Faraday Discussions

SUPPORTING INFORMATION

Structural and elemental influence of various MOFs on the performance of Fe@C catalysts for Fischer-Tropsch synthesis

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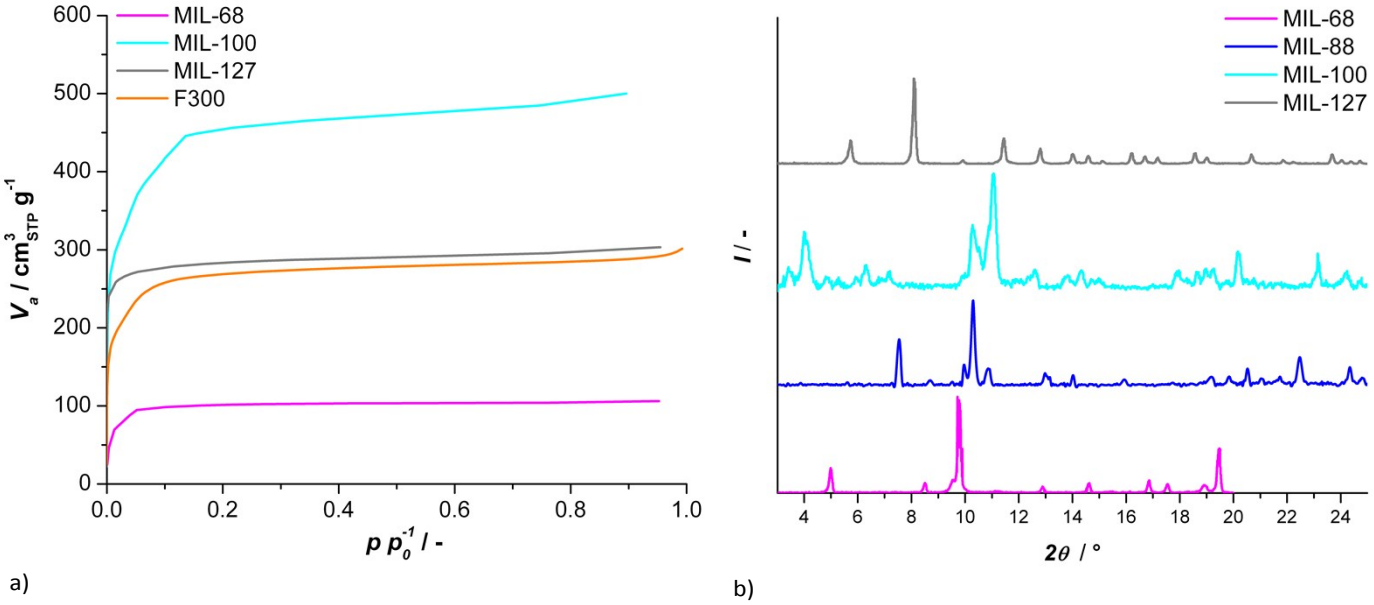
MOF Identification



a) b)

Figure S1. a) N_2 physisorption at 77 K and b) PXRD patterns for the various MOFs. Isotherm shapes and diffraction patterns match with literature[1-12].

