Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for:

Computational exploration of Fe55@C240-catalyzed Fischer-Tropsch synthesis.

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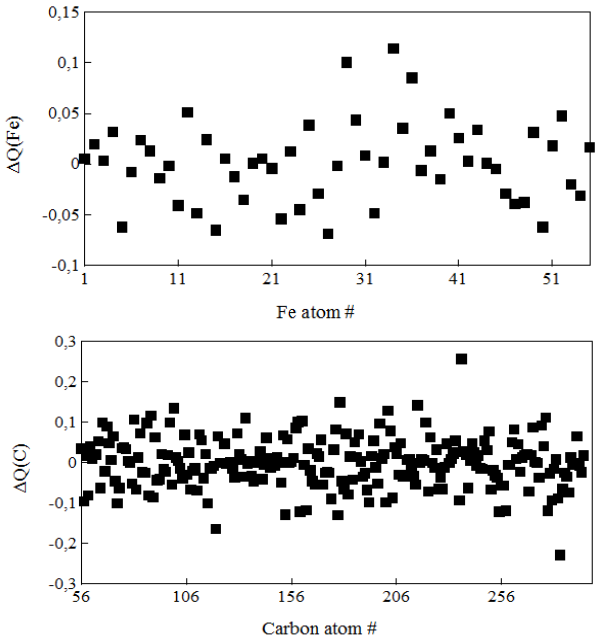

Figure S1 Charge differences in Fe and C upon CO binding on Fe55@C240. $\Delta Q = q(CO_{ads}\text{-Fe55@C240}) - q(\text{Fe55@C240})$.

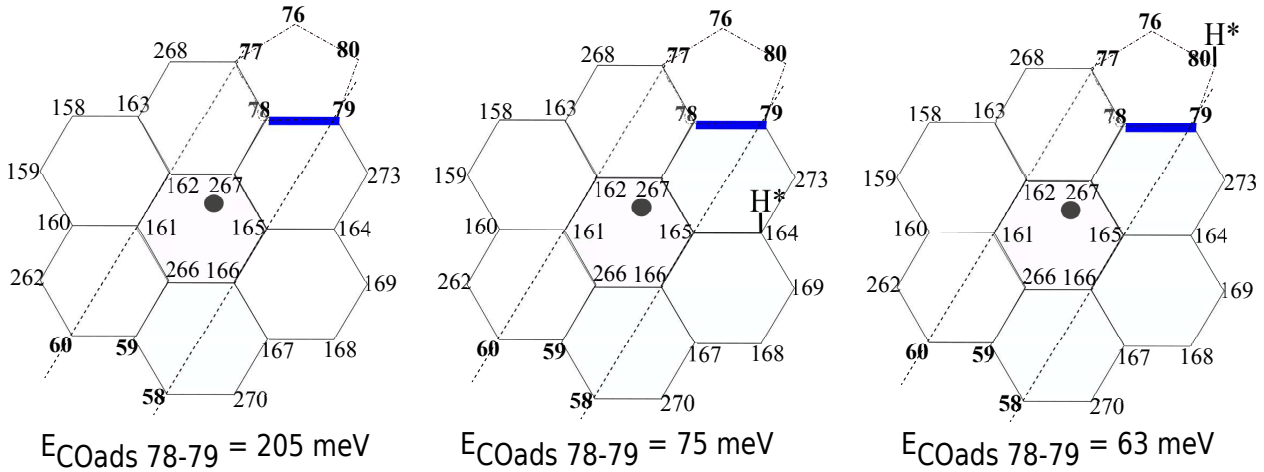

Figure S2 H-assisted CO adsorption. CO adsorption energy at the bridge C78-79 ($E_{COads78-79}$) and its enhancement in the presence of H* at positions C164 and C80.

Fe_{corner} in Fe55@C240 (12 Fe)			
$Fe_{\#}$ / Pointing to 2/3 5MR wheels	Bond to $C_{\#}$	BO > 0.1 (Sum of BO per Fe)	$\Delta E_{CO}{}^{*}$ (meV)
Fe1/2-5MR	222/226/293	0.1643/0.1271/0.2057 (0.5)	
Fe2/3-5MR	116/117/118/119	0.1226/0.2226/0.2433/0.1517 (0.74)	
Fe3/2-5MR	177/178/235/279	0.1024/0.2264/0.2090/0.2248 (0.76)	
Fe4/3-5MR	152/153/154/155/**156/157**	0.1601/0.2187/0.2034/0.1384/0.1014/0.1094 (0.93)	95
Fe5/2-5MR	126/129/243	0.1952/0.2217/0.2237 (0.64)	
Fe6/3-5MR	**212/213**/214/215/216/217	0.1332/0.1097/0.1320/0.1836/0.2234/0.1960 (0.98)	256
Fe7/3-5MR	182/183/184/185/186/187	0.2364/0.1679/0.1169/0.1225/0.1811/0.2431 (1.07)	
Fe8/3-5MR	**134/135**/136/137/138/139	0.1850/0.1774/0.2110/0.2385/0.2383/0.2205 (1.27)	128
Fe9/3-5MR	**170/171**/172/173/174/175	0.1093/0.1152/0.1801/0.2407/0.2260/0.1579 (1.03)	118
Fe10/2-5MR	162/165/267	0.1874/0.1953/0.2165 (0.6)	
Fe11/2-5MR	**200**/205/207/208/**287**	0.2520/0.1254/0.2404/0.1203/0.2373 (0.97)	329
Fe12/2-5MR	193/196/282	0.1572/0.1962/0.2101 (0.56)	

Table S1 DDEC6 bond orders (BOs) calculated from the method of Manz et al. [1] and reported for the corner irons (Fe_{corner}).In the first column is indicated the corner iron numbers and if the Fe_{corner} is pointing to a 6MR wheel surrounding by two or three 5MR in reference of Figure 8 of the manuscript. In the last column, CO adsorption energies ΔE_{CO} in the most favorable bridge sites were added. The carbons $C_{\#}$ involved in the bridge sites are highlighted in bold in column 2. Most Fe_{corner} pointing to 3-5MR wheels have a sