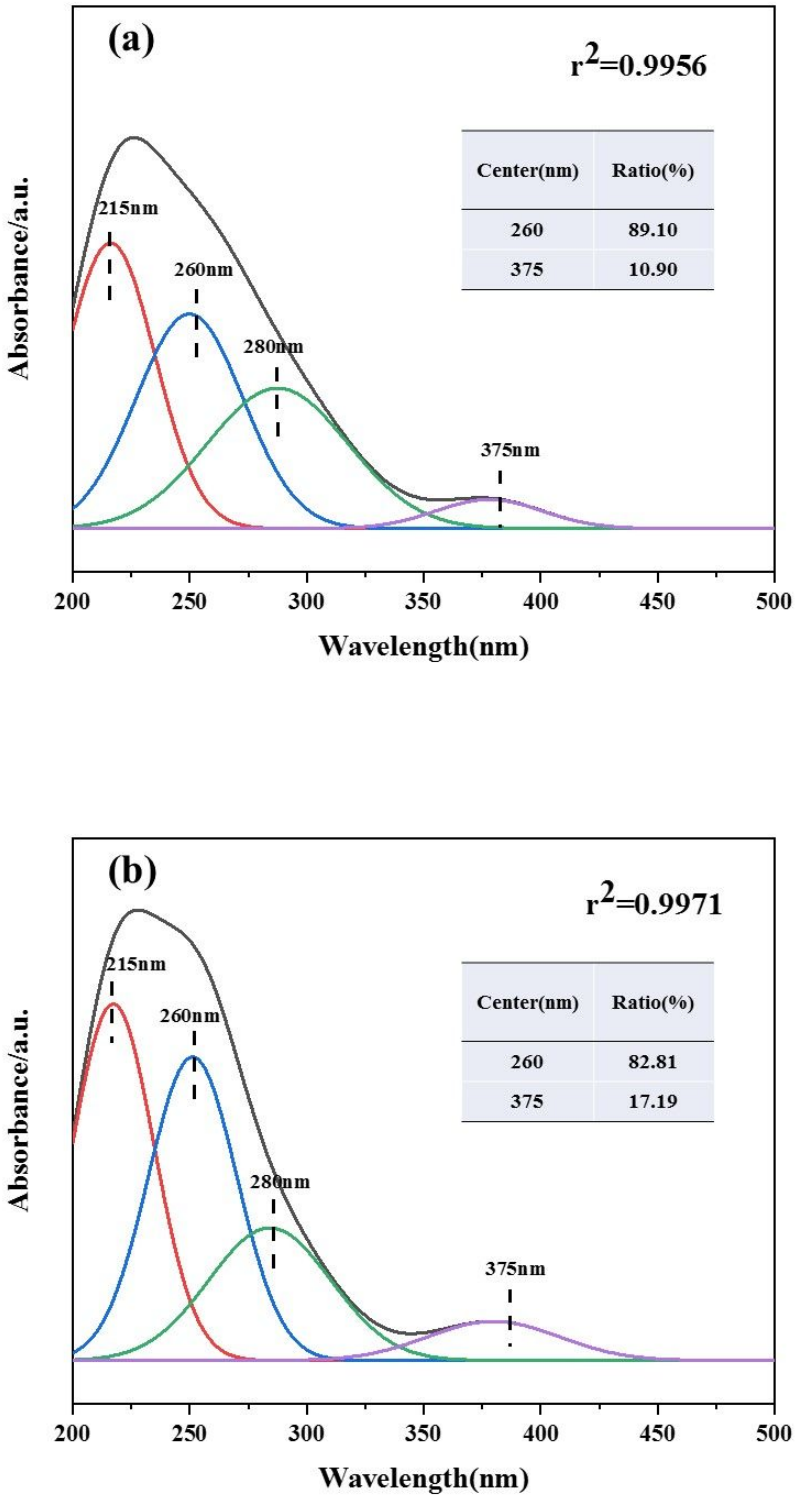

Figure S1 Deconvolution of UV-Vis spectra for (a)FTS-50 and (b)FTS-50-D

Table S3 Conversion and selectivity with error range of all NaOH-treated samples

Catalysts	X (%)	Selectivity (%)		
		CAT	HQ	DHB
FTS-50-D	44.3±0.9	42.9±1.2	49.4±1.7	92.3±2.9
FTS-100-D	42.6±1.1	41.6±1.6	46.2±1.1	87.8±2.8
FTS-150-D	42.1±1.5	41.3±1.5	44.8±1.8	86.1±3.1
FTS-50-H-D	42.6±1.3	40.1±1.0	49.7±1.2	89.8±2.2
FS-25-D	40.0±1.6	42.3±0.9	45.1±1.6	87.4±2.5
TS-25-D	35.4±1.7	33.3±1.5	45.0±1.2	78.3±2.7
Mixture-2	39.6±1.1	41.0±1.9	45.6±1.6	86.6±3.5

Table S4 Conversion of hydrogen peroxide and the selectivity in all FTS samples

Catalysts	Si/metal[a]	X_{hy} (%)	S_{hy} (%)		
			CAT	HQ	DHB
FTS-50	28	57.3	13.26	12.83	26.10
FTS-100	36	58.0	12.13	11.47	23.60
FTS-150	37	54.1	11.92	11.26	23.18
FTS-50-H	29	60.3	13.66	13.94	27.59
FTS-50-D	27	77.1	25.84	29.94	55.79
FTS-100-D	36	78.3	24.11	26.39	50.50
FTS-150-D	38	80.6	23.15	25.21	48.37
FTS-50-H-D	28	76.3	23.67	29.32	52.99
FS-25	24	51.7	13.68	9.69	23.37
TS-25	26	52.0	8.50	6.65	15.15
FS-25-D	20	76.4	23.50	25.40	48.91
TS-25-D	27	67.3	19.17	25.46	44.63

Reaction conditions: water 10 mL, phenol/H_2O_2 molar ratio 1:1, phenol 1.0 g, catalyst 50 mg, reaction temperature 338 K, reaction time 2 h

[a]Si/metal: the molar ratio of Si/metal in the sample, measured by X-ray fluorescence spectrometer (XRF)

The conversion of hydrogen peroxide (X_{hy}) and the selectivity of dihydroxybenzenes (S_{hy}) were obtained as follows:

$$X_{hy} = \frac{C_{hy0} - C_{hy1}}{C_{hy0}} \times 100\%$$

$$S_{hy} = \frac{C_{HQ} + C_{CAT}}{C_{hy0} - C_{hy1}} \times 100\%$$

Where C_{hy0} and C_{hy1} represent for the initial molar concentration of hydrogen peroxide and molar concentration of hydrogen peroxide after reaction, respectively. C_{CAT} and C_{HQ} are the molar concentrations of CAT and HQ after reaction, respectively.