Supporting Information

Investigating Synergistic Cooperativity of Metal-Brønsted Acid Site Pair in *MFI*-type Zeolites by Synchrotron X-ray Powder Diffraction

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Materials and methods

Materials

M/X-Z zeolites (M = Cu, Fe; X = Al, Ga, B)

Synthesis of M/X-Z samples was attempted by the "acidic co-hydrolysis route". Metal nitrate (0.00048 mol) was added to the solution of tetraethyl orthosilicate (TEOS) (10 g) and DI water (32.5 g). the pH of the mixture was adjusted to 1.0 by drop-wise adding sulfuric acid. After the pH adjustment, the mixture was stirred at room temperature for 20 h to get a complete co-hydrolysis and condensation of TEOS with the metal salt. After that, the source of the Brønsted acid site (1.2 mmol), 0.75 g of aluminum (aluminum sulfate octadecahydrate as an example), and tetrapropylammonium hydroxide (TPAOH) (4.8 mmol) was added into the mixture with the dripping of NaOH solution to get a basic gel (pH = 9.8). The final gel composition was $1SiO_2$: 0.01 Metal: 40 H_2O: 0.1 TPAOH. Finally, the slurry was transferred into the 100 mL Teflon-lined stainless-steel autoclave and statically crystallized at 180 °C for 72 h. After that, the zeolite was separated by centrifugation, followed by washing with DI water, and air drying at 70 °C for overnight. The obtained as-synthesized samples were calcinated at 550 °C for 5 h to remove the organic template. H-form of the zeolite was prepared by ammonia treatment. The zeolite was firstly converted into NH_4-form by ion exchange with 1.0 M ammonia solution at room temperature for 24 h (1g solid to 100 mL solution). The zeolite samples were separated by centrifugation, followed by washing with DI water, and air drying at 70 °C for overnight. The NH_4-form samples were converted to H-form by calcination at 500 °C under dry air for 4h.

Method

High-resolution synchrotron PXRD

Synchrotron PXRD measurements for structural determination were collected at beamline BL02B2 at SPring-8, Japan. The energy of the incident X-ray flux was set at 17.7 keV[1]. The wavelength (λ = 0.700261 Å) and the 2θ-zero point (ZP = 0.00020°) were calibrated using a diffraction pattern obtained from a high-quality CeO_2 powder (NIST SRM674b). High-resolution synchrotron PXRD data were obtained from the zeolite samples (loaded in 0.5-mm borosilicate capillaries) using the Microstrip sYstem for Time rEsolved experimeNts (MYTHEN) detectors, with a modular system constructed by six MYTHEN detectors. The patterns were collected in the 2θ range 2-70° with 0.006° data binning. Each synchrotron PXRD pattern was collected for 5 min for each 2θ-step, i.e., 10 min in total for MYTHEN data summation. This procedure produced good quality patterns of a high signal-to-noise ratio. It should be particularly noted that the R-factors using the MYTHEN detectors are artificially high. Therefore, the quality of the Rietveld refinement should be best judged by the difference between the fitted and observed data.

Using the TOPAS software, the lattice parameters were obtained using Le Bail and Rietveld refinement analyses of the diffraction patterns were performed. The starting coordinates used were based on the H-ZSM-5 zeolite model by Heo *et al.* for the refinement[2]. The background curve was fitted by a Chebyshev polynomial with an average of 20 coefficients. The Thompson-Cox-Hastings (pseudo-Voigt) function was applied to describe the diffraction peaks[3]. The scale factor and lattice parameters were allowed to vary for all the histograms.

The final refined structural parameters for each data histogram were carried out using the Rietveld method with the fractional coordinates (*x, y, z*) and isotropic displacement factors (B_{eq}) for all atoms. In addition, the R_{wp} and *gof* values ($gof = R_{wp}/R_{exp}$) helped assess the quality of fit, where R_{exp} represents the quality of the data. So, the R_{wp} value should be close to R_{exp} for a good fit.

Fourier-Transform infrared spectroscopy (FTIR)

FTIR in an attenuated total reflection (ATR) mode was measured using Thermo Scientific Nicolet iS50 equipped with a single bounce diamond crystal and a deuterated triglycine sulfate (DTGS) detector.

X-ray absorption fine structure (XAFS)

The XAFS data of a series of zeolite catalysts were collected at Beamline BL07A of the Taiwan Light Source (Taiwan). A Si (111) double crystal monochromator (DCM) was used to scan the photon energy.

Temperature-programmed desorption of ammonia (NH_3-TPD)

Typically, 100 mg of sample was pre-treated in a helium stream (30 mL min^{-1}) at 600 °C for 2 h. The adsorption of NH3 was carried out at 50 °C for 1 h. The catalyst was flushed with helium at 100 °C for 2 h to remove physisorbed NH3 from the catalyst surface. The TPD profile was recorded at a heating rate of 10 °C min-1 from 100 °C to 600 °C.`

Pyridine-assisted FT-IR (Py-FTIR)

Wafers with a weight of 25 mg and radius of 6.5 mm were degassed for 1 h under vacuum at 600 °C. Then pyridine was admitted, and after equilibration, the samples were outgassed for 0.5 h at increasing temperatures (150, 200, 250, 350, and 450 °C). The spectra were recorded on a Nicolet iS50 FT-IR spectrometer.

Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES).

The chemical composition of the samples was determined using a 5900 ICP-OES from Agilent Technologies. For the ICP-OES spectroscopy analysis, 0.5 mg of zeolite powder was first dissolved in a mixture of HF solution (2 mL, 39%, Merck) and aqua regia, and stirred for at least 12 hours. After dissolution, the solution was diluted and filtered using a 0.45-μm microfilter. Boric acid was added to the solution to minimize fluoride interferences during the measurement.

Styrene oxidation

The catalytic performance of M/X-Z for styrene oxidation was evaluated by the following procedure: 0.5 mmol of 4-chlorostyrene, 0.05 g M/X-Z, 1.5 mmol of 30% H_2O_2 and 5 mL CH_3CN were added into a 10 mL flask and then stirred at different temperature (50/70/90/110 °C) for 24 h. The reaction solution was analyzed by gas chromatography (Agilent 6890 N, flame ion detector, a 0.45 μm × 5mm× 30m capillary column). The conversion of styrene and the selectivity of products were calculated by an internal standard method with dimethoxybenzene as the internal standard sample. Meanwhile, the main products were testified by GC–MS (Agilent 7890/5975C GC/MSD).

GVL decarboxylation

The catalytic performance of M/X-Z for alkene oxidation was evaluated by the following procedure: 0.10 g of catalyst and 1.00 g of γ-valerolactone were added into the stainless-steel batch-stirred reactor (100 mL). Subsequently, the reactor was purged with N_2 three times to replace the air from the reactor. Then the reactor was heated to 250 °C to react for 12 h under stirred with 700 rpm. Finally, the reactor was cooled

down to room temperature with cold water after the reaction immediately. For the liquid and gas products, it was collected in a gas storage bag and qualitatively analyzed by the GC–MS, while the liquid products were dissolved in acetone and quantified and analyzed by the GC-MS.

Density functional theory calculation (DFT)

The DFT calculations were performed using the projector-augmented wave method as implemented in the Vienna Ab initio Simulation Package (VASP). The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was used. A uniform 2×2×2 *k*-mesh grid in the Brillouin zone was used to optimize the crystal structures of Fe/X-Z and Cu/X-Z without and with GVL (or 4-chlorostyrene) adsorption. The kinetic energy cutoff for the wave functions was set at 450 eV. All the atomic positions of the Fe/X-Z and Cu/X-Z without and with GVL (or 4-chlorostyrene) adsorption were relaxed until the forces on each atom were less than 0.015 eV/Å. The binding energy for Fe/X-Z and Cu/X-Z with GVL (or 4-chlorostyrene) adsorption was calculated as E (binding) = E (total) – E (Fe/X-Z and Cu/X-Z) – E (molecule); where E (total) and E (Fe/X-Z and Cu/X-Z) are the total energies of Fe/X-Z and Cu/X-Z with and without GVL (or 4-chlorostyrene) adsorption; E (molecule) is the energy of a GVL (or 4-chlorostyrene) molecule.

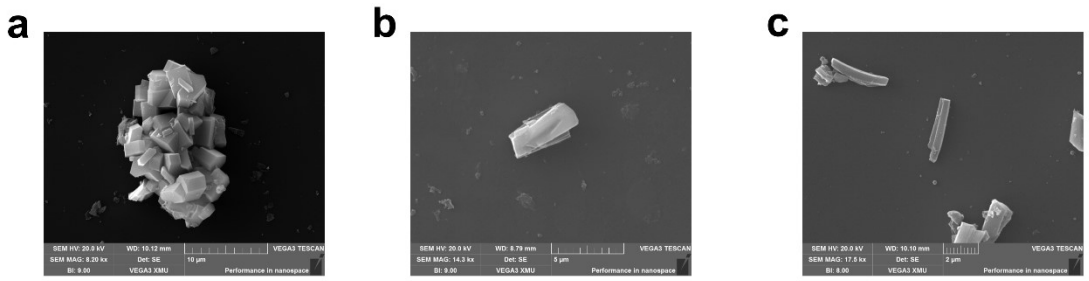


Figure S1. Morphology analysis by SEM. SEM images of (a) Fe/Al-Z, (b) Fe/Ga-Z, and (c) Fe/B-Z.

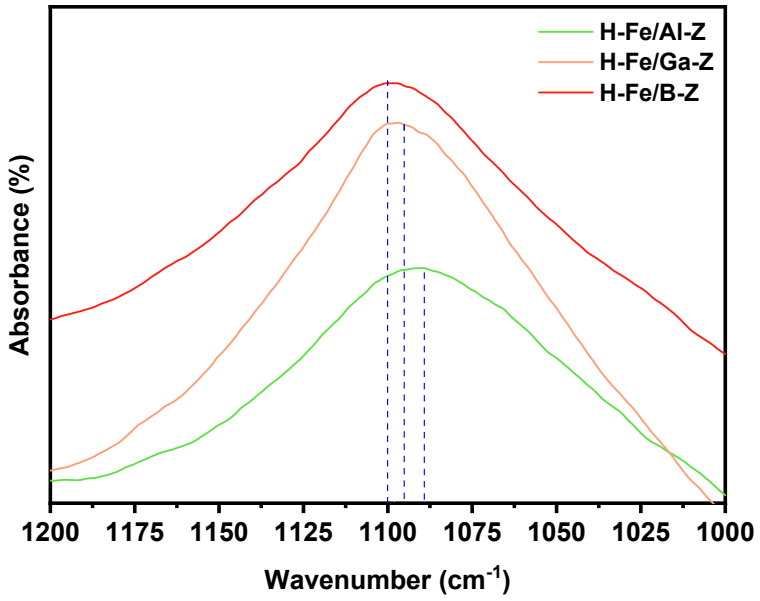


Figure S2. FTIR spectra of Fe/Al-Z, Fe/Ga-Z, and Fe/B-Z.

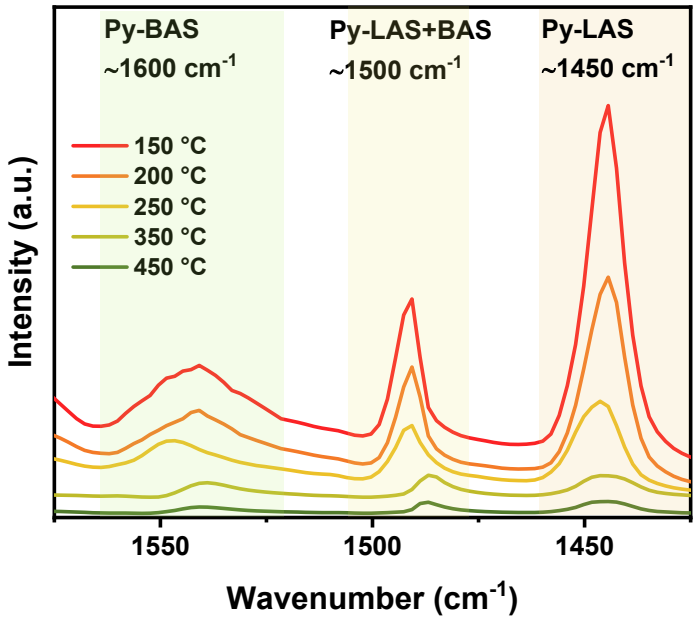


Figure S3. Py-FTIR spectra of Fe/Al-Z.

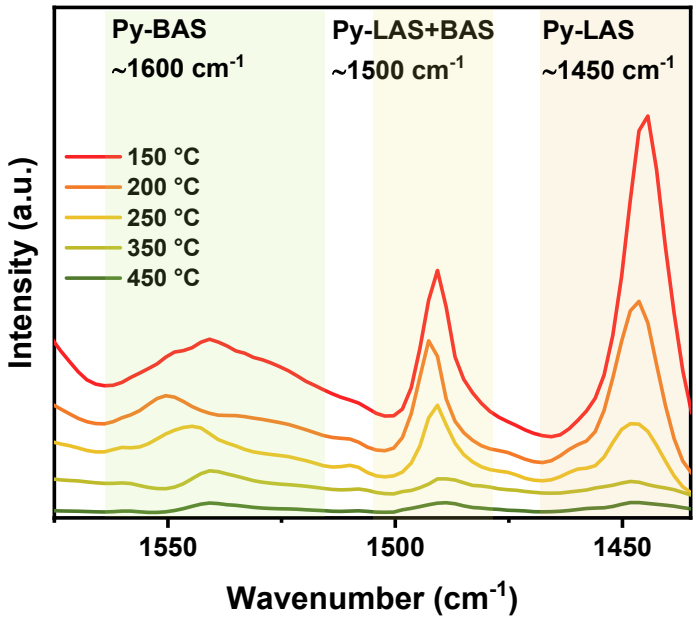


Figure S4. Py-FTIR spectra of Fe/Ga-Z.

