Electronic Supplementary Information (ESI) for:

Formulation and Catalytic Performance of MOF-derived Fe@C/Al composites for High-Temperature Fischer-Tropsch Synthesis

Lide Oar-Arteta, María José Valero-Romero, Tim Wezendonk, Freek Kapteijn and Jorge Gascon

Metal loading in the samples calculated from TGA in air

$$\frac{Fe_2O_3}{Al_2O_3} = \frac{x\ g\ Fe{-}BTC \cdot \frac{0.2\ g\ Fe}{g\ Fe{-}BTC} \cdot \frac{1\ mol\ Fe}{55.845\ g\ Fe} \cdot \frac{1\ mol\ Fe2O3}{2\ mol\ Fe} \cdot \frac{159.7\ g\ Fe2O3}{1 mol\ Fe2O3}}{(1-x) g\ AlOOH \cdot \frac{1\ mol\ AlOOH}{60\ g\ AlOOH} \cdot \frac{1\ mol\ Al2O3}{2\ mol\ AlOOH} \cdot \frac{102\ g\ Al2O3}{1\ mol\ Al2O3}} \quad \text{(S1)}$$

$$W_{Fe\ (Fe-BTC-500C)}[mg] = \frac{x\ mg\ Fe_2O_3}{159.69 \frac{g}{mol}} \cdot \frac{2\ mol\ Fe}{mol\ Fe_2O_3} \cdot \frac{55.845\ g}{mol\ Fe} \quad \text{(S2)}$$

$$W_{Al\ (AlOOH-500C)}[mg] = \frac{x\ mg\ Al_2O_3}{101.96 \frac{g}{mol}} \cdot \frac{2\ mol\ Al}{mol\ Al_2O_3} \cdot \frac{26.98\ g}{mol\ Al} \quad \text{(S3)}$$

Table S1. Fe loading in the different catalysts

Fe-BTC/AlOOH mass ratio	Initial wt% Fe	Catalyst wt.% Fe	Sample Designation	Increase in Fe content after pyrolysis, %
100/0	22	38	38Fe@C	42
90/10	21	33	33Fe@C/Al	36
70/30	17	25	25Fe@C/Al	32
50/50	10	15	15Fe@C/Al	33

Table S2. Fe/Fe_3O_4 ratios calculated according to the Rietveld method and crystallite sizes of Al_2O_3, Fe_3O_4, and Fe according to the Scherrer equation for the pure 38Fe@C and the composites.

Material	Fe/Fe_3O_4	Particle size /nm		
		Al_2O_3	Fe_3O_4	Fe
38Fe@C	0.07	n.a.	5.6	3.8
33Fe@C/Al	0.26	n.d.	5.2	11
25Fe@C/Al	2.63	5.4	7	26
15Fe@C/Al	5.93	4.9	6.5	36
Al_2O_3	n.a.	5	n.a.	n.a.

n.d.: not detected
n.a.: not applicable

Table S3. Textural properties of the fresh catalysts (1st row) after the initial mechanical test (2nd row) and after HT-FTS experiments (3rd row).

Samples		S_{BET} (cm^2/g)	V_{meso} (cm^3/g)	V_{Total} (cm^3/g)
38Fe@C	Fresh	274	0.24	0.33
	FT-PT	277	0.14	0.24
	HT-FTS (3 h)	57	0.065	0.073
15Fe@C/Al	Fresh	160	0.27	0.28
	FT-PT	132	0.24	0.24
	HT-FTS (50 h)	112	0.23	0.23