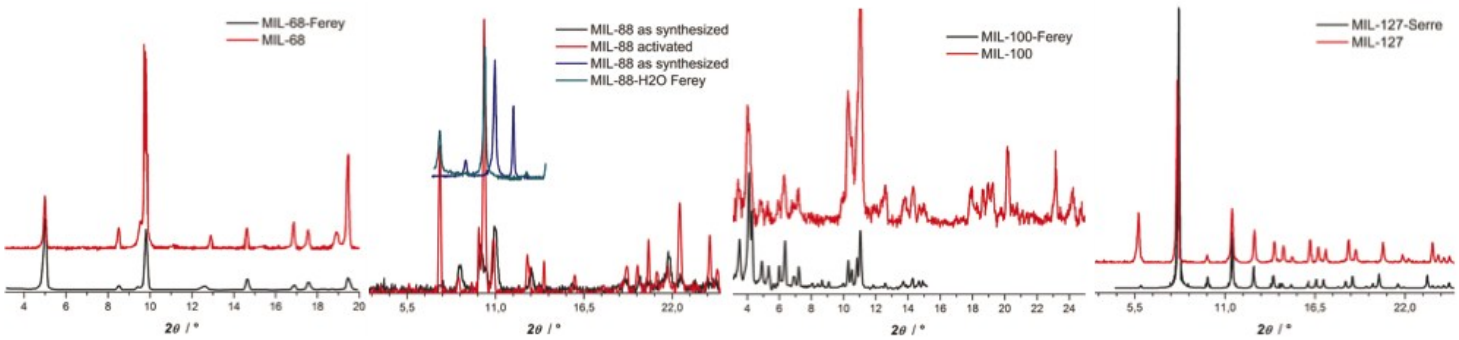


Figure S2. Comparison of the XRD angle and relative intensity for the various MOFs and reported XRD patterns from literature.

Table S1. N_2 physisorption calculations for the various MOFs, comprising BET area (S_{BET}) and total pore volume (V_p). Values agree with reported BET area and pore volume in literature.

MOF	S_{BET} $m^2\ g^{-1}$	V_p $cm^3\ g^{-1}$
MIL-68	400	0.16
MIL-100	1777	0.99
MIL-127	1131	0.47
F300	1021	0.45

Fe@C Characterization

Table S2. Data of N_2 physisorption per gram of catalyst, not taken into account the high Fe_2O_3 loading of the Fe@C materials.

Catalyst	S_{BET} $m^2\ g^{-1}$	S_{Ext} $m^2\ g^{-1}$	V_P $cm^3\ g^{-1}$	V_μ $cm^3\ g^{-1}$
Fe@C-MIL68	314	161	0.28	0.06
Fe@C-MIL88A	224	163	0.16	0.03
Fe@C-MIL100	260	136	0.18	0.06
Fe@C-MIL127	323	172	0.30	0.06
Fe@C-MIL101NH_2	283	120	0.25	0.07
Fe@C-F300	280	140	0.29	0.06

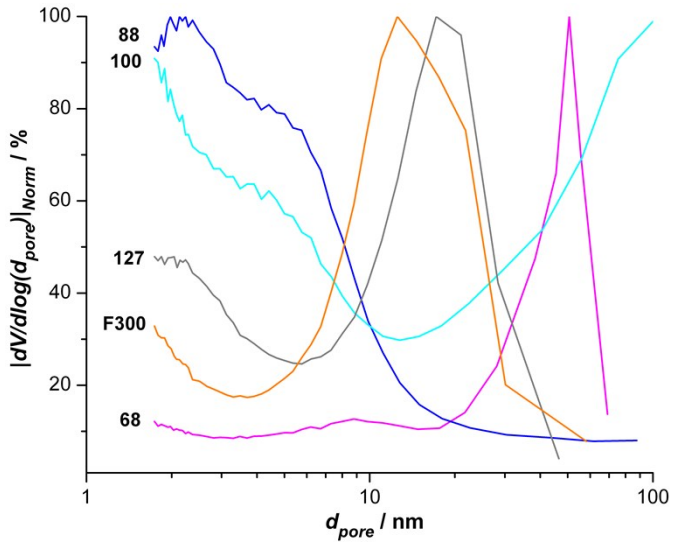


Figure S3. BJH transformation of isotherms displaying the normalized pore size distribution of Fe@C catalysts.