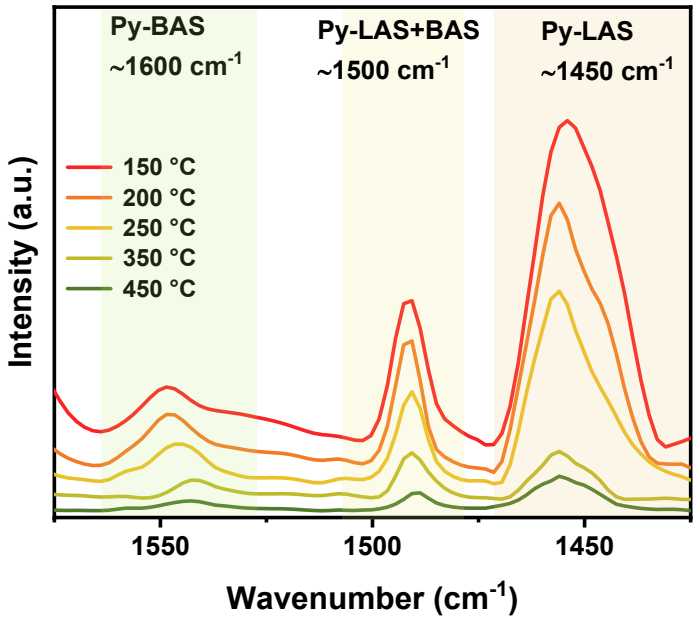


Figure S5. Py-FTIR spectra of Fe/B-Z.

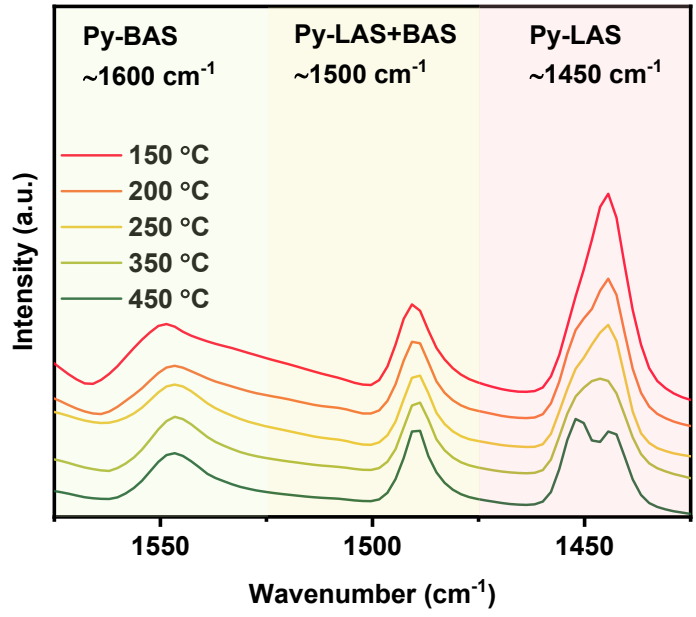


Figure S6. Py-FTIR spectra of Cu/Al-Z.

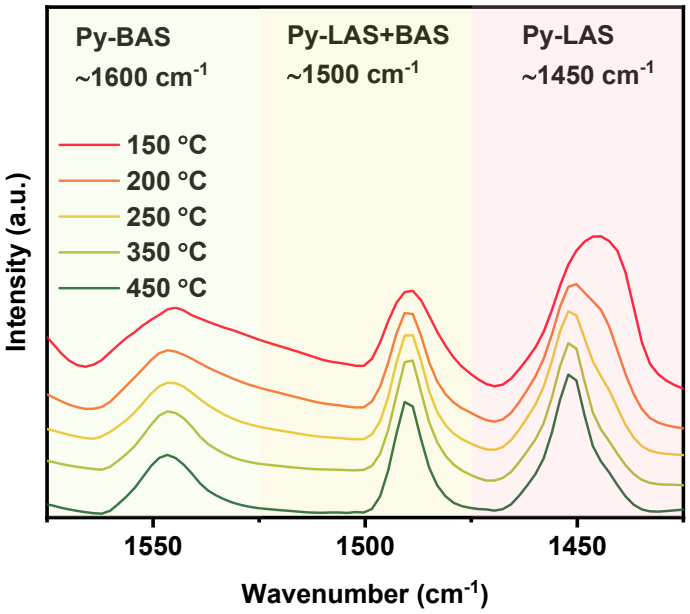


Figure S7. Py-FTIR spectra of Cu/Ga-Z.

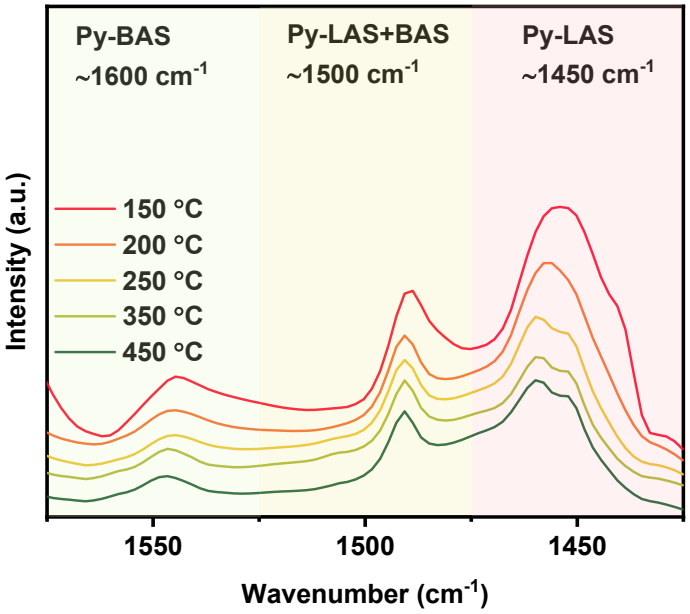


Figure S8. Py-FTIR spectra of Cu/B-Z.

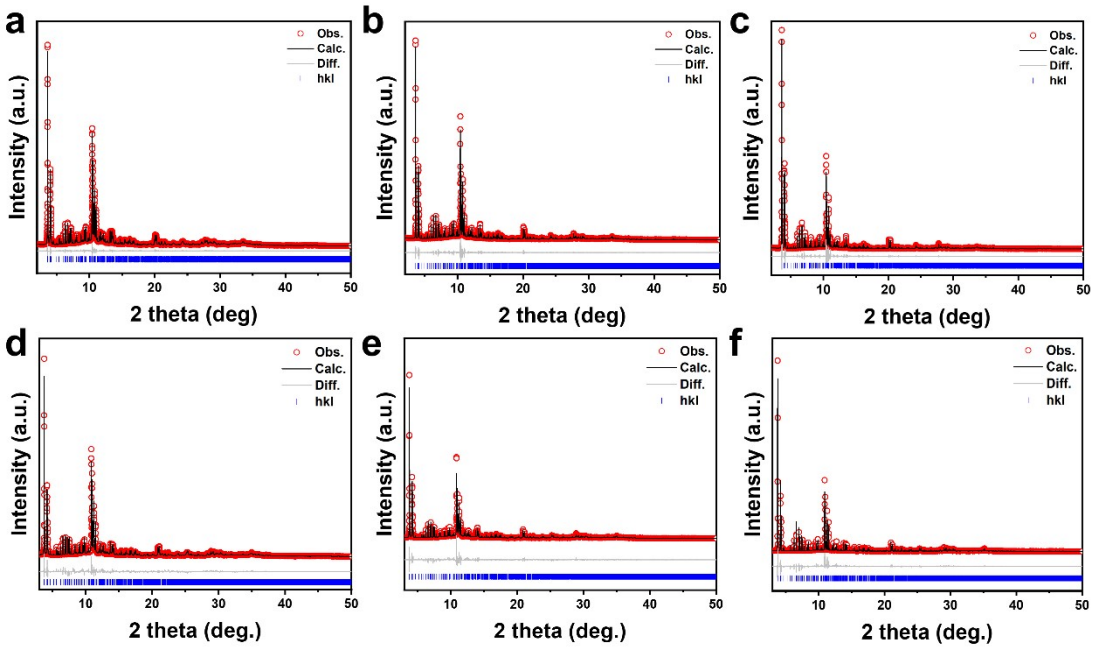


Figure S9. The Rietveld refinement profiles of high-resolution synchrotron PXRD of (a) Fe/Al-Z, (b) Fe/Ga-Z, (c) Fe/B-Z, (d) Cu/Al-Z, (e) Cu/Ga-Z, and (f) Cu/B-Z. The structural and atomic parameters are summarized in **Tables S13–S18**.

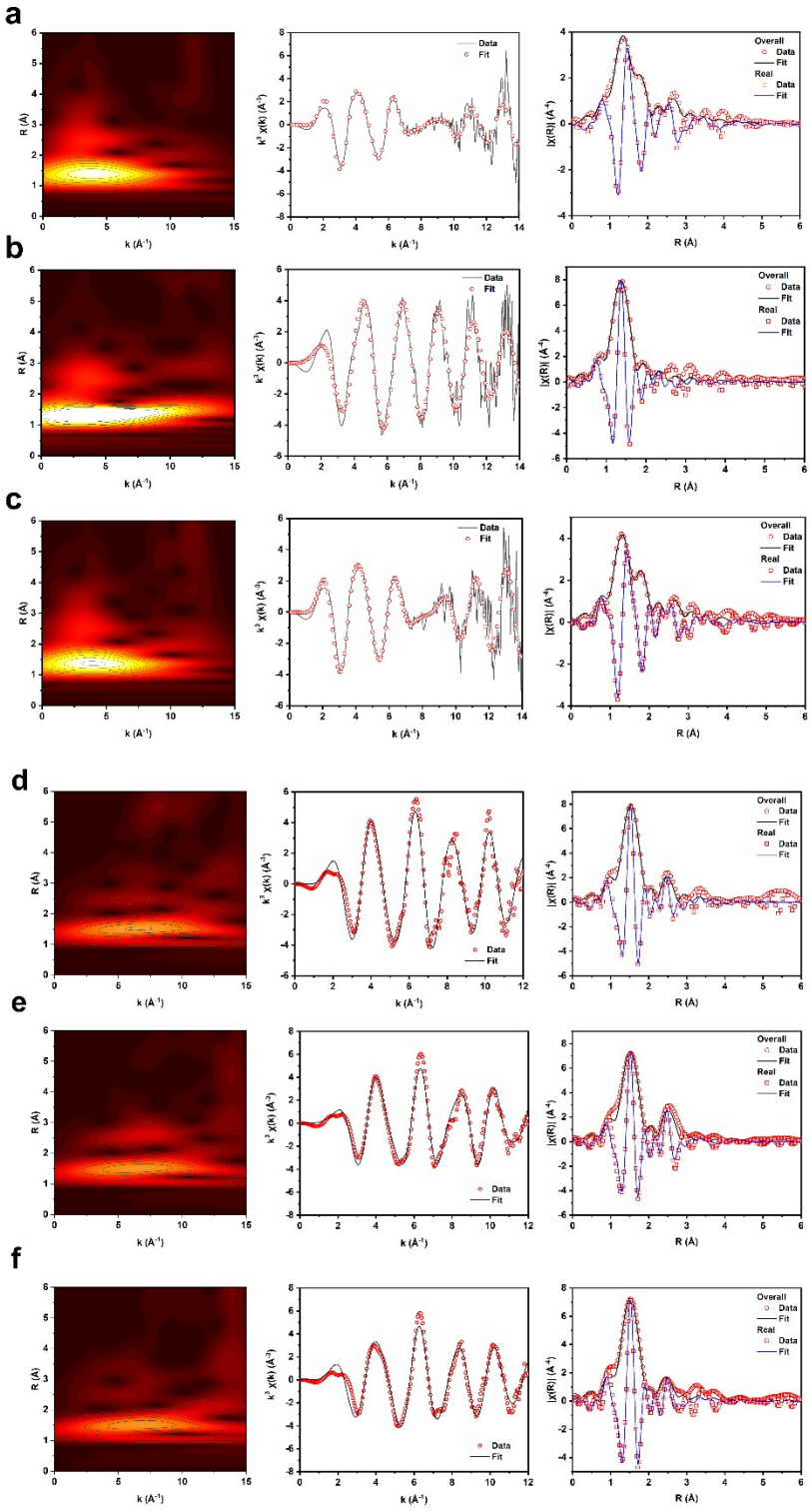


Figure S10. Wavelet transform for k^3 weighted EXAFS signal of (a) Fe/Al-Z, (b) Fe/Ga-Z, (c) Fe/B-Z, (d) Cu/Al-Z, (e) Cu/Ga-Z, and (f) Cu/B-Z, and the corresponding Fe and Cu K-edge EXAFS (red) and fitting profile (black) in k^3 weighted k-space and R-space.

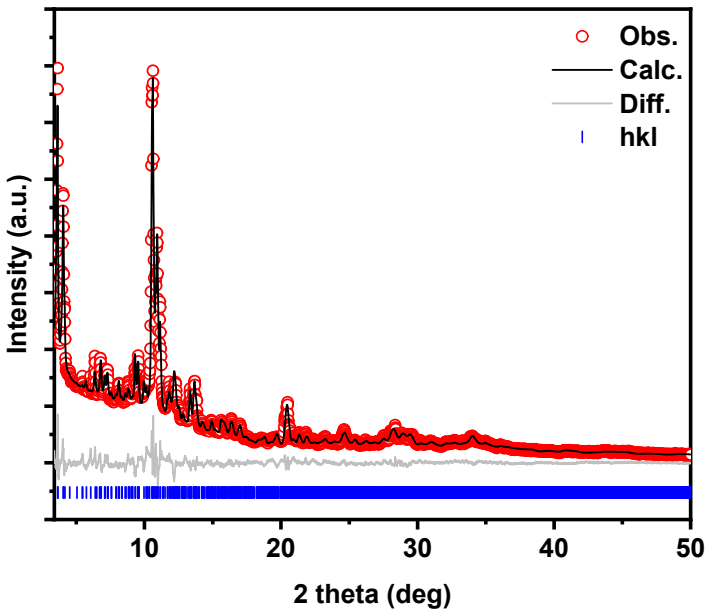


Figure S11. PXRD data and Rietveld refinement of 4-chlorostyrene pre-adsorbed on Fe/Al-Z.

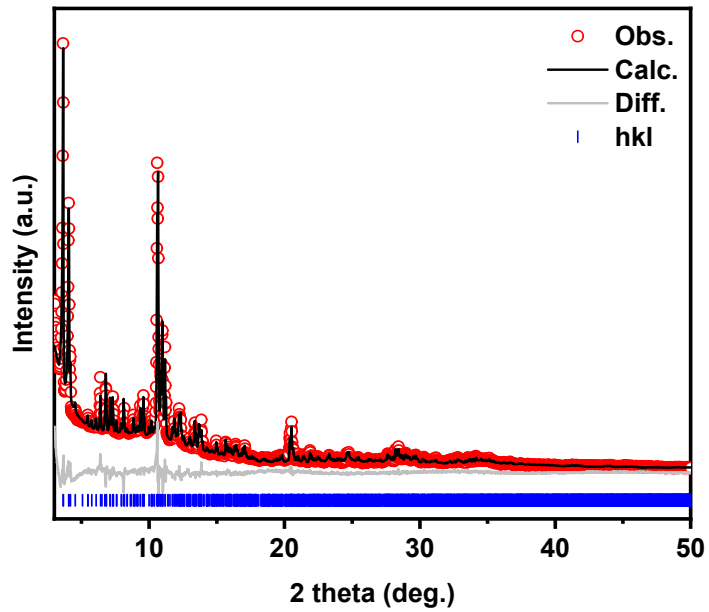


Figure S12. PXRD data and Rietveld refinement of 4-chlorostyrene pre-adsorbed on Fe/B-Z.

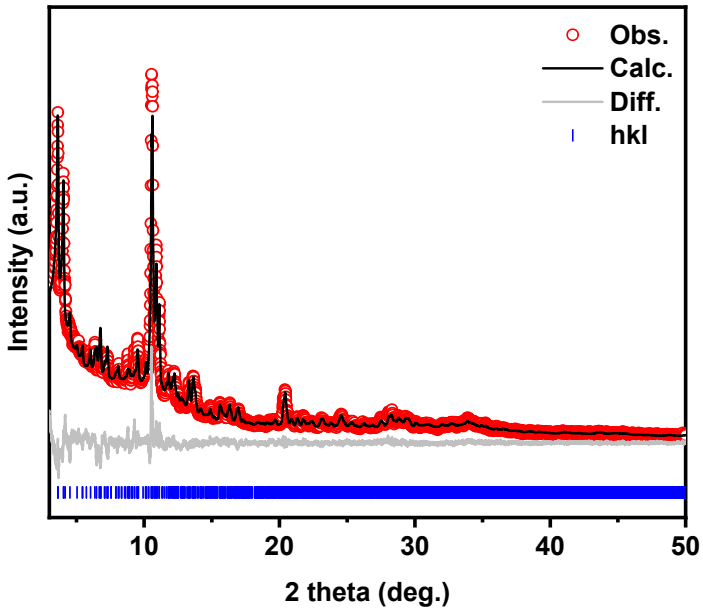


Figure S13. PXRD data and Rietveld refinement of GVL pre-adsorbed on Fe/Al-Z.

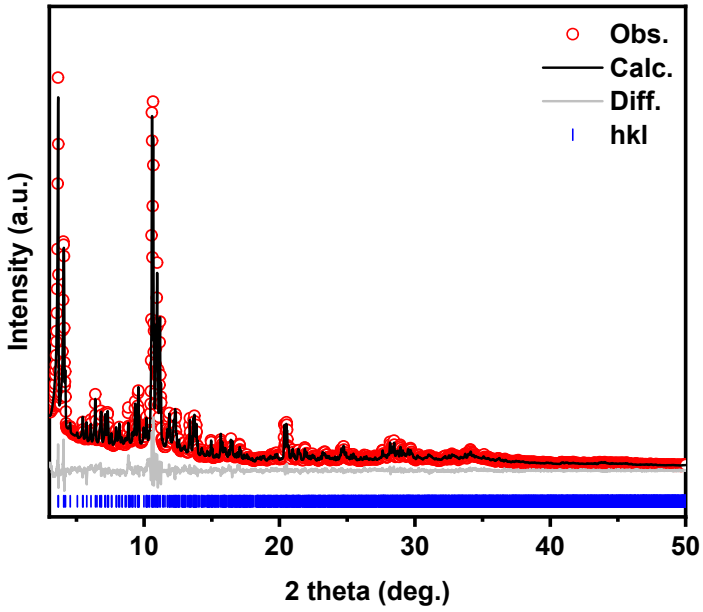


Figure S14. PXRD data and Rietveld refinement of GVL pre-adsorbed on Fe/B-Z.

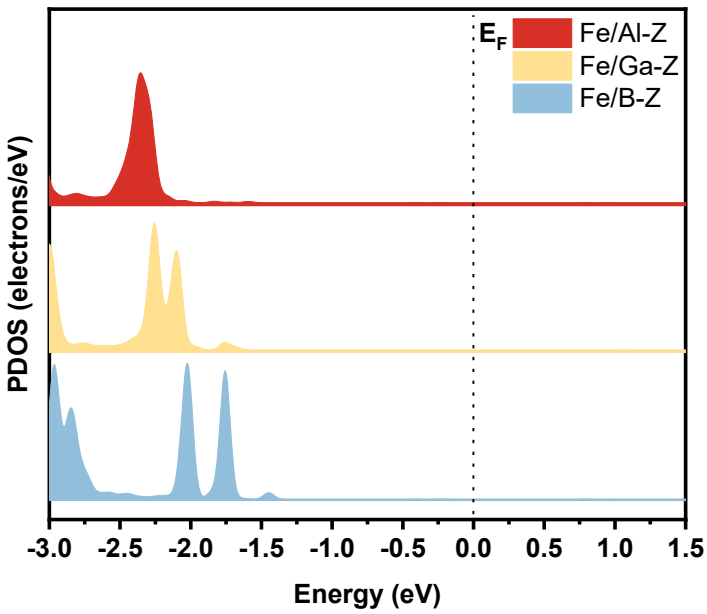


Figure S15. Projected density of states of substrate molecule orbitals for Fe/X-Z with pre-adsorbed GVL.

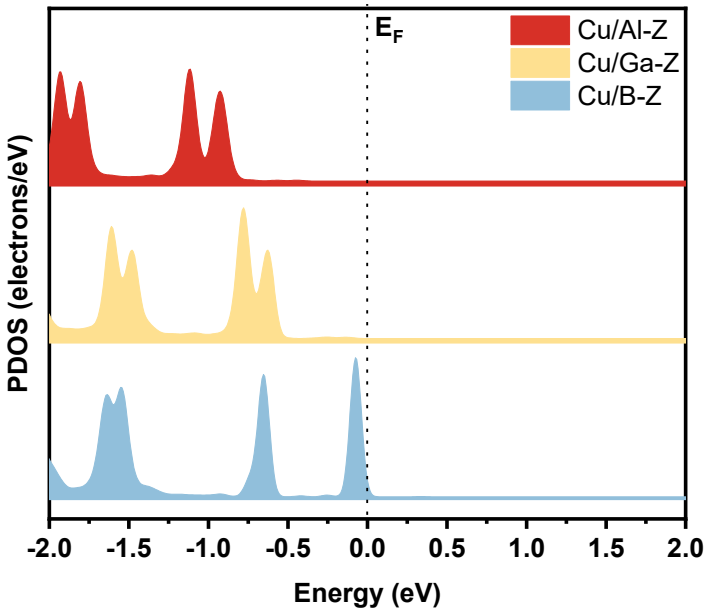


Figure S16. Projected density of states of substrate molecule orbitals for Cu/X-Z with pre-adsorbed GVL.

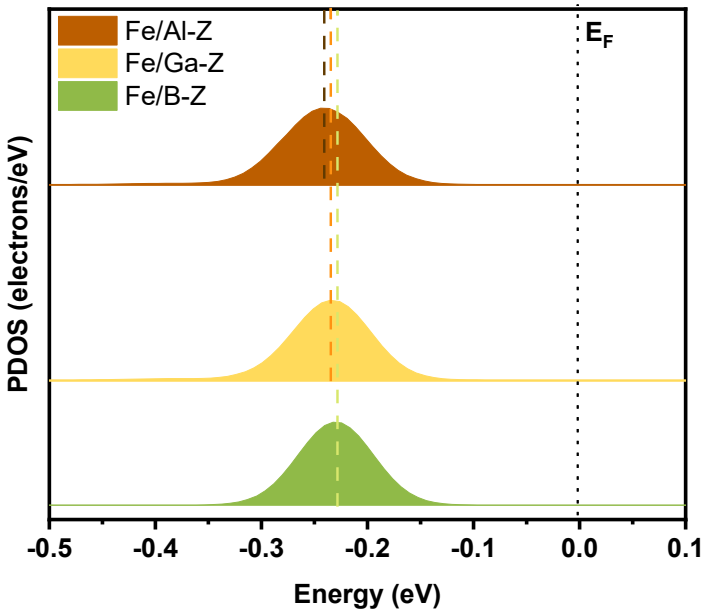


Figure S17. Projected density of states of substrate molecule orbitals for Fe/X-Z with pre-adsorbed 4-chlorostyrene.

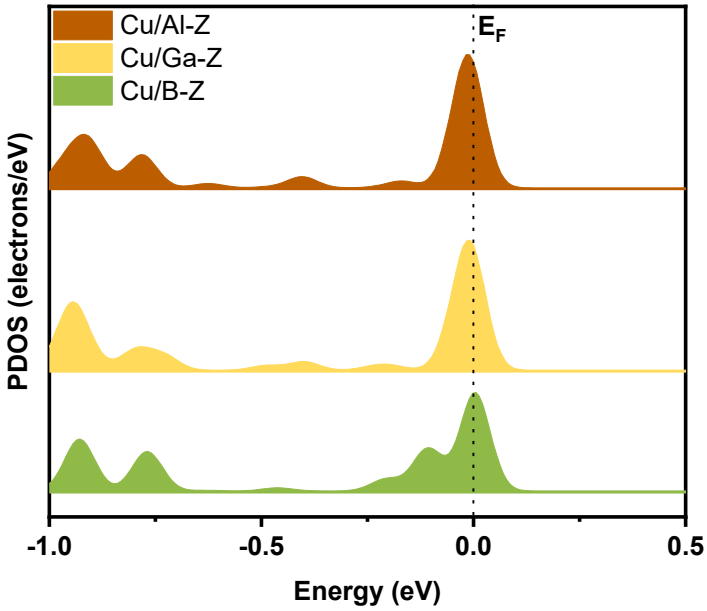


Figure S18. Projected density of states of substrate molecule orbitals for Cu/X-Z with pre-adsorbed 4-chlorostyrene.

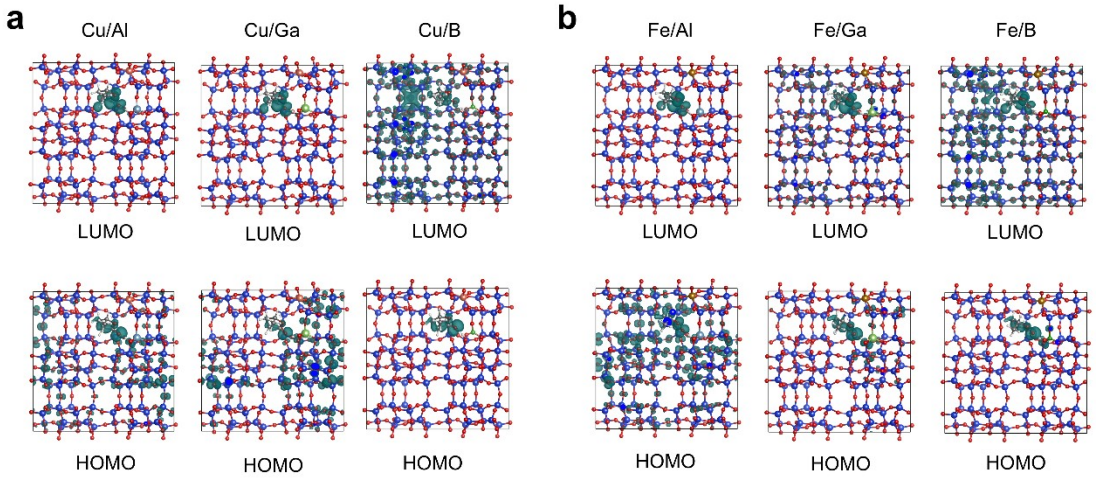


Figure S19. Electronic charge densities of LUMO and HOMO for (a) Cu/X-Z and (b) Fe/X-Z with pre-adsorbed GVL.

