Supplementary Materials: Replacement of Chromium by Non-toxic Metals in Lewis-Acid MOFs: Assessment of Stability as Glucose Conversion Catalysts

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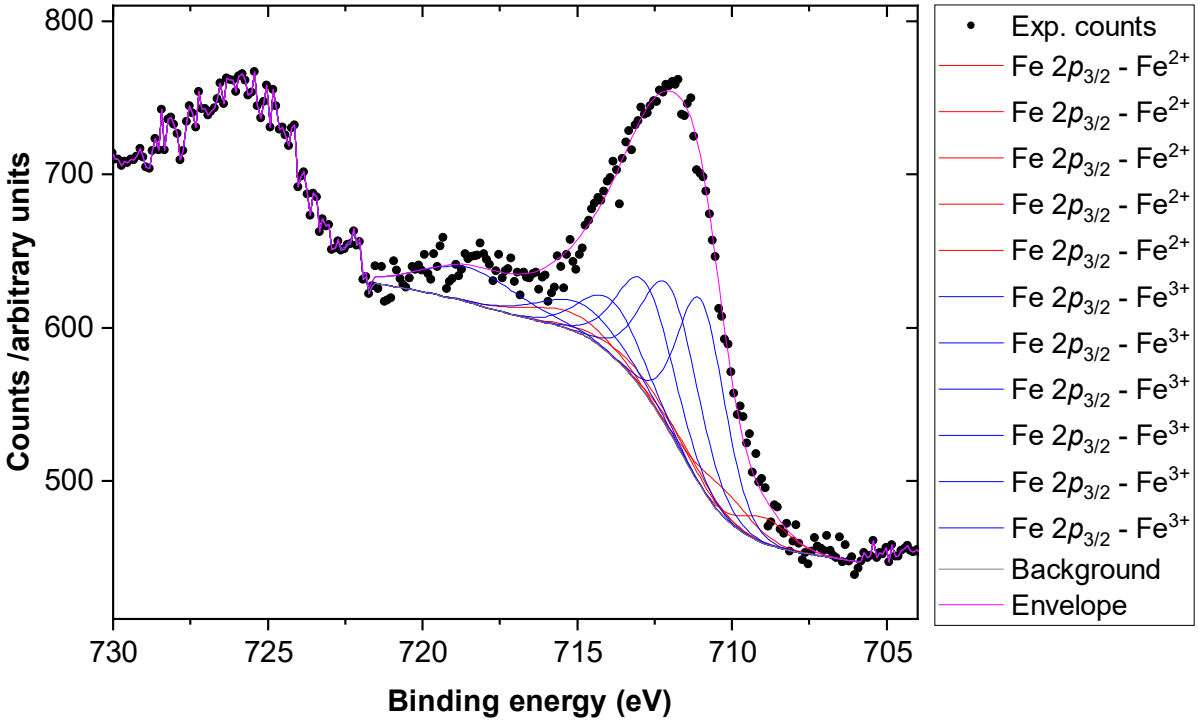

Figure S1. XPS of MIL-88B (Fe) in the Fe 2$p_{3/2}$ region. The fitted contributions are shown with reference spectra in the literature used for guidance.

Table S1. Assignment of key bands in the IR spectra[1].

Band /cm^{-1}	Assignment
1685 (*)	Free C=O
1595 strong	ν_{ass} (–CO_2) bound
1490	C=C stretch (aromatic)
1395 strong	ν_{sym} (–CO_2) bound
1135 (*)	C–OH stretch
875	C–H bending (aromatic)
750	C–H bending (aromatic)

Additional bands (*) in the spectrum of the MIL-53(Fe,Sc) sample (see Figure 8 in the manuscript) suggest the presence of some un-coordinated carboxylic groups. This is not due to the presence of crystalline benzene-1,4-dicarboxylic acid (which is not seen in the powder XRD), suggesting a more defective structure for the mixed-metal material.