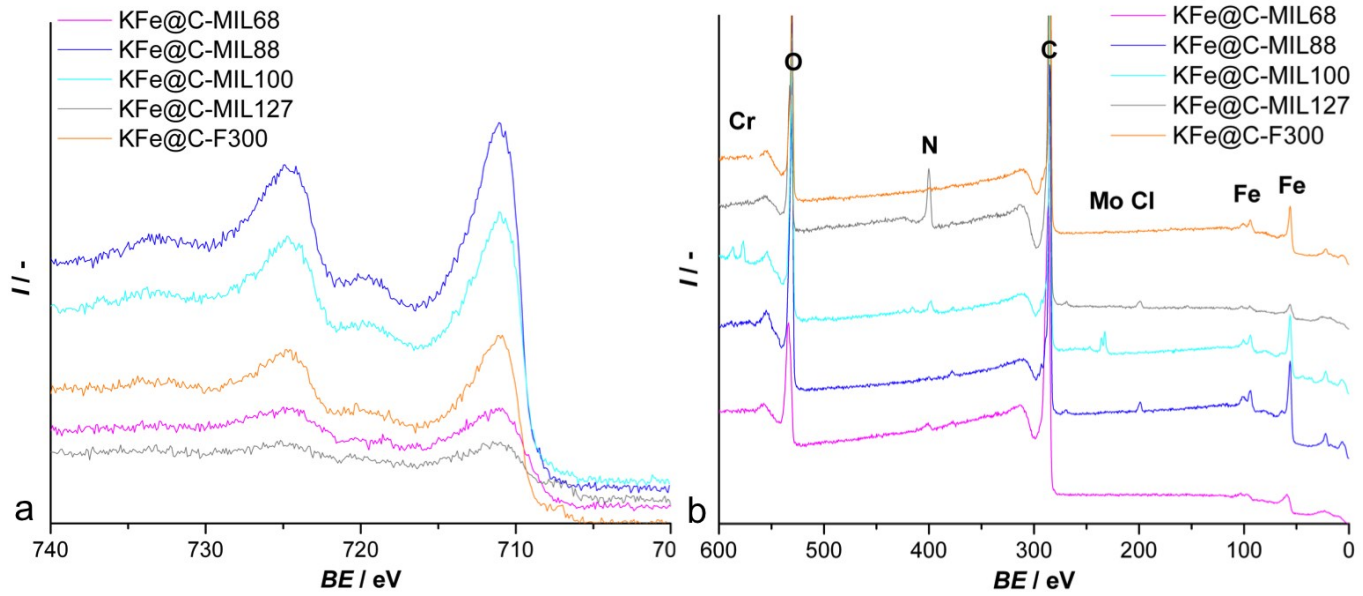
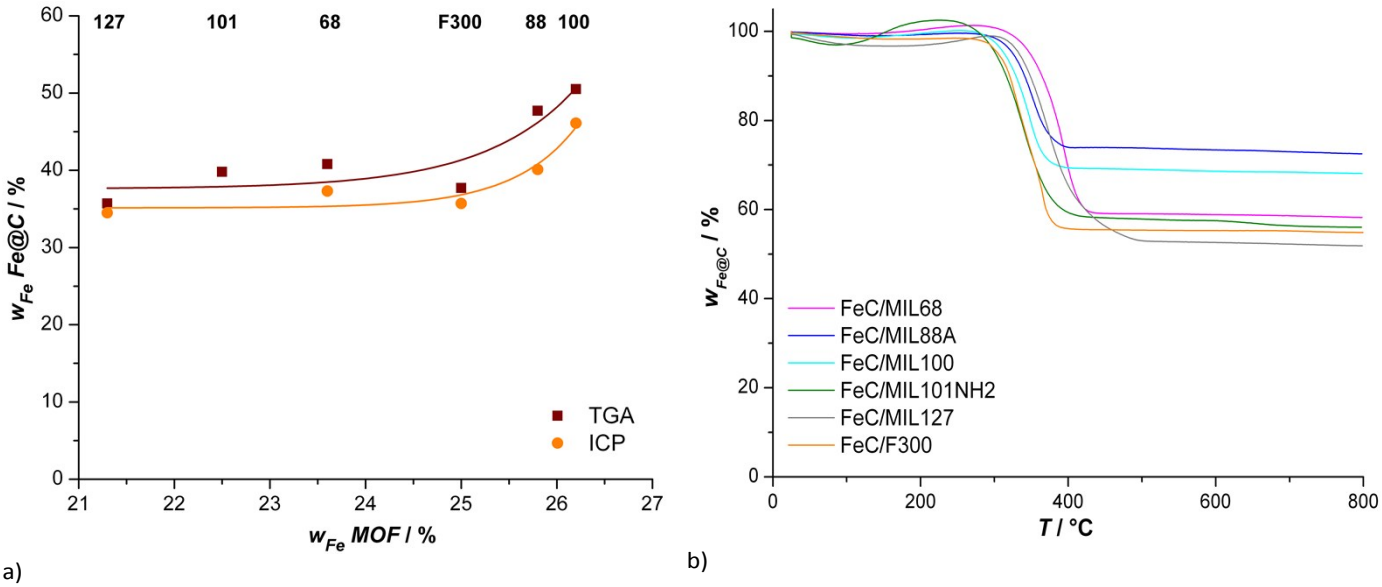


Figure S4. a) Core-level Fe*2p* spectra for passivated catalysts and b) their associating survey spectra displaying surface impurities.



a) b)

Figure S5. a) TGA and ICP analysis showing the non-linear relation between Fe loading in the MOF and in the resulting Fe@C catalyst and b) TGA profiles of Fe@C catalysts in air.