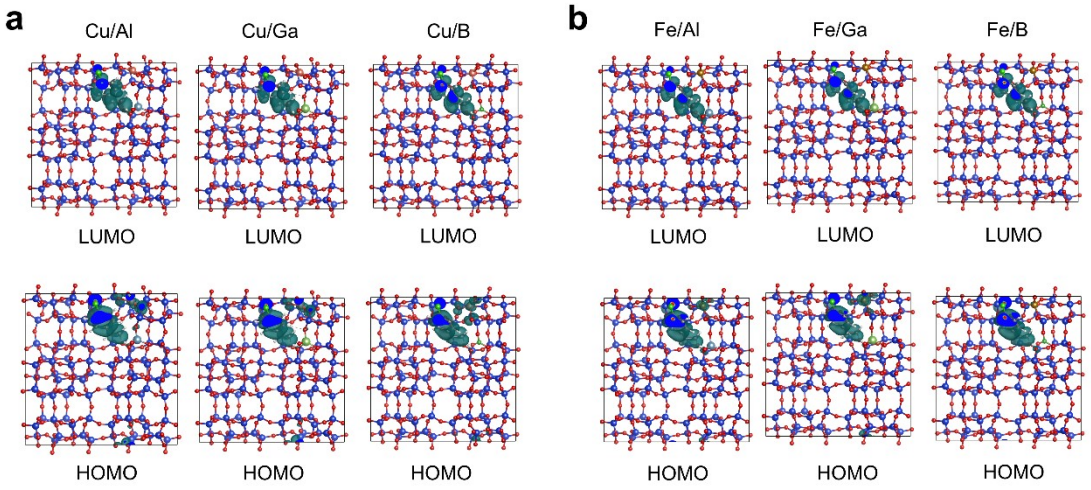
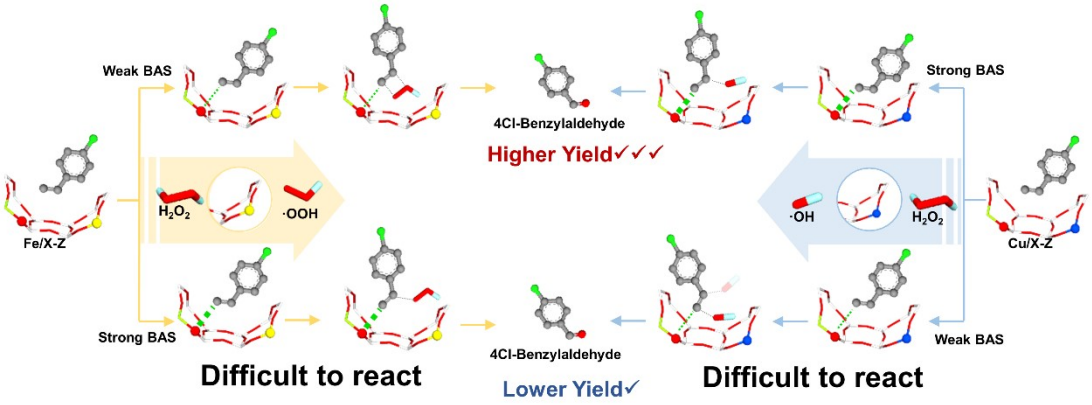


Figure S20. Electronic charge densities of LUMO and HOMO for (a) Cu/X-Z and (b) Fe/X-Z with pre-adsorbed 4-chlorostyrene.



Scheme S1. Proposed reaction mechanism of the oxidation of 4-chlorostyrene over Fe/X-Z and Cu/X-Z with varying BAS strengths.

Table S1. Crystallographic data of the synchrotron PXRD measurement of the zeolite samples labelled.

	Fe/Al-Z	**Fe/Ga-Z**	**Fe/B-Z**	**Cu/Al-Z**	**Cu/Ga-Z**	**Cu/B-Z**
X-ray energy (keV)	17.7	17.7	17.7	17	17	17
Beamline	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2
Wavelength (Å) (synchrotron)	0.700261	0.700261	0.700261	0.729589	0.729589	0.729589
2θ – zero point (°)	0.00020	0.00020	0.00020	-0.00019	-0.00019	-0.00019
Space group	*Pnma*	*Pnma*	*Pnma*	*Pnma*	*Pnma*	*Pnma*
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
a (Å)	20.13162(15)	20.11702(17)	20.08193(27)	20.14844(16)	20.12378(21)	20.04048(11)
b (Å)	19.93828(16)	19.91554(19)	19.86314(31)	19.94904(16)	19.91965(24)	19.85013(10)
c (Å)	13.41994(14)	13.40324(15)	13.37000(22)	13.42828(14)	13.40730(18)	13.36017(7)
V (Å^3)	5386.63(8)	5369.89(9)	5333.16(14)	5397.39(8)	5374.43(11)	5314.76(5)
2θ range for refinement (°)	2-50	2-50	2-50	3-50	3-50	3-50
Detector	MYTHEN	MYTHEN	MYTHEN	MYTHEN	MYTHEN	MYTHEN
Number of parameters	27	27	29	27	27	27
Number of *hkl*s	5241	5246	5246	4648	4647	4580
Refinement methods	LeBail	LeBail	LeBail	LeBail	LeBail	LeBail
$R_{wp}/R_{exp}/R_p$ (%)	2.905/0.694/2.059	5.906/0.791/3.657	10.759/0.737/6.108	3.404/0.831/2.342	5.631/0.760/3.520	6.780/0.761/4.275
Gof	4.189	7.465	14.594	4.095	7.414	8.913

R_{wp}: weighted profile; R_{exp}: expected; R_p: profile; *gof:* goodness-of-fit.

Table S2. element content of the zeolite samples.

Sample	Si (Atom%)	M (Fe, Cu) (Atomic %)	X (Al. Ga, B) (Atomic %)	Si:M	Si:X
Fe/Al-Z	88.20	1.92	9.88	1: 0.021	1: 0.112
Fe/Ga-Z	93.41	2.09	4.51	1: 0.022	1: 0.048
Fe/B-Z	96.82	1.45	1.73	1: 0.015	1: 0.018
Cu/Al-Z	91.79	1.23	6.98	1: 0.013	1: 0.076
Cu/Ga-Z	93.19	0.94	5.87	1: 0.010	1: 0.063
Cu/B-Z	95.48	0.84	3.68	1: 0.009	1: 0.038

Table S3 Summary of the acidity of the zeolite samples. Values were determined by combined NH_3-TPD and Py-FTIR results.

Catalyst	**Weak acid[a] (mmol g^{-1})**	**Strong acid[a] (mmol g^{-1})**	**strong/weak acid ratio [a]**	**Total acid [a] (mmol g^{-1})**	**B/L acid ratio [b]**
Fe/Al-Z	1.315	0.335	0.255	1.650	0.50
Fe/Ga-Z	0.761	0.163	0.211	0.924	0.481
Fe/B-Z	0.449	0.003	0.006	0.452	0.213
Cu/Al-Z	1.054	0.738	0.700	1.792	0.796
Cu/Ga-Z	0.463	0.203	0.437	0.666	0.664
Cu/B-Z	0.278	0.105	0.377	0.383	0.617

a. From NH_3-TPD
b. From Py-FTIR

Table S4 Crystallographic data of the synchrotron PXRD measurements of the pyridine pre-adsorbed zeolite samples.

	Py-Fe/Al-Z	**Py-Fe/Ga-Z**	**Py-Fe/B-Z**	**Py-Cu/Al-Z**	**Py-Cu/Ga-Z**	**Py-Cu/B-Z**
X-ray energy (keV)	17.7	17.7	17.7	17	17	17
Beamline	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2	Spring-8 BL02B2
Wavelength (Å)	0.700261	0.700261	0.700261	0.729589	0.729589	0.729589
2θ – zero point (°)	0.00020	0.00020	0.00020	-0.00019	-0.00019	-0.00019
Space group	*Pnma*	*Pnma*	*Pnma*	*Pnma*	*Pnma*	*Pnma*
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
a (Å)	20.07500(32)	20.11925(10)	20.08267(24)	20.11861(20)	20.10727(13)	20.03008(10)
b (Å)	19.87873(27)	19.89772(10)	19.85981(29)	19.95147(20)	19.92729(14)	19.83891(10)
c (Å)	13.40706(22)	13.42167(9)	13.38353(23)	13.44488(19)	13.41986(12)	13.35547(8)
V (Å^3)	5350.30(14)	5373.06(5)	5337.86(14)	5396.72(11)	5377.12(7)	5307.13(5)
2θ range for refinement (°)	2-50	2-50	2-50	3-50	3-50	3-50
Detector	MYTHEN	MYTHEN	MYTHEN	MYTHEN	MYTHEN	MYTHEN
Number of parameters	28	24	24	27	27	27
Number of *hkl*s	5256	5249	5212	4644	4658	4576
Refinement methods	LeBail	LeBail	LeBail	LeBail	LeBail	LeBail
$R_{wp}/R_{exp}/R_p$ (%)	3.689/0.726/2.547	3.558/0.746/2.513	9.897/0.759/5.893	3.263/0.865/2.232	3.936/0.736/2.724	7.055/0.733/4.255
Gof	5.084	4.770	13.042	3.770	5.346	9.622

R_{wp}: weighted profile; R_{exp}: expected; R_p: profile; *gof:* goodness-of-fit.

Table S5 Atomic parameters of Py-Fe/Al-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.36489	0.05895	0.76052	1	1.3968	8d
framework	O2	0.30581	0.06876	0.92451	1	1.3968	8d
	O3	0.20497	0.05808	0.01484	1	1.3968	8d
	O4	0.08619	0.06535	0.92424	1	1.3968	8d
	O5	0.13149	0.04593	0.75060	1	1.3968	8d
	O6	0.25258	0.05714	0.72809	1	1.3968	8d
	O7	0.37456	0.85138	0.74921	1	1.3968	8d
	O8	0.28716	0.83291	0.91950	1	1.3968	8d
	O9	0.19531	0.84373	0.05442	1	1.3968	8d
	O10	0.06315	0.84501	0.93008	1	1.3968	8d
	O11	0.10665	0.84750	0.71981	1	1.3968	8d
	O12	0.23507	0.83455	0.75581	1	1.3968	8d
	O13	0.30894	0.94376	0.81333	1	1.3968	8d
	O14	0.06832	0.95430	0.81205	1	1.3968	8d
	O15	0.41385	0.13021	0.56598	1	1.3968	8d
	O16	0.42853	0.98767	0.58886	1	1.3968	8d
	O17	0.41367	0.87903	0.58130	1	1.3968	8d
	O18	0.17407	0.13535	0.60737	1	1.3968	8d
	O19	0.20533	-0.01364	0.62343	1	1.3968	8d
	O20	0.18998	0.85092	0.60966	1	1.3968	8d
	O21	0.99350	0.05423	0.79371	1	1.3968	8d
	O22	0.99546	0.85280	0.79006	1	1.3968	8d
	O23	0.40563	0.75000	0.65828	1	1.3968	4c
	O24	0.19533	0.75000	0.63190	1	1.3968	4c
	O25	0.29224	0.75000	0.06621	1	1.3968	4c
	O26	0.11226	0.75000	0.04182	1	1.3968	4c
	Si1	0.41588	0.06002	0.65566	1	0.6984	8d
	Si2	0.30885	0.02717	0.81515	1	0.6984	8d
	Si3	0.28282	0.06965	0.03070	1	0.6984	8d
	Si4	0.10963	0.05713	0.02639	1	0.6984	8d
	Si5	0.06686	0.03197	0.80184	1	0.6984	8d
	Si6	0.18062	0.06305	0.66747	1.4655	0.6984	8d
	Si7	0.42248	0.82219	0.67922	1	0.6984	8d
	Si8	0.31064	0.86594	0.80821	1	0.6984	8d
	Si9	0.26734	0.82841	0.03037	1	0.6984	8d
	Si10	0.11923	0.82804	0.03326	1	0.6984	8d
	Si11	0.07491	0.86887	0.82600	1	0.6984	8d
	Si12	0.18000	0.83054	0.69340	1	0.6984	8d
Pyridine1	C1	0.29611	0.25616	-0.12414	0.5574	8	8d
	C2	0.24489	0.26873	-0.05686	0.5574	8	8d
	C3	0.17946	0.25882	-0.08599	0.5574	8	8d
	C4	0.16463	0.23654	-0.18144	0.5574	8	8d
	C5	0.21586	0.22398	-0.24871	0.5574	8	8d
	C6	0.28128	0.23389	-0.21955	0.5574	8	8d
Pyridne2	C11	1.49595	1.06343	0.99928	0.8615	8	8d
	C12	1.52140	1.11003	1.06661	0.8615	8	8d
	C13	1.52747	1.17675	1.03839	0.8615	8	8d
	C14	1.50844	1.19743	0.94382	0.8615	8	8d
	C15	1.48300	1.15082	0.87651	0.8615	8	8d
	C16	1.47693	1.08410	0.90476	0.8615	8	8d

Table S6 Atomic parameters of Py-Fe/Ga-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.38268	0.03934	0.77104	1	2.1229	8d
framework	O2	0.31300	0.05796	0.92671	1	2.1229	8d
	O3	0.20511	0.05954	0.01852	1	2.1229	8d
	O4	0.09447	0.06888	0.92945	1	2.1229	8d
	O5	0.12441	0.04678	0.72699	1	2.1229	8d
	O6	0.24949	0.06889	0.75204	1	2.1229	8d
	O7	0.38450	0.84531	0.76885	1	2.1229	8d
	O8	0.30274	0.83968	0.91213	1	2.1229	8d
	O9	0.17806	0.84774	0.03699	1	2.1229	8d
	O10	0.08236	0.84801	0.92496	1	2.1229	8d
	O11	0.12400	0.84654	0.73464	1	2.1229	8d
	O12	0.24606	0.84447	0.78334	1	2.1229	8d
	O13	0.31719	0.94580	0.82964	1	2.1229	8d
	O14	0.07406	0.95174	0.81895	1	2.1229	8d
	O15	0.41565	0.12973	0.59613	1	2.1229	8d
	O16	0.40656	0.98884	0.59120	1	2.1229	8d
	O17	0.39583	0.85995	0.54944	1	2.1229	8d
	O18	0.19785	0.13575	0.63850	1	2.1229	8d
	O19	0.19555	-0.00584	0.60311	1	2.1229	8d
	O20	0.20627	0.85657	0.60028	1	2.1229	8d
	O21	1.00118	0.05020	0.79470	1	2.1229	8d
	O22	0.99382	0.84499	0.77493	1	2.1229	8d
	O23	0.42618	0.75000	0.66379	1	2.1229	4c
	O24	0.20461	0.75000	0.64077	1	2.1229	4c
	O25	0.28291	0.75000	0.07395	1	2.1229	4c
	O26	0.10080	0.75000	0.08383	1	2.1229	4c
	Si1	0.42004	0.05590	0.67607	1	1.0615	8d
	Si2	0.31375	0.03331	0.82453	1	1.0615	8d
	Si3	0.27790	0.05802	0.03514	1	1.0615	8d
	Si4	0.12600	0.06903	0.02551	1	1.0615	8d
	Si5	0.07350	0.03000	0.81142	1	1.0615	8d
	Si6	0.18643	0.05876	0.67353	1.3352	1.0615	8d
	Si7	0.42408	0.82079	0.67652	1	1.0615	8d
	Si8	0.31398	0.86789	0.82429	1	1.0615	8d
	Si9	0.27296	0.83727	0.02946	1	1.0615	8d
	Si10	0.11590	0.82225	0.04499	1	1.0615	8d
	Si11	0.07819	0.87413	0.80908	1	1.0615	8d
	Si12	0.19243	0.82855	0.69073	1	1.0615	8d
Pyridine1	C1	0.03586	-0.26355	0.35748	0.5843	8	8d
	C2	-0.03098	-0.24679	0.36829	0.5843	8	8d
	C3	-0.04886	-0.19467	0.43145	0.5843	8	8d
	C4	-0.00080	-0.15914	0.48387	0.5843	8	8d
	C5	0.06603	-0.17591	0.47304	0.5843	8	8d
	C6	0.08389	-0.22804	0.40988	0.5843	8	8d

Table S7 Atomic parameters of Py-Fe/B-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37686	0.04813	0.75883	1	1.3739	8d
framework	O2	0.31082	0.05507	0.91713	1	1.3739	8d
	O3	0.20112	0.06355	0.00433	1	1.3739	8d
	O4	0.10336	0.06510	0.93051	1	1.3739	8d
	O5	0.11462	0.05350	0.71909	1	1.3739	8d
	O6	0.23998	0.07514	0.77006	1	1.3739	8d
	O7	0.38211	0.84393	0.78430	1	1.3739	8d
	O8	0.30744	0.82999	0.91451	1	1.3739	8d
	O9	0.18633	0.85661	0.04354	1	1.3739	8d
	O10	0.07853	0.85774	0.91971	1	1.3739	8d
	O11	0.12928	0.83790	0.73223	1	1.3739	8d
	O12	0.24089	0.85367	0.76425	1	1.3739	8d
	O13	0.31564	0.95104	0.81424	1	1.3739	8d
	O14	0.07100	0.94595	0.81238	1	1.3739	8d
	O15	0.41916	0.13031	0.60349	1	1.3739	8d
	O16	0.40138	1.00008	0.56399	1	1.3739	8d
	O17	0.39111	0.85156	0.53447	1	1.3739	8d
	O18	0.19802	0.13670	0.62161	1	1.3739	8d
	O19	0.19283	0.00538	0.59552	1	1.3739	8d
	O20	0.20297	0.86667	0.59320	1	1.3739	8d
	O21	0.99966	0.05396	0.78808	1	1.3739	8d
	O22	1.00021	0.86091	0.76028	1	1.3739	8d
	O23	0.43089	0.75000	0.67678	1	1.3739	4c
	O24	0.20800	0.75000	0.65755	1	1.3739	4c
	O25	0.27639	0.75000	0.06768	1	1.3739	4c
	O26	0.10781	0.75000	0.06329	1	1.3739	4c
	Si1	0.42603	0.04914	0.66672	1	0.6870	8d
	Si2	0.31552	0.03263	0.83019	1.2786	0.6870	8d
	Si3	0.27740	0.04952	0.03991	1	0.6870	8d
	Si4	0.12019	0.06579	0.03123	1	0.6870	8d
	Si5	0.07302	0.03374	0.81956	1	0.6870	8d
	Si6	0.18431	0.06092	0.66666	1	0.6870	8d
	Si7	0.42603	0.82580	0.66790	1	0.6870	8d
	Si8	0.31308	0.87107	0.81985	1	0.6870	8d
	Si9	0.26675	0.83436	0.03648	1	0.6870	8d
	Si10	0.11622	0.82232	0.03135	1	0.6870	8d
	Si11	0.07850	0.86881	0.80555	1	0.6870	8d
	Si12	0.19522	0.83413	0.68868	1	0.6870	8d
Pyridine1	C1	0.04470	-0.23737	0.30234	0.4561	8	8d
	C2	-0.02150	-0.25693	0.31341	0.4561	8	8d
	C3	-0.04038	-0.29362	0.39692	0.4561	8	8d
	C4	0.00606	-0.31097	0.46940	0.4561	8	8d
	C5	0.07226	-0.29141	0.45831	0.4561	8	8d
	C6	0.09112	-0.25472	0.37479	0.4561	8	8d

Table S8 Atomic parameters of Py-Cu/Al-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37683	0.04816	0.74754	1	1.73028	8d
framework	O2	0.29809	0.05837	0.92673	1	1.73028	8d
	O3	0.21354	0.05358	0.04447	1	1.73028	8d
	O4	0.08659	0.05702	0.90951	1	1.73028	8d
	O5	0.11294	0.03731	0.72367	1	1.73028	8d
	O6	0.25456	0.05534	0.74653	1	1.73028	8d
	O7	0.37972	0.83551	0.76924	1	1.73028	8d
	O8	0.30661	0.85235	0.91195	1	1.73028	8d
	O9	0.21161	0.84457	0.01736	1	1.73028	8d
	O10	0.09950	0.84568	0.89937	1	1.73028	8d
	O11	0.12851	0.84325	0.73351	1	1.73028	8d
	O12	0.24376	0.85654	0.75179	1	1.73028	8d
	O13	0.29490	0.93761	0.82243	1	1.73028	8d
	O14	0.06969	0.94733	0.82745	1	1.73028	8d
	O15	0.40670	0.13603	0.60248	1	1.73028	8d
	O16	0.40599	0.99239	0.58265	1	1.73028	8d
	O17	0.39184	0.85596	0.56116	1	1.73028	8d
	O18	0.18491	0.13497	0.62303	1	1.73028	8d
	O19	0.18690	0.00013	0.60171	1	1.73028	8d
	O20	0.20119	0.86092	0.58828	1	1.73028	8d
	O21	0.99829	0.04366	0.79344	1	1.73028	8d
	O22	0.98284	0.84344	0.79409	1	1.73028	8d
	O23	0.42394	0.75000	0.63228	1	1.73028	4c
	O24	0.19235	0.75000	0.62993	1	1.73028	4c
	O25	0.29512	0.75000	0.06288	1	1.73028	4c
	O26	0.08843	0.75000	0.07474	1	1.73028	4c
	Si1	0.41990	0.05046	0.66656	1	0.86514	8d
	Si2	0.30985	0.03005	0.82155	1	0.86514	8d
	Si3	0.28108	0.06204	0.03101	1	0.86514	8d
	Si4	0.12670	0.06599	0.01801	1	0.86514	8d
	Si5	0.07896	0.03510	0.80796	1	0.86514	8d
	Si6	0.18143	0.05175	0.67912	1	0.86514	8d
	Si7	0.42141	0.82333	0.67058	1	0.86514	8d
	Si8	0.31151	0.87186	0.81409	1	0.86514	8d
	Si9	0.28364	0.82978	0.01591	1	0.86514	8d
	Si10	0.12084	0.82212	0.03599	1	0.86514	8d
	Si11	0.06746	0.86416	0.81743	1	0.86514	8d
	Si12	0.18891	0.82671	0.66548	1.2588	0.86514	8d
Pyridine1	C1	0.43910	-0.61872	-0.10331	0.7707	8	8d
	C2	0.45177	-0.68734	-0.10663	0.7707	8	8d
	C3	0.49518	-0.71558	-0.03825	0.7707	8	8d
	C4	0.52603	-0.67611	0.03329	0.7707	8	8d
	C5	0.51335	-0.60750	0.03659	0.7707	8	8d
	C6	0.46994	-0.57927	-0.03179	0.7707	8	8d

Table S9 Atomic parameters of Py-Cu/Ga-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37115	0.05338	0.73877	1	1.73028	8d
framework	O2	0.29811	0.06846	0.91865	1	1.73028	8d
	O3	0.20658	0.05291	0.02585	1	1.73028	8d
	O4	0.09055	0.06139	0.91139	1	1.73028	8d
	O5	0.11633	0.06366	0.71292	1	1.73028	8d
	O6	0.24231	0.06636	0.75527	1	1.73028	8d
	O7	0.37792	0.82977	0.76290	1	1.73028	8d
	O8	0.31106	0.84951	0.90643	1	1.73028	8d
	O9	0.19279	0.84983	0.01429	1	1.73028	8d
	O10	0.09498	0.84282	0.92890	1	1.73028	8d
	O11	0.10994	0.84340	0.71516	1	1.73028	8d
	O12	0.24678	0.86012	0.74223	1	1.73028	8d
	O13	0.30036	0.94221	0.80679	1	1.73028	8d
	O14	0.06981	0.95310	0.82639	1	1.73028	8d
	O15	0.41049	0.11876	0.59935	1	1.73028	8d
	O16	0.41309	0.99160	0.60043	1	1.73028	8d
	O17	0.40538	0.87180	0.56497	1	1.73028	8d
	O18	0.19275	0.13100	0.61485	1	1.73028	8d
	O19	0.19208	0.00555	0.58138	1	1.73028	8d
	O20	0.19447	0.86146	0.57770	1	1.73028	8d
	O21	0.99912	0.05077	0.77639	1	1.73028	8d
	O22	1.00011	0.84962	0.79174	1	1.73028	8d
	O23	0.41884	0.75000	0.66564	1	1.73028	4c
	O24	0.18917	0.75000	0.64342	1	1.73028	4c
	O25	0.28740	0.75000	0.05324	1	1.73028	4c
	O26	0.10720	0.75000	0.06186	1	1.73028	4c
	Si1	0.42528	0.05528	0.66165	1	0.86514	8d
	Si2	0.30748	0.03036	0.81113	1	0.86514	8d
	Si3	0.28124	0.05841	0.02461	1	0.86514	8d
	Si4	0.12326	0.06258	0.01881	1	0.86514	8d
	Si5	0.07288	0.02706	0.80679	1	0.86514	8d
	Si6	0.18729	0.06060	0.67089	1.3346	0.86514	8d
	Si7	0.42449	0.82800	0.66878	1	0.86514	8d
	Si8	0.30633	0.87313	0.80566	1	0.86514	8d
	Si9	0.27574	0.83032	0.01955	1	0.86514	8d
	Si10	0.11869	0.82598	0.03602	1	0.86514	8d
	Si11	0.07019	0.86645	0.81723	1	0.86514	8d
	Si12	0.18497	0.82688	0.67716	1	0.86514	8d
Pyridine1	C1	0.05862	0.73253	-0.66085	0.4879	8	8d
	C2	0.08377	0.67720	-0.60975	0.4879	8	8d
	C3	0.04579	0.64725	-0.53577	0.4879	8	8d
	C4	-0.01694	0.67190	-0.51229	0.4879	8	8d
	C5	-0.04207	0.72723	-0.56340	0.4879	8	8d
	C6	-0.00408	0.75717	-0.63737	0.4879	8	8d

Table S10 Atomic parameters of Py-Cu/B-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37508	0.06038	0.75351	1	2.2312	8d
framework	O2	0.30733	0.05869	0.92335	1	2.2312	8d
	O3	0.20230	0.05912	0.02514	1	2.2312	8d
	O4	0.09469	0.06431	0.91276	1	2.2312	8d
	O5	0.11415	0.05582	0.72545	1	2.2312	8d
	O6	0.24312	0.04591	0.74803	1	2.2312	8d
	O7	0.37226	0.84182	0.76217	1	2.2312	8d
	O8	0.30750	0.84712	0.92267	1	2.2312	8d
	O9	0.19684	0.84769	0.02825	1	2.2312	8d
	O10	0.08685	0.83435	0.92849	1	2.2312	8d
	O11	0.11645	0.84412	0.72622	1	2.2312	8d
	O12	0.24474	0.84269	0.76831	1	2.2312	8d
	O13	0.31583	0.95031	0.81533	1	2.2312	8d
	O14	0.08271	0.94847	0.82126	1	2.2312	8d
	O15	0.41965	0.13151	0.60694	1	2.2312	8d
	O16	0.41241	0.99690	0.58170	1	2.2312	8d
	O17	0.39948	0.86931	0.57510	1	2.2312	8d
	O18	0.19420	0.13006	0.61971	1	2.2312	8d
	O19	0.19092	0.00208	0.58938	1	2.2312	8d
	O20	0.19728	0.86770	0.58179	1	2.2312	8d
	O21	0.99691	0.04943	0.79070	1	2.2312	8d
	O22	0.99689	0.85216	0.78442	1	2.2312	8d
	O23	0.42376	0.75000	0.65543	1	2.2312	4c
	O24	0.19367	0.75000	0.64587	1	2.2312	4c
	O25	0.28429	0.75000	0.06250	1	2.2312	4c
	O26	0.10859	0.75000	0.05833	1	2.2312	4c
	Si1	0.42321	0.05822	0.66328	1	1.1156	8d
	Si2	0.30949	0.02954	0.81041	1	1.1156	8d
	Si3	0.27936	0.06171	0.03265	1	1.1156	8d
	Si4	0.12076	0.06316	0.02537	1	1.1156	8d
	Si5	0.07167	0.02922	0.81379	1	1.1156	8d
	Si6	0.18663	0.05912	0.67035	1	1.1156	8d
	Si7	0.42420	0.82784	0.67272	1	1.1156	8d
	Si8	0.30723	0.86909	0.81622	1	1.1156	8d
	Si9	0.27286	0.82842	0.03087	1	1.1156	8d
	Si10	0.11989	0.82699	0.03182	1	1.1156	8d
	Si11	0.07201	0.87121	0.81751	1	1.1156	8d
	Si12	0.18796	0.82687	0.68439	1.0842	1.1156	8d
Pyridine1	C1	-0.04342	-0.22608	0.45025	0.3862	8	8d
	C2	-0.01757	-0.16891	0.49685	0.3862	8	8d
	C3	0.04681	-0.14797	0.47449	0.3862	8	8d
	C4	0.08561	-0.18343	0.40621	0.3862	8	8d
	C5	0.05975	-0.24060	0.35962	0.3862	8	8d
	C6	-0.00464	-0.26153	0.38200	0.3862	8	8d

Table S11. Occupancies of different T sites for Fe/X-Z by Rietveld refinement.

Occupancies	Fe/Al-Z	Fe/Ga-Z	Fe/B-Z
T1	1.3364	1.1594	0.9679
T2	1.2157	1.2235	**1.2786**
T3	1.1597	1.1788	1.1410
T4	0.8413	0.9102	0.6391
T5	0.9910	1.1033	1.0068
T6	**1.4655**	**1.3352**	1.2703
T7	0.6662	0.7214	0.6399
T8	1.1055	1.0372	1.2354
T9	1.1902	1.1406	1.2216
T10	0.9400	0.8666	0.8288
T11	0.7569	0.8250	0.9490
T12	0.9840	0.9800	1.0955

Table S12. Occupancies of different T sites for Cu/X-Z by Rietveld refinement.

Occupancies	Cu/Al-Z	Cu/Ga-Z	Cu/B-Z
T1	1.0790	1.1871	1.0000
T2	1.1216	1.0289	1.0483
T3	1.0290	1.0604	1.0010
T4	1.0002	1.0002	1.0003
T5	1.1109	1.1277	1.0148
T6	1.1861	**1.3346**	1.0617
T7	1.0574	1.0001	1.0098
T8	1.1698	1.0457	1.0389
T9	1.1310	1.1031	1.0461
T10	1.0514	1.0088	1.0070
T11	1.0263	1.0000	1.0005
T12	**1.2588**	1.1170	**1.0842**

Table S13. Fitting parameters for Fe K-edge EXAFS for the sample labelled.

Sample	Path	C.N.	R/Å	σ^2	ΔE	R-factor	k-range/Å^{-1}
Fe/Al	Fe–O	1.32 (8)	1.873(10)	0.0009(90)	-0.5 (4)	0.009	3-11
Fe/Al	Fe–O	3.06 (8)	2.059 (5)	0.0062(51)	-0.5 (4)	0.009	3-11
Fe/Al	Fe–O	4.44 (41)	3.001(13)	0.0210(86)	-0.5 (4)	0.009	3-11
Fe/Ga	Fe–O	3.01 (11)	1.825 (8)	0.0027(15)	-9.1 (5)	0.004	3-11
Fe/B	Fe–O	2.01 (6)	1.872(31)	0.0016(16)	-2.2 (3)	0.003	3-11
Fe/B	Fe–O	2.40 (5)	2.059 (4)	0.0022(27)	-2.2 (3)	0.003	3-11
Fe/B	Fe–O	4.88 (39)	2.974 (11)	0.0260(86)	-2.2 (3)	0.003	3-11

C.N. is the average coordination number around the central atoms. R and σ^2 are the average path length (Å) and the Debye factor (Å^2), respectively. The ΔE_0 values of the first shell are constrained to share the same value in the fitting models. The s_0^2 was fixed as 0.9 for all fitting.

Table S14. Fitting parameters for Cu K-edge EXAFS for the sample labeled.

Sample	Path	C.N.	R/Å	σ^2	ΔE	R-factor	k-range/Å^{-1}
Cu/Al	Cu–N/O	3.3(1)	1.959(7)	0.027(1)	-0.8(4)	0.008	3-11
Cu/Al	Cu–N/O	1.7(4)	2.864(21)	0.005	-0.8(4)	0.008	3-11
Cu/Ga	Cu–N/O	3.0(2)	1.950(10)	0.003(2)	-1.1(5)	0.020	3-11
Cu/Ga	Cu–N/O	1.6(4)	2.932(24)	0.002	-1.1(5)	0.020	3-11
Cu/B	Cu–N/O	3.3(1)	1.952(7)	0.003(1)	-2.3(3)	0.006	3-11
Cu/B	Cu–N/O	2.4(3)	2.846(14)	0.008(6)	-2.3(3)	0.006	3-11

C.N. is the average coordination number around the central atoms. R and σ^2 are the average path length (Å) and the Debye factor (Å^2), respectively. The ΔE_0 values of the first shell are constrained to share the same value in the fitting models. The s_0^2 was fixed as 0.9 for all fitting.

Table S15. Atomic parameters of Fe/Al-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite framework	O1	0.37995	0.06505	0.77466	1	1.2	8d
	O2	0.29840	0.06294	0.93825	1	1.2	8d
	O3	0.20062	0.05667	0.01049	1	1.2	8d
	O4	0.09196	0.04483	0.91863	1	1.2	8d
	O5	0.11423	0.05946	0.74148	1	1.2	8d
	O6	0.25062	0.06483	0.74034	1	1.2	8d
	O7	0.41931	0.84891	0.73863	1	1.2	8d
	O8	0.31426	0.84127	0.93028	1	1.2	8d
	O9	0.16434	0.83846	0.02039	1	1.2	8d
	O10	0.11745	0.87118	0.92897	1	1.2	8d
	O11	0.11951	0.85409	0.74143	1	1.2	8d
	O12	0.27462	0.85547	0.77080	1	1.2	8d
	O13	0.31258	0.99712	0.80324	1	1.2	8d
	O14	0.07323	0.87609	0.80518	1	1.2	8d
	O15	0.40009	0.25031	0.60888	1	1.2	8d
	O16	0.40615	0.97417	0.59746	1	1.2	8d
	O17	0.39894	0.88471	0.57718	1	1.2	8d
	O18	0.19543	0.13149	0.62111	1	1.2	8d
	O19	0.18527	-0.00006	0.57673	1	1.2	8d
	O20	0.19536	0.85570	0.58349	1	1.2	8d
	O21	1.00277	0.06246	0.79792	1	1.2	8d
	O22	0.99991	0.84253	0.79040	1	1.2	8d
	O23	0.42805	0.75000	0.67261	1	1.2	4c
	O24	0.19073	0.75000	0.63547	1	1.2	4c
	O25	0.32987	0.75000	0.05097	1	1.2	4c
	O26	0.11494	0.75000	0.04384	1	1.2	4c
	Si1	0.42871	0.06027	0.65935	1	0.6	8d
	Si2	0.31207	0.03855	0.81976	1	0.6	8d
	Si3	0.27885	0.05952	0.03252	1	0.6	8d
	Si4	0.12157	0.06155	0.04353	1	0.6	8d
	Si5	0.06426	0.03098	0.81211	1	0.6	8d
	Si6	0.19647	0.06422	0.67826	1.4655*	0.6	8d
	Si7	0.42832	0.82882	0.67608	1	0.6	8d
	Si8	0.31083	0.86841	0.82170	1	0.6	8d
	Si9	0.29063	0.82889	0.03312	1	0.6	8d
	Si10	0.11895	0.82988	0.03223	1	0.6	8d
	Si11	0.07387	0.86996	0.81198	1	0.6	8d
	Si12	0.18908	0.82651	0.67832	1	0.6	8d

Table S16. Atomic parameters of Fe/Ga-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite framework	O1	0.38133	0.05960	0.76617	1	1.4398	8d
	O2	0.30580	0.06053	0.91424	1	1.4398	8d
	O3	0.19432	0.06084	0.01228	1	1.4398	8d
	O4	0.09846	0.06169	0.91886	1	1.4398	8d
	O5	0.11918	0.05443	0.71804	1	1.4398	8d
	O6	0.25548	0.04437	0.75660	1	1.4398	8d
	O7	0.39208	0.84730	0.78530	1	1.4398	8d
	O8	0.30764	0.84096	0.91430	1	1.4398	8d
	O9	0.19398	0.84655	0.02954	1	1.4398	8d
	O10	0.08007	0.85374	0.92174	1	1.4398	8d
	O11	0.11128	0.84363	0.73470	1	1.4398	8d
	O12	0.22848	0.83628	0.76170	1	1.4398	8d
	O13	0.31080	0.93679	0.82497	1	1.4398	8d
	O14	0.07270	0.93017	0.81185	1	1.4398	8d
	O15	0.41660	0.13504	0.58744	1	1.4398	8d
	O16	0.40266	0.99628	0.56227	1	1.4398	8d
	O17	0.40404	0.86416	0.57133	1	1.4398	8d
	O18	0.19309	0.14498	0.62759	1	1.4398	8d
	O19	0.19514	-0.01980	0.61480	1	1.4398	8d
	O20	0.19471	0.85979	0.59974	1	1.4398	8d
	O21	1.00748	0.04953	0.78963	1	1.4398	8d
	O22	1.00359	0.85114	0.75091	1	1.4398	8d
	O23	0.42003	0.75000	0.65462	1	1.4398	4c
	O24	0.19853	0.75000	0.63479	1	1.4398	4c
	O25	0.29195	0.75000	0.08286	1	1.4398	4c
	O26	0.10733	0.75000	0.07404	1	1.4398	4c
	Si1	0.42315	0.05762	0.67142	1	0.7199	8d
	Si2	0.31296	0.03522	0.82653	1	0.7199	8d
	Si3	0.28049	0.06251	0.03372	1	0.7199	8d
	Si4	0.12151	0.06057	0.03645	1	0.7199	8d
	Si5	0.07382	0.02748	0.81817	1	0.7199	8d
	Si6	0.19081	0.06168	0.67409	1.3352*	0.7199	8d
	Si7	0.42749	0.83008	0.69250	1	0.7199	8d
	Si8	0.30938	0.86737	0.82959	1	0.7199	8d
	Si9	0.27677	0.82878	0.04337	1	0.7199	8d
	Si10	0.11663	0.81993	0.03769	1	0.7199	8d
	Si11	0.07222	0.86890	0.80191	1	0.7199	8d
	Si12	0.18079	0.82814	0.67462	1	0.7199	8d

Table S17. Atomic parameters of Fe/B-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.36796	0.05042	0.74038	1	0.9609	8d
framework	O2	0.30322	0.06319	0.92658	1	0.9609	8d
	O3	0.20163	0.05992	0.01475	1	0.9609	8d
	O4	0.09144	0.03945	0.90694	1	0.9609	8d
	O5	0.12457	0.07261	0.74069	1	0.9609	8d
	O6	0.22629	0.06964	0.77696	1	0.9609	8d
	O7	0.39382	0.83980	0.77672	1	0.9609	8d
	O8	0.31058	0.83573	0.93479	1	0.9609	8d
	O9	0.18804	0.84068	-0.00241	1	0.9609	8d
	O10	0.11011	0.84887	0.90099	1	0.9609	8d
	O11	0.12777	0.84581	0.73324	1	0.9609	8d
	O12	0.25737	0.84408	0.76581	1	0.9609	8d
	O13	0.30304	0.93787	0.81241	1	0.9609	8d
	O14	0.08562	0.95326	0.82506	1	0.9609	8d
	O15	0.41559	0.13509	0.64600	1	0.9609	8d
	O16	0.40494	0.98840	0.58940	1	0.9609	8d
	O17	0.39952	0.86555	0.55371	1	0.9609	8d
	O18	0.18533	0.12592	0.61261	1	0.9609	8d
	O19	0.18412	0.03370	0.58815	1	0.9609	8d
	O20	0.20354	0.85679	0.59221	1	0.9609	8d
	O21	0.99431	0.04966	0.77471	1	0.9609	8d
	O22	0.99423	0.84906	0.78463	1	0.9609	8d
	O23	0.42449	0.75000	0.70717	1	0.9609	4c
	O24	0.20688	0.75000	0.67519	1	0.9609	4c
	O25	0.27058	0.75000	0.01086	1	0.9609	4c
	O26	0.10459	0.75000	0.06982	1	0.9609	4c
	Si1	0.41936	0.05714	0.67305	1	0.4804	8d
	Si2	0.30802	0.02944	0.82280	1.2786*	0.4804	8d
	Si3	0.28244	0.05460	0.04556	1	0.4804	8d
	Si4	0.11743	0.06626	0.03184	1	0.4804	8d
	Si5	0.07212	0.03750	0.81429	1	0.4804	8d
	Si6	0.18327	0.04427	0.68045	1	0.4804	8d
	Si7	0.42237	0.82315	0.66708	1	0.4804	8d
	Si8	0.31068	0.87140	0.82534	1	0.4804	8d
	Si9	0.27739	0.83304	0.02539	1	0.4804	8d
	Si10	0.11548	0.82555	0.04495	1	0.4804	8d
	Si11	0.07427	0.86774	0.81369	1	0.4804	8d
	Si12	0.19103	0.82381	0.67879	1	0.4804	8d
Water1	O1	0.48146	0.36773	0.45202	0.5452	7	8d