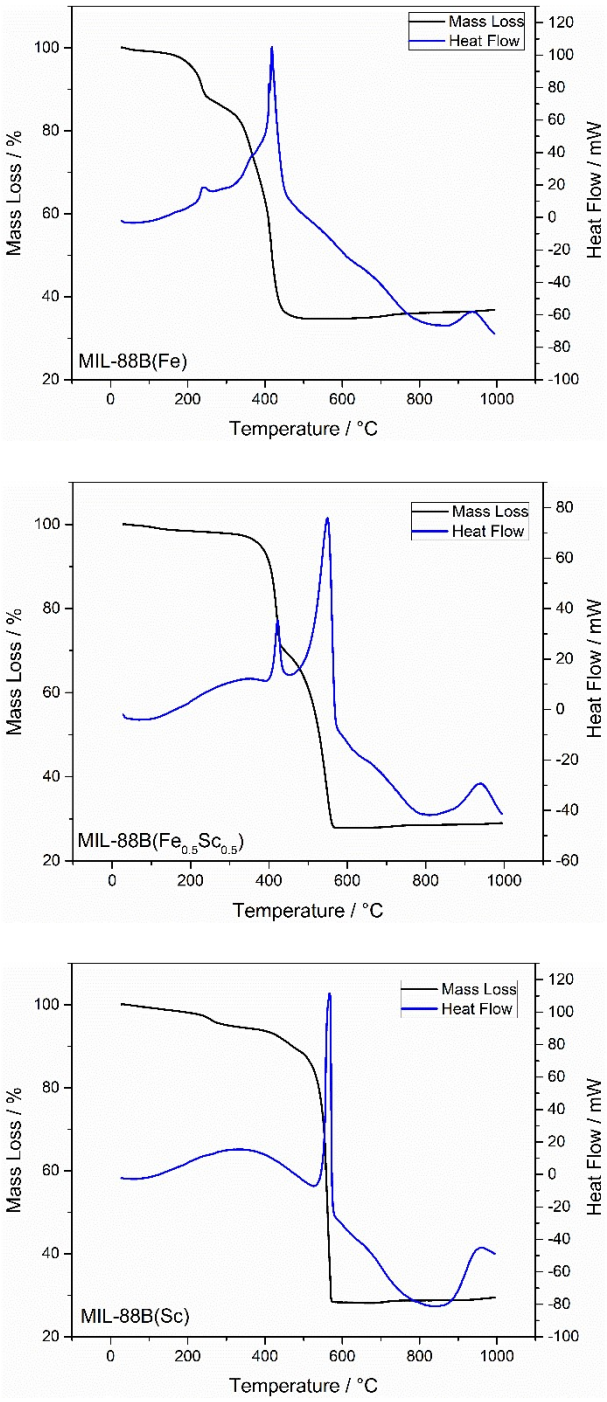

Figure S2. Thermogravimetric analysis of MIL-88B catalysts.

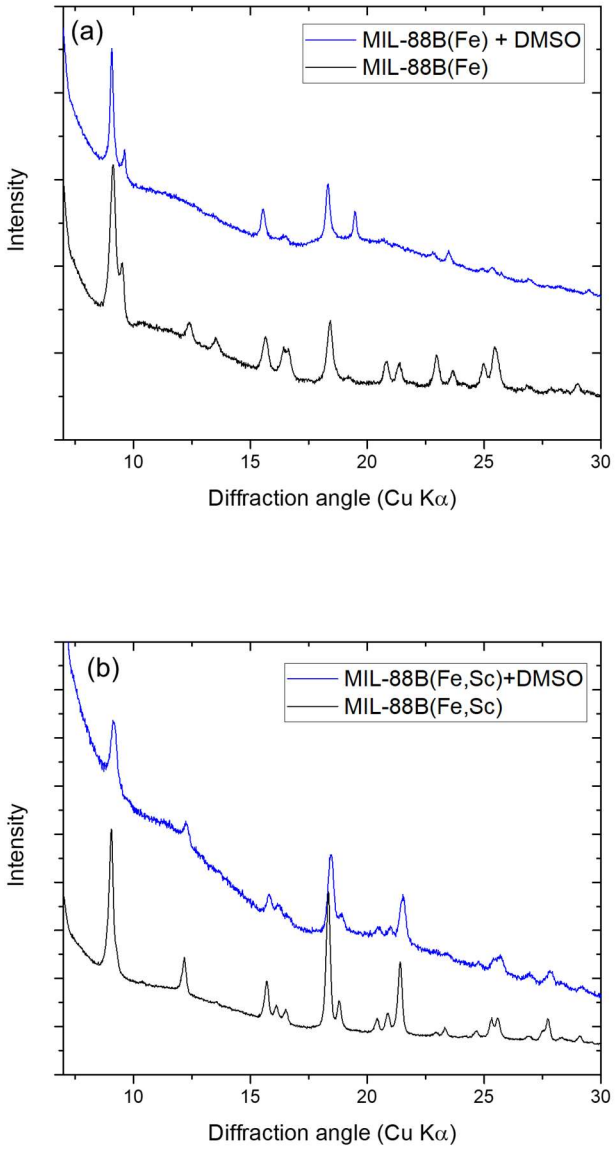

Figure S3. Powder XRD of (**a**) MIL-88B (Fe) and (**b**) MIL-88 (Fe,Sc) on samples immersed in DMSO.

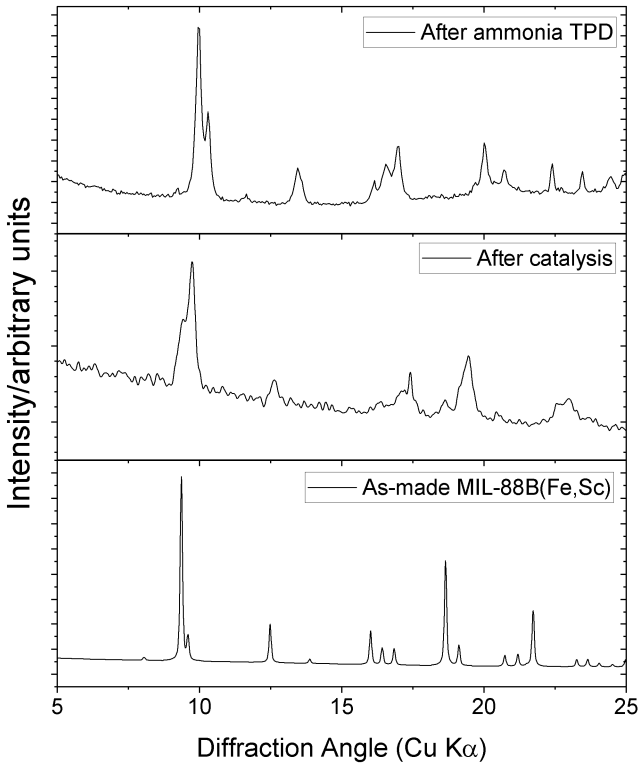

Figure S4. Powder XRD of MIL-88 (Fe,Sc) as-made, after catalysis, and after ammonia TPD. Note the sample after catalysis is contaminated with carbonaceous material (humins) and so the signal:noise ratio in the data is lower than in the other samples.

References

Solid-State Vibrational Spectra and Structures of Terephthalic Acid and the Terephthalate Ion, Tripathi, G. N. R.; Sheng, S.J. *J. Molec. Struct.*, **1979**, *57*, 21−34.