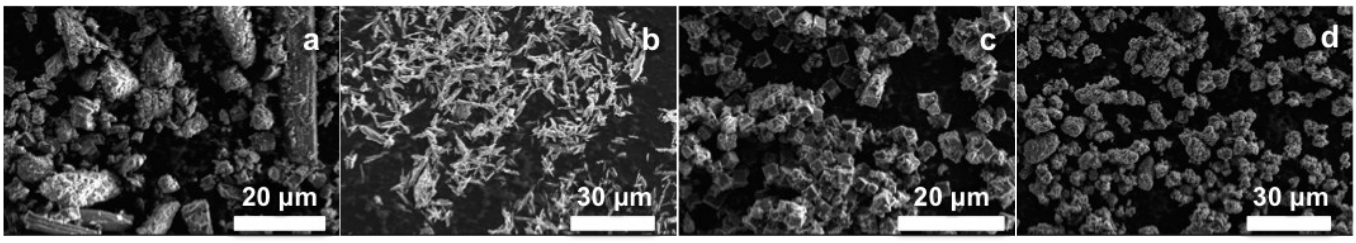


Figure S6. SEM images of pyrolyzed MOFs a) Fe@C-MIL68, b) Fe@C-MIL88, c) Fe@C-MIL127 and d) Fe@C-F300.