Table S18. Atomic parameters of Cu/Al-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	Beq	Wyckoff
Zeolite	O1	0.38292	0.05969	0.76470	1	1.2	8d
framework	O2	0.30991	0.06035	0.91453	1	1.2	8d
	O3	0.19925	0.04396	0.02637	1	1.2	8d
	O4	0.09250	0.05904	0.93912	1	1.2	8d
	O5	0.11301	0.06095	0.69945	1	1.2	8d
	O6	0.24093	0.04684	0.75345	1	1.2	8d
	O7	0.39521	0.85010	0.77988	1	1.2	8d
	O8	0.31640	0.84709	0.89548	1	1.2	8d
	O9	0.19990	0.84678	0.04076	1	1.2	8d
	O10	0.09168	0.83705	0.93887	1	1.2	8d
	O11	0.10799	0.84922	0.73094	1	1.2	8d
	O12	0.23713	0.86111	0.78160	1	1.2	8d
	O13	0.31313	0.93952	0.80765	1	1.2	8d
	O14	0.07981	0.93925	0.83211	1	1.2	8d
	O15	0.42831	0.15378	0.63664	1	1.2	8d
	O16	0.39939	1.00792	0.57081	1	1.2	8d
	O17	0.39321	0.86854	0.54115	1	1.2	8d
	O18	0.18847	0.14147	0.61464	1	1.2	8d
	O19	0.19712	-0.00808	0.60575	1	1.2	8d
	O20	0.20133	0.86754	0.59088	1	1.2	8d
	O21	1.00052	0.06068	0.75599	1	1.2	8d
	O22	1.00213	0.84925	0.79446	1	1.2	8d
	O23	0.41989	0.75000	0.66265	1	1.2	4c
	O24	0.19451	0.75000	0.60233	1	1.2	4c
	O25	0.30322	0.75000	0.09781	1	1.2	4c
	O26	0.08779	0.75000	0.08809	1	1.2	4c
	Si1	0.42525	0.05959	0.68484	1	0.6	8d
	Si2	0.31354	0.03220	0.82342	1	0.6	8d
	Si3	0.27579	0.06253	0.02584	1	0.6	8d
	Si4	0.12404	0.05455	0.01350	1	0.6	8d
	Si5	0.07146	0.03555	0.81274	1	0.6	8d
	Si6	0.19149	0.06400	0.67078	1	0.6	8d
	Si7	0.42616	0.83196	0.66609	1	0.6	8d
	Si8	0.31359	0.86384	0.82773	1	0.6	8d
	Si9	0.28994	0.81987	0.02762	1	0.6	8d
	Si10	0.12176	0.81615	0.04350	1	0.6	8d
	Si11	0.06907	0.86692	0.80583	1	0.6	8d
	Si12	0.18408	0.82669	0.68732	1.2588*	0.6	8d
Water1	O1	0.50920	0.25123	-0.13938	0.4171	8	8d
Water2	O2	0.50697	-0.02271	-0.06333	0.3971	8	8d
Water3	O3	-0.50826	0.16454	-0.04125	0.7816	8	8d
Water4	O4	-0.73969	0.24463	-0.10154	0.6393	8	8d
Water5	O5	-0.52583	-0.21553	-0.06154	0.4389	8	8d

Table S19. Atomic parameters of Cu/Ga-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37457	0.05369	0.77299	1	1.73028	8d
framework	O2	0.30270	0.06622	0.91221	1	1.73028	8d
	O3	0.20333	0.05209	0.01384	1	1.73028	8d
	O4	0.09571	0.06158	0.92047	1	1.73028	8d
	O5	0.11842	0.05225	0.71586	1	1.73028	8d
	O6	0.24506	0.05807	0.75603	1	1.73028	8d
	O7	0.39861	0.84194	0.78950	1	1.73028	8d
	O8	0.31507	0.84758	0.90637	1	1.73028	8d
	O9	0.18333	0.84471	0.02910	1	1.73028	8d
	O10	0.08878	0.85064	0.90931	1	1.73028	8d
	O11	0.10683	0.84985	0.74288	1	1.73028	8d
	O12	0.23777	0.84202	0.75938	1	1.73028	8d
	O13	0.30892	0.93744	0.82488	1	1.73028	8d
	O14	0.07227	0.93686	0.82515	1	1.73028	8d
	O15	0.41537	0.14335	0.62519	1	1.73028	8d
	O16	0.39892	0.98777	0.56410	1	1.73028	8d
	O17	0.40016	0.86953	0.56708	1	1.73028	8d
	O18	0.19322	0.15115	0.62909	1	1.73028	8d
	O19	0.20424	-0.01749	0.61817	1	1.73028	8d
	O20	0.19680	0.85901	0.59980	1	1.73028	8d
	O21	1.00655	0.05534	0.77681	1	1.73028	8d
	O22	1.00098	0.85193	0.75080	1	1.73028	8d
	O23	0.42186	0.75000	0.63774	1	1.73028	4c
	O24	0.18365	0.75000	0.61364	1	1.73028	4c
	O25	0.29574	0.75000	0.07985	1	1.73028	4c
	O26	0.09478	0.75000	0.10587	1	1.73028	4c
	Si1	0.42149	0.05327	0.66977	1	0.86514	8d
	Si2	0.31209	0.03267	0.83037	1	0.86514	8d
	Si3	0.27907	0.06183	0.03274	1	0.86514	8d
	Si4	0.11874	0.05807	0.03030	1	0.86514	8d
	Si5	0.07391	0.02963	0.82086	1	0.86514	8d
	Si6	0.19348	0.06171	0.66472	1.3346*	0.86514	8d
	Si7	0.43022	0.82861	0.68293	1	0.86514	8d
	Si8	0.31121	0.86714	0.82330	1	0.86514	8d
	Si9	0.27795	0.82692	0.03767	1	0.86514	8d
	Si10	0.11834	0.81607	0.03232	1	0.86514	8d
	Si11	0.07271	0.86383	0.81411	1	0.86514	8d
	Si12	0.18731	0.82692	0.67519	1	0.86514	8d
Water1	O1	0.35314	0.23586	-0.12051	0.3406	8	8d
Water2	O2	0.48732	0.49544	0.06707	0.4175	8	8d
Water3	O3	0.61909	0.30742	0.56819	0.5779	8	8d
Water4	O4	0.51675	0.28235	0.90390	0.6172	8	8d

Table S20. Atomic parameters of Cu/B-Z derived from synchrotron PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.37439	0.06183	0.75485	1	1.73028	8d
framework	O2	0.30843	0.06014	0.92019	1	1.73028	8d
	O3	0.19967	0.06045	0.03227	1	1.73028	8d
	O4	0.09096	0.06092	0.91501	1	1.73028	8d
	O5	0.11881	0.05304	0.72666	1	1.73028	8d
	O6	0.24172	0.04834	0.73954	1	1.73028	8d
	O7	0.37975	0.84450	0.76134	1	1.73028	8d
	O8	0.31314	0.84467	0.91851	1	1.73028	8d
	O9	0.19003	0.84636	0.02615	1	1.73028	8d
	O10	0.09219	0.83758	0.93354	1	1.73028	8d
	O11	0.11418	0.84383	0.73161	1	1.73028	8d
	O12	0.24904	0.85774	0.77817	1	1.73028	8d
	O13	0.31183	0.96003	0.81917	1	1.73028	8d
	O14	0.07785	0.94729	0.82187	1	1.73028	8d
	O15	0.42134	0.12905	0.61701	1	1.73028	8d
	O16	0.40273	0.99599	0.57894	1	1.73028	8d
	O17	0.40140	0.87114	0.57054	1	1.73028	8d
	O18	0.19283	0.12880	0.61905	1	1.73028	8d
	O19	0.19170	-0.00143	0.59485	1	1.73028	8d
	O20	0.19928	0.86818	0.57730	1	1.73028	8d
	O21	0.99872	0.04775	0.79441	1	1.73028	8d
	O22	0.99952	0.84781	0.78421	1	1.73028	8d
	O23	0.42804	0.75000	0.65033	1	1.73028	4c
	O24	0.19182	0.75000	0.64219	1	1.73028	4c
	O25	0.28222	0.75000	0.07094	1	1.73028	4c
	O26	0.09929	0.75000	0.08109	1	1.73028	4c
	Si1	0.42599	0.05721	0.66306	1	0.86514	8d
	Si2	0.30768	0.02957	0.81107	1	0.86514	8d
	Si3	0.27727	0.06332	0.02911	1	0.86514	8d
	Si4	0.12257	0.06249	0.02250	1	0.86514	8d
	Si5	0.06984	0.03118	0.81126	1	0.86514	8d
	Si6	0.18793	0.06159	0.67112	1	0.86514	8d
	Si7	0.42398	0.82858	0.67892	1	0.86514	8d
	Si8	0.31146	0.86726	0.81668	1	0.86514	8d
	Si9	0.27839	0.82553	0.03141	1	0.86514	8d
	Si10	0.12425	0.82453	0.03381	1	0.86514	8d
	Si11	0.07494	0.86972	0.81423	1	0.86514	8d
	Si12	0.18733	0.82701	0.68146	1.0842*	0.86514	8d
Water1	O1	0.49092	0.30494	-0.07982	0.4289	8	8d

Table S21. Catalytic performance of 4-chlorostyrene of the zeolite sample labelled.

Catalyst	Reaction temp. (°C)	Conv.$_{(4Cl\text{-}styrene)}$ (%)	Sel.$_{(4Cl\text{-}benzaldehyde)}$ (%)	Activation energy (kJ)
Fe/Al-Z	50	7.2	54.1	87.685
	70	35.0	74.7	
	90	24.1	74.0	
Fe/Ga-Z	50	6.9	67.5	51.578
	70	33.6	71.5	
	90	51.6	73.4	
Fe/B-Z	50	9.3	74.5	49.533
	70	57.4	75.4	
	90	65.3	78.6	
Cu/Al-Z	50	No reaction	-	50.060
	70	36.9	57.8	
	90	30.3	76.6	
	110	73.0	75.6	
Cu/Ga-Z	50	No reaction	-	70.744
	70	10.6	37.0	
	90	23.6	85.5	
	110	78.6	65.9	
Cu/B-Z	50	No reaction	-	84.369
	70	9.6	67.3	
	90	13.3	78.3	
	110	61.5	72.9	
Na-Fe/Al-Z	70	16.3	76.0	-
Na-Fe/Ga-Z	70	12.7	62.0	-
Na-Fe/B-Z	70	15.2	71.5	-
H-ZSM-5	70	14.7	55.1	-
Na-ZSM-5	70	No reaction	-	-

Table S22. Crystallographic data of the synchrotron PXRD measurement of the 4-chlorostrene (4Cl-sty) and GVL pre-adsorbed zeolite sample labelled.

	4Cl-sty-Fe/Al-Z	**4Cl-sty-Fe/B-Z**	**GVL-Fe/Al-Z**	**GVL-Fe/B-Z**
Diffractometer	Rigaku SmartLab	Rigaku SmartLab	Rigaku SmartLab	Rigaku SmartLab
Wavelength (Å)	0.7093	0.7093	0.7093	0.7093
2θ – zero point (°)	-0.00557(17)	-0.00817(16)	-0.00154(28)-	-0.00335
Space group	*Pnma*	*Pnma*	*Pnma*	*Pnma*
Crystal system	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
a (Å)	20.11775(58)	20.01241(48)	20.12910(72)	20.04154(30)
b (Å)	19.92743(53)	19.88942(54)	19.95968(86)	19.86729(33)
c (Å)	13.40824(40)	13.36641(37)	13.44821(56)	13.37965(25)
V (Å^3)	5375.30(27)	5320.29(24)	5403.09(38)	5327.39(15)
2θ range for refinement (°)	3-50	3-50	3-50	3-50
Detector	D/tex Ultra 250-HE	D/tex Ultra 250-HE	D/tex Ultra 250-HE	D/tex Ultra 250-HE
Number of parameters	24	24	24	24
Number of *hkl*s	5036	8187	5073	4986
Refinement methods	LeBail	LeBail	LeBail	LeBail
$R_{wp}/R_{exp}/R_p$ (%)	2.329/2.828/1.791	4.467/3.051/3.239	4.073/6.008/3.012	4.253/6.069/3.290
Gof	0.824	1.464	0.678	0.701

R_{wp}: weighted profile; R_{exp}: expected; R_p: profile; *gof:* goodness-of-fit.