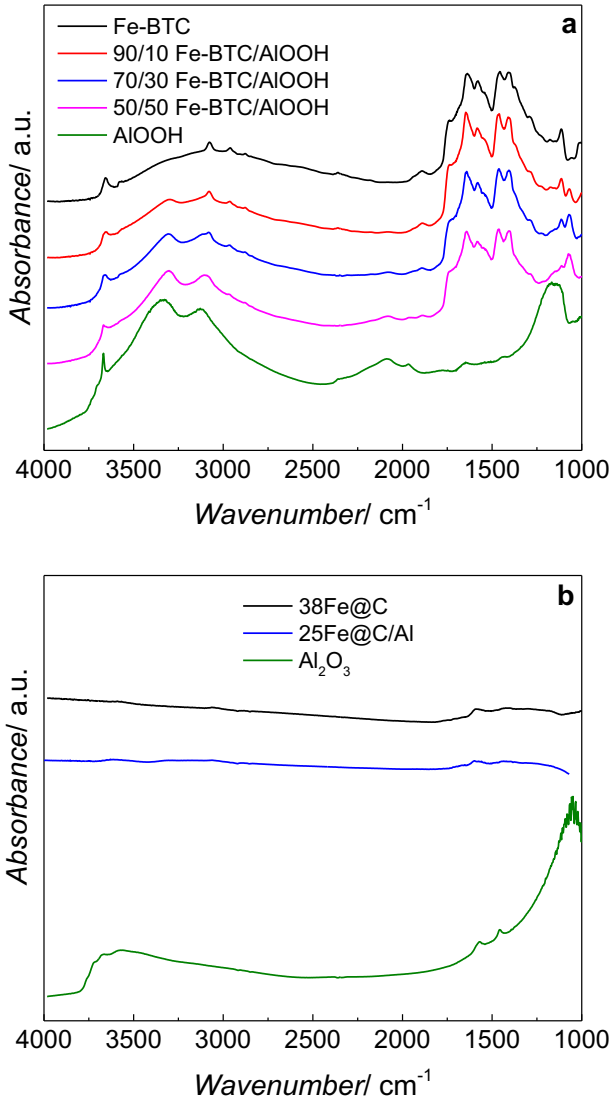

Figure S1. DRIFT spectra of all materials before (a) and after (b) pyrolysis at 500 °C