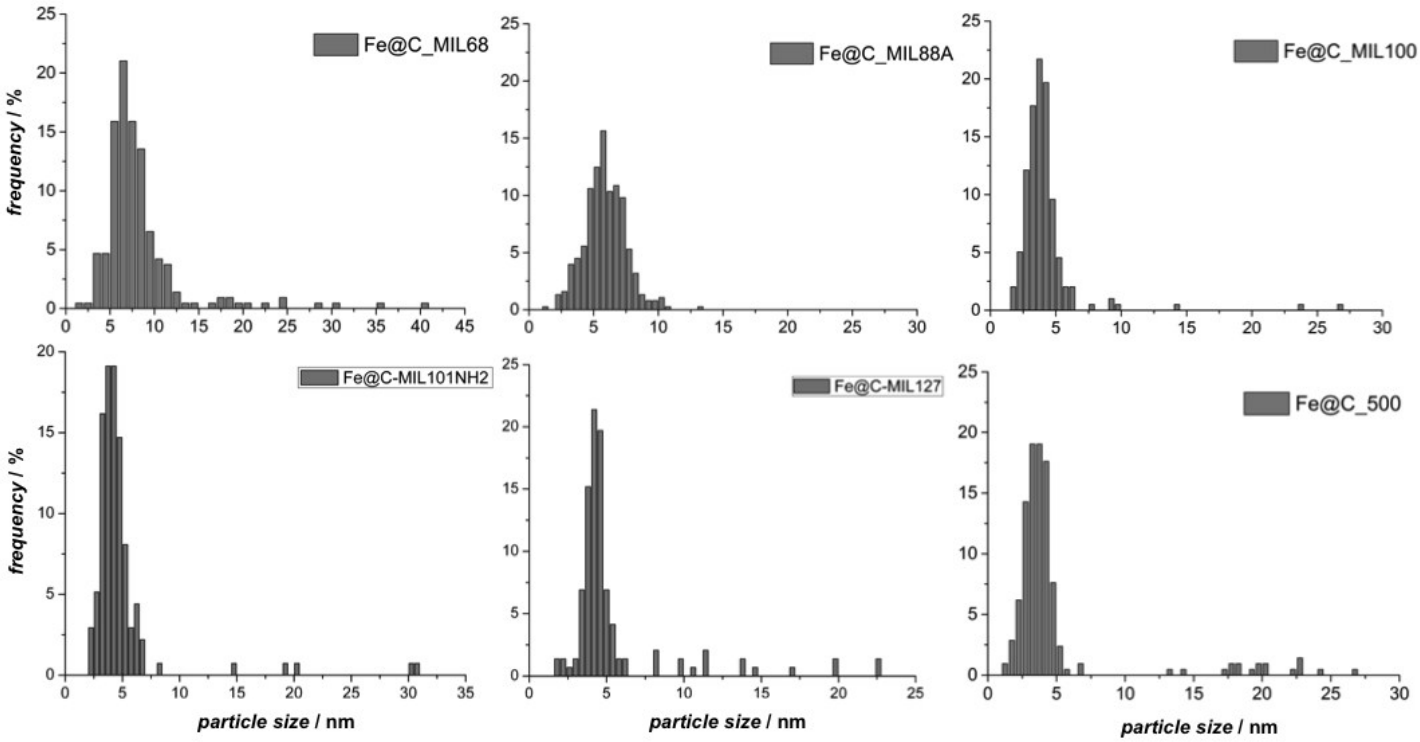


Figure S7. Particle size distribution determined by TEM in the Fe@C catalysts derived from different MOFs by pyrolysis at 500 °C.

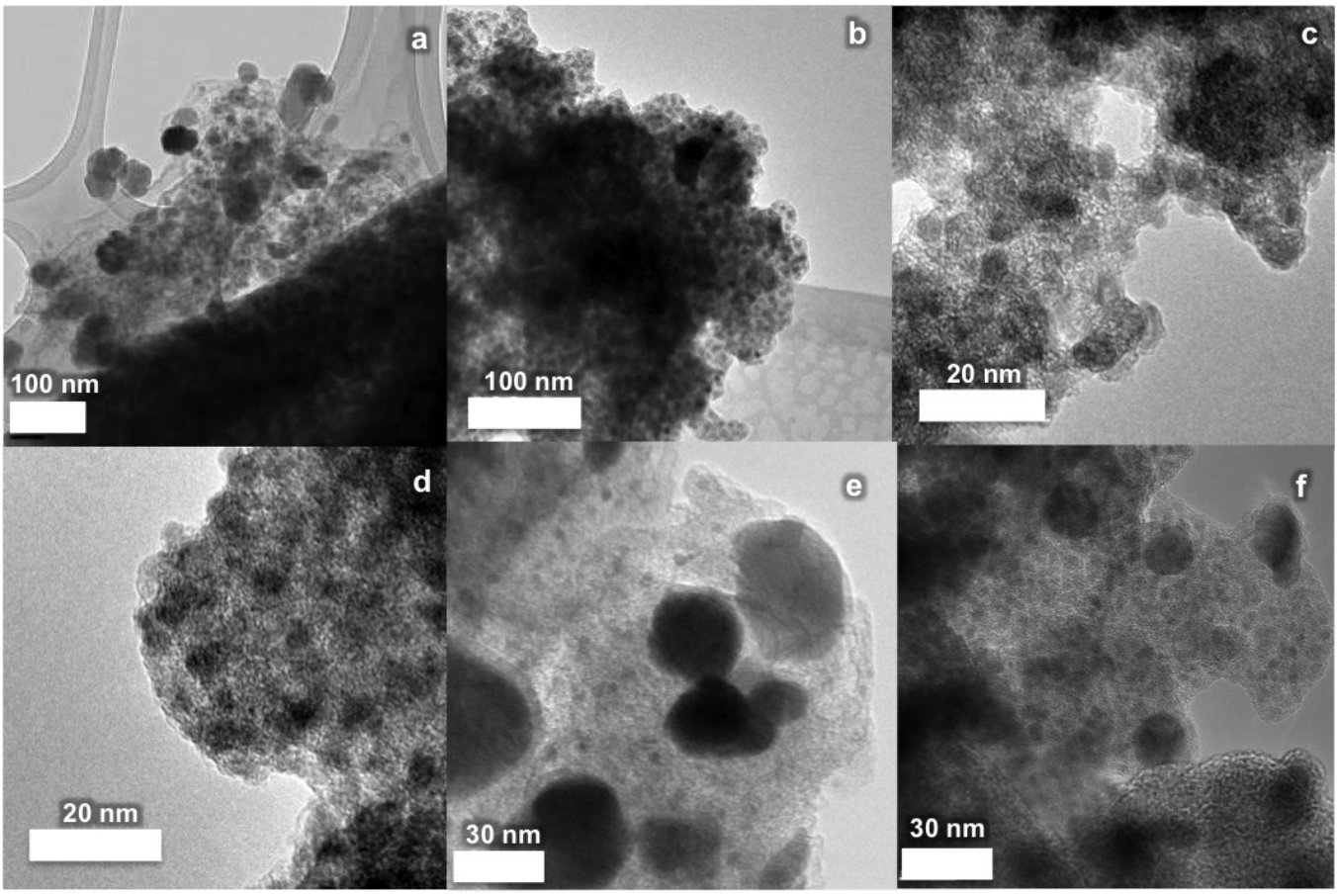
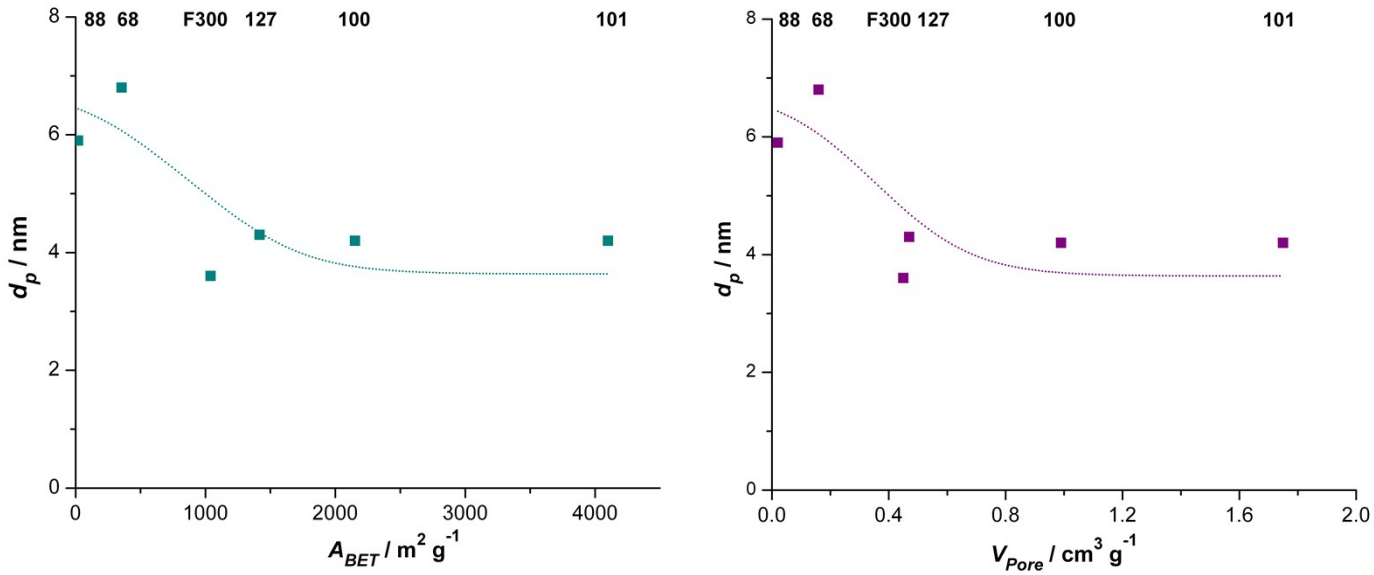