Table S23. Atomic parameters of 4Cl-sty-Fe/Al-Z derived from PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.38399	0.05878	0.76741	1	0.1941	8d
framework	O2	0.28158	0.05573	0.93411	1	0.1941	8d
	O3	0.18726	0.04622	0.02763	1	0.1941	8d
	O4	0.0833	0.0704	0.9258	1	0.1941	8d
	O5	0.11522	0.04014	0.71712	1	0.1941	8d
	O6	0.25712	0.03818	0.74286	1	0.1941	8d
	O7	0.37293	0.84347	0.76652	1	0.1941	8d
	O8	0.31422	0.83556	0.93155	1	0.1941	8d
	O9	0.20253	0.84841	-0.01042	1	0.1941	8d
	O10	0.08887	0.83149	0.91674	1	0.1941	8d
	O11	0.12424	0.844	0.73922	1	0.1941	8d
	O12	0.22386	0.84756	0.77626	1	0.1941	8d
	O13	0.3093	0.94395	0.8213	1	0.1941	8d
	O14	0.0881	0.95694	0.80367	1	0.1941	8d
	O15	0.4167	0.13068	0.60315	1	0.1941	8d
	O16	0.41828	0.99026	0.59621	1	0.1941	8d
	O17	0.40663	0.87397	0.59093	1	0.1941	8d
	O18	0.1878	0.11457	0.61751	1	0.1941	8d
	O19	0.23153	0.0079	0.61313	1	0.1941	8d
	O20	0.19795	0.84274	0.58141	1	0.1941	8d
	O21	0.9988	0.05178	0.78692	1	0.1941	8d
	O22	0.99935	0.83687	0.77263	1	0.1941	8d
	O23	0.43513	0.75	0.62121	1	0.1941	4c
	O24	0.20272	0.75	0.62301	1	0.1941	4c
	O25	0.313	0.75	0.04502	1	0.1941	4c
	O26	0.09524	0.75	0.0782	1	0.1941	4c
	Si1	0.42606	0.06764	0.66273	1	0.097	8d
	Si2	0.32293	0.03747	0.83325	1	0.097	8d
	Si3	0.26831	0.0716	0.03174	1	0.097	8d
	Si4	0.12128	0.07527	0.02309	1	0.097	8d
	Si5	0.07129	0.02925	0.81017	1	0.097	8d
	Si6	0.18292	0.05472	0.68203	1.4655	0.097	8d
	Si7	0.433	0.82948	0.6832	1	0.097	8d
	Si8	0.31414	0.86191	0.82342	1	0.097	8d
	Si9	0.27583	0.84036	0.04001	1	0.097	8d
	Si10	0.11537	0.82756	0.04262	1	0.097	8d
	Si11	0.07958	0.86622	0.81762	1	0.097	8d
	Si12	0.1933	0.83018	0.67705	1	0.097	8d
4-Cl-sty	Cl1	0.42768	-0.02431	-0.04426	0.8511	8	8d
	C2	0.44962	0.068549	-0.02199	0.8511	8	8d
	C3	0.498821	0.086401	0.04602	0.8511	8	8d
	C4	0.514738	0.152872	0.062259	0.8511	8	8d
	C5	0.481573	0.20371	0.010441	0.8511	8	8d
	C6	0.432138	0.185687	-0.05789	0.8511	8	8d
	C7	0.416608	0.119063	-0.07356	0.8511	8	8d
	C8	0.496921	0.268667	0.026017	0.8511	8	8d
	C9	0.544947	0.295024	-0.03224	0.8511	8	8d

Table S24. Atomic parameters of 4Cl-sty-Fe/B-Z derived from PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite framework	O1	0.37846	0.04456	0.7543	1	0.6848	8d
	O2	0.30255	0.05825	0.92132	1	0.6848	8d
	O3	0.19771	0.06239	0.03627	1	0.6848	8d
	O4	0.09774	0.06008	0.90918	1	0.6848	8d
	O5	0.11632	0.0525	0.73301	1	0.6848	8d
	O6	0.25356	0.04071	0.73525	1	0.6848	8d
	O7	0.37667	0.8333	0.76649	1	0.6848	8d
	O8	0.31233	0.84136	0.91544	1	0.6848	8d
	O9	0.19782	0.84948	0.03346	1	0.6848	8d
	O10	0.09304	0.83247	0.91558	1	0.6848	8d
	O11	0.11448	0.84535	0.74292	1	0.6848	8d
	O12	0.2269	0.84348	0.74855	1	0.6848	8d
	O13	0.31314	0.94349	0.81784	1	0.6848	8d
	O14	0.083	0.94816	0.81488	1	0.6848	8d
	O15	0.42729	0.12889	0.59605	1	0.6848	8d
	O16	0.41533	0.9871	0.58405	1	0.6848	8d
	O17	0.39958	0.86522	0.56047	1	0.6848	8d
	O18	0.18625	0.12612	0.60881	1	0.6848	8d
	O19	0.19668	0.008	0.5778	1	0.6848	8d
	O20	0.19989	0.87331	0.57849	1	0.6848	8d
	O21	0.99577	0.04711	0.79585	1	0.6848	8d
	O22	0.99936	0.85809	0.79922	1	0.6848	8d
	O23	0.42216	0.75	0.6502	1	0.6848	4c
	O24	0.18939	0.75	0.65863	1	0.6848	4c
	O25	0.28173	0.75	0.04457	1	0.6848	4c
	O26	0.09582	0.75	0.05746	1	0.6848	4c
	Si1	0.42525	0.05682	0.6514	1	0.3424	8d
	Si2	0.31554	0.0252	0.82444	1.2786	0.3424	8d
	Si3	0.27542	0.06648	0.02767	1	0.3424	8d
	Si4	0.123	0.06121	0.01425	1	0.3424	8d
	Si5	0.0693	0.02965	0.79928	1	0.3424	8d
	Si6	0.18213	0.06262	0.66263	1	0.3424	8d
	Si7	0.42143	0.82977	0.67589	1	0.3424	8d
	Si8	0.30501	0.87318	0.8045	1	0.3424	8d
	Si9	0.27615	0.82871	0.02818	1	0.3424	8d
	Si10	0.12053	0.8229	0.03505	1	0.3424	8d
	Si11	0.06846	0.86274	0.81932	1	0.3424	8d
	Si12	0.18557	0.82948	0.66918	1	0.3424	8d
4-Cl-sty	Cl1	-0.06098	0.5132	0.45773	0.4062	8	8d
	C2	-0.07135	0.424641	0.513972	0.4062	8	8d
	C3	-0.04573	0.368587	0.465033	0.4062	8	8d
	C4	-0.05303	0.305011	0.505011	0.4062	8	8d
	C5	-0.08644	0.295725	0.595812	0.4062	8	8d
	C6	-0.11217	0.35211	0.644907	0.4062	8	8d
	C7	-0.10459	0.415465	0.604272	0.4062	8	8d
	C8	-0.0937	0.233775	0.635156	0.4062	8	8d
	C9	-0.04498	0.212526	0.697187	0.4062	8	8d

Table S25. Atomic parameters of GVL-Fe/Al-Z derived from PXRD.

Species	Atom	x	y	z	SOF	B_{eq}	Wyckoff
Zeolite	O1	0.39307	0.05508	0.75835	1	0.0783	8d
framework	O2	0.30006	0.05278	0.9248	1	0.0783	8d
	O3	0.19555	0.06785	0.03664	1	0.0783	8d
	O4	0.09335	0.06499	0.92963	1	0.0783	8d
	O5	0.1077	0.05233	0.73747	1	0.0783	8d
	O6	0.25159	0.03222	0.75088	1	0.0783	8d
	O7	0.37149	0.8291	0.75601	1	0.0783	8d
	O8	0.31226	0.83354	0.93241	1	0.0783	8d
	O9	0.18104	0.84347	0.02251	1	0.0783	8d
	O10	0.09732	0.84165	0.92837	1	0.0783	8d
	O11	0.11863	0.84584	0.74045	1	0.0783	8d
	O12	0.22675	0.83588	0.74783	1	0.0783	8d
	O13	0.31746	0.94589	0.81134	1	0.0783	8d
	O14	0.07893	0.96925	0.8524	1	0.0783	8d
	O15	0.41833	0.13184	0.60776	1	0.0783	8d
	O16	0.40526	0.9989	0.5674	1	0.0783	8d
	O17	0.39508	0.85595	0.55118	1	0.0783	8d
	O18	0.19649	0.12847	0.59526	1	0.0783	8d
	O19	0.20624	-0.00915	0.57762	1	0.0783	8d
	O20	0.1995	0.86953	0.58716	1	0.0783	8d
	O21	0.99816	0.06328	0.79917	1	0.0783	8d
	O22	1.00053	0.84426	0.76162	1	0.0783	8d
	O23	0.43516	0.75	0.66466	1	0.0783	4c
	O24	0.19814	0.75	0.6766	1	0.0783	4c
	O25	0.29264	0.75	0.06819	1	0.0783	4c
	O26	0.10279	0.75	0.07787	1	0.0783	4c
	Si1	0.42263	0.06215	0.65924	1	0.0391	8d
	Si2	0.31424	0.02616	0.81001	1	0.0391	8d
	Si3	0.27196	0.06216	0.03914	1	0.0391	8d
	Si4	0.11708	0.07182	0.02464	1	0.0391	8d
	Si5	0.07281	0.03726	0.82548	1	0.0391	8d
	Si6	0.18078	0.05318	0.68277	1.4655	0.0391	8d
	Si7	0.42254	0.83121	0.66751	1	0.0391	8d
	Si8	0.31033	0.85628	0.80372	1	0.0391	8d
	Si9	0.27183	0.8257	0.02391	1	0.0391	8d
	Si10	0.12367	0.83036	0.02057	1	0.0391	8d
	Si11	0.06119	0.87702	0.81605	1	0.0391	8d
	Si12	0.18274	0.82418	0.65791	1	0.0391	8d
GVL1	O1	-0.23101	-0.25501	0.20205	0.4062	8	8d
	C2	-0.28835	-0.25249	0.169251	0.4062	8	8d
	C3	-0.30461	-0.26493	0.062113	0.4062	8	8d
	C4	-0.37816	-0.28321	0.075302	0.4062	8	8d
	C5	-0.39424	-0.23823	0.163103	0.4062	8	8d
	C6	-0.45596	-0.26036	0.222006	0.4062	8	8d
	O7	-0.33719	-0.22493	0.225266	0.4062	8	8d

Table S26. Atomic parameters of GVL-Fe/B-Z derived from PXRD.

Species	Atom	x	y	z	SOF	Beq	Wyckoff
Zeolite framework	O1	0.3767	0.05686	0.75479	1	0.887	8d
	O2	0.30619	0.05106	0.93662	1	0.887	8d
	O3	0.20404	0.0635	0.03351	1	0.887	8d
	O4	0.09899	0.05903	0.90753	1	0.887	8d
	O5	0.11556	0.04714	0.72618	1	0.887	8d
	O6	0.24291	0.0406	0.74579	1	0.887	8d
	O7	0.37887	0.83434	0.76967	1	0.887	8d
	O8	0.30478	0.83507	0.91662	1	0.887	8d
	O9	0.20903	0.84221	0.02826	1	0.887	8d
	O10	0.08594	0.83661	0.91963	1	0.887	8d
	O11	0.12537	0.83796	0.73282	1	0.887	8d
	O12	0.23988	0.84741	0.77008	1	0.887	8d
	O13	0.31517	0.93993	0.81996	1	0.887	8d
	O14	0.0811	0.94061	0.82238	1	0.887	8d
	O15	0.41755	0.13087	0.60403	1	0.887	8d
	O16	0.40589	0.9998	0.57135	1	0.887	8d
	O17	0.38962	0.85873	0.57453	1	0.887	8d
	O18	0.20098	0.11991	0.63244	1	0.887	8d
	O19	0.19218	0.00993	0.60727	1	0.887	8d
	O20	0.20698	0.8583	0.60123	1	0.887	8d
	O21	0.9902	0.04613	0.79892	1	0.887	8d
	O22	0.98764	0.8525	0.78882	1	0.887	8d
	O23	0.43218	0.75	0.64883	1	0.887	4c
	O24	0.18441	0.75	0.65766	1	0.887	4c
	O25	0.28109	0.75	0.05715	1	0.887	4c
	O26	0.09823	0.75	0.06307	1	0.887	4c
	Si1	0.42281	0.06252	0.66092	1	0.4435	8d
	Si2	0.3094	0.02423	0.82168	1	0.4435	8d
	Si3	0.27533	0.06012	0.03387	1	0.4435	8d
	Si4	0.12119	0.06761	0.01499	1	0.4435	8d
	Si5	0.06856	0.02724	0.80209	1	0.4435	8d
	Si6	0.18494	0.05095	0.6706	1.2786	0.4435	8d
	Si7	0.41951	0.82336	0.67547	1	0.4435	8d
	Si8	0.30499	0.87383	0.80578	1	0.4435	8d
	Si9	0.27572	0.82787	0.04124	1	0.4435	8d
	Si10	0.12292	0.83469	0.04091	1	0.4435	8d
	Si11	0.07247	0.87495	0.80975	1	0.4435	8d
	Si12	0.19067	0.82734	0.67882	1	0.4435	8d
GVL1	O1	0.08929	-0.28655	0.36562	0.7346	8	8d
	C2	0.051614	-0.32146	0.417244	0.7346	8	8d
	C3	0.041815	-0.39536	0.399448	0.7346	8	8d
	C4	0.016477	-0.41427	0.503944	0.7346	8	8d
	C5	-0.02031	-0.34952	0.529036	0.7346	8	8d
	C6	-0.03127	-0.33879	0.641701	0.7346	8	8d
	O7	0.007312	-0.29126	0.4793	0.7346	8	8d

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