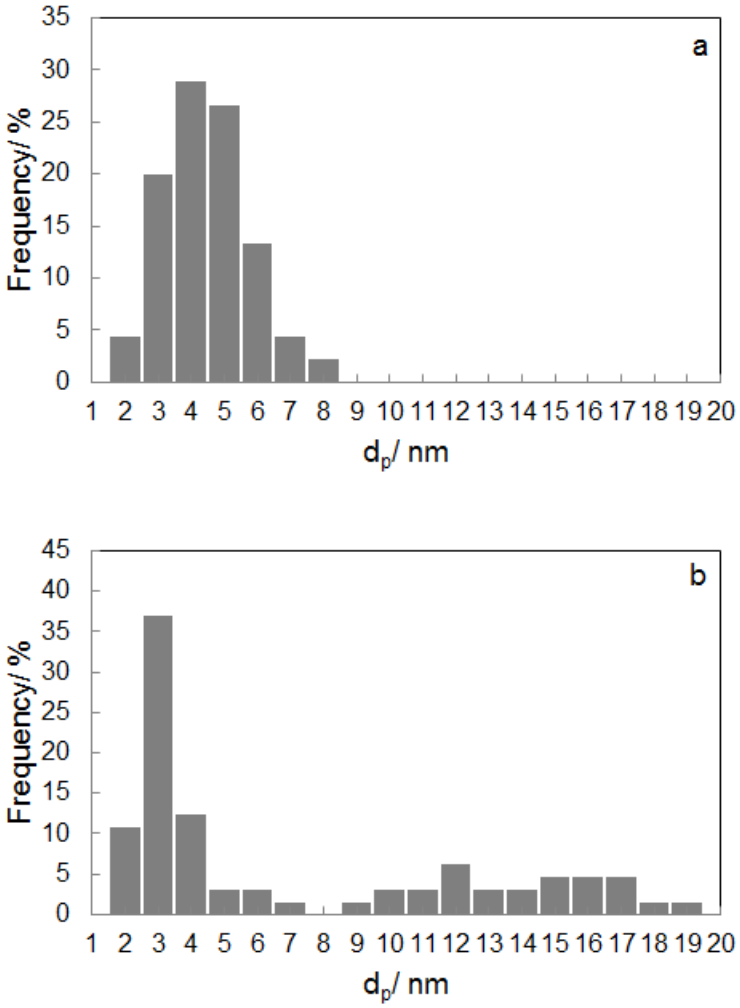

Figure S2. Particle size distribution (PSD) determined by TEM analysis of (a) 38Fe@C and (b) 33Fe@C/Al.

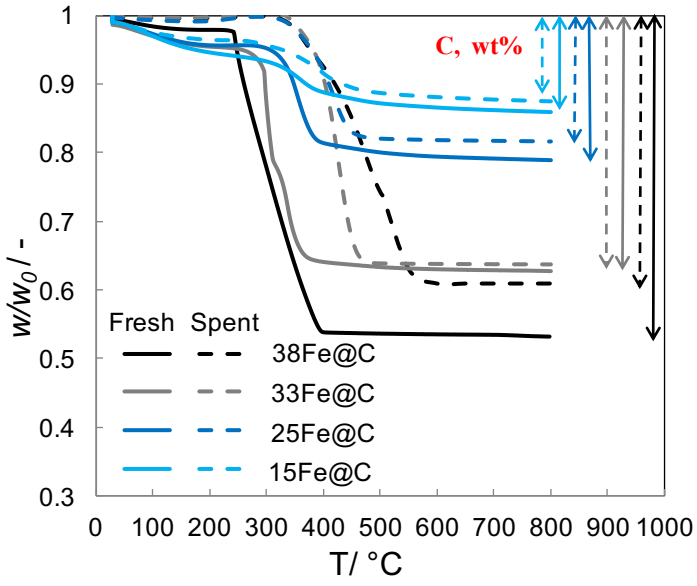

Figure S3. TGA for the fresh and the spent catalysts after testing them in HTFTS at 340 °C, 15 bar and $H_2/CO = 1$, *GHSV* = 55 $mmol_{CO,STP}\ g_{Fe}^{-1} min^{-1}$.

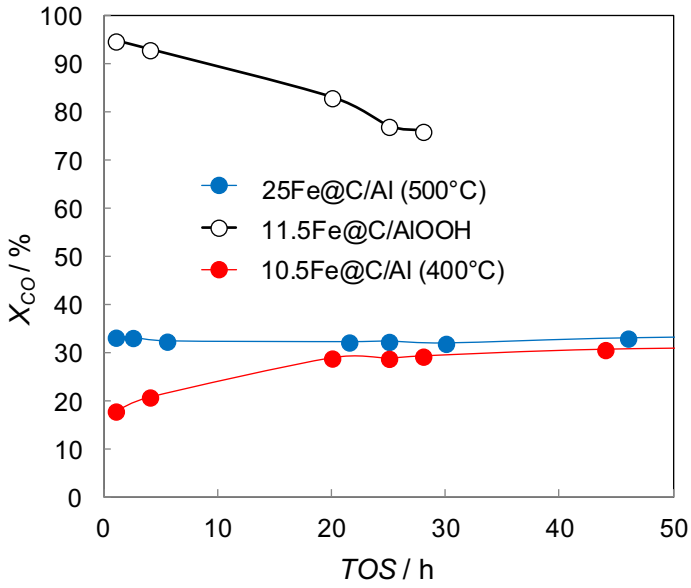

Figure S4. Time-on-stream (*TOS*) evolution of X_{CO} for the 25Fe@C/Al, 11.5Fe@C/Al and 10.5Fe@C/Al composites. HT-FTS conditions are 340 °C, 15 bar, $H_2/CO = 1$, *GHSV* = 55 $mmol_{CO,STP}\ g_{Fe}^{-1} min^{-1}$.