Figure S8. TEM of a) Fe@C-MIL68, b) Fe@C-MIL88, c) Fe@C-MIL100, d) Fe@C-MIL101NH2, e) Fe@C-MIL127 and f) Fe@C-F300



a) b)

Figure S9. Relation between the average Fe particle size and the BET area (a) and pore volume (b) for the Fe@C catalysts derived from the various Fe-MIL-X typologies (X= 88, 68, 127, 100 and 101) and Fe-BTC F300.

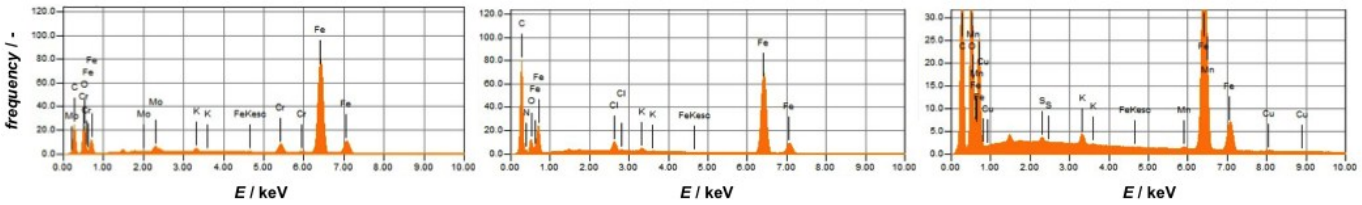


Figure S10. Elemental analysis from EDX spectra for *left*) KFe@C-MIL100, *middle*) KFe@C-MIL127 and *right*) KFe@C-F300 catalysts showing impurities in the bulk phase.

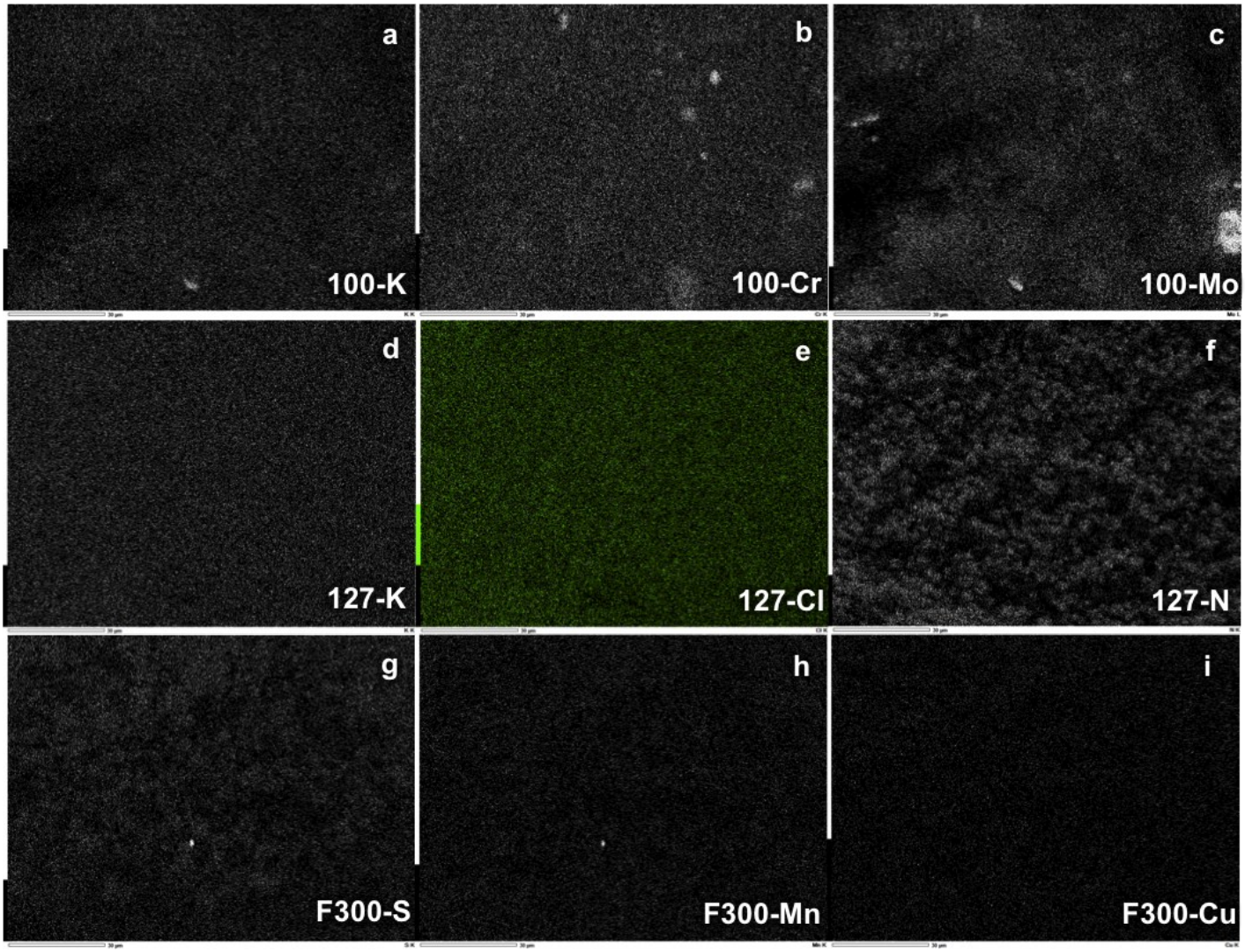


Figure S11. EDX mapping images of selected Fe@C catalysts, clearly showing agglomeration of metal impurities in the Fe@C-MIL100 sample and dispersed elements in Fe@C-MIL127 and Fe@C -F-300.

Notes and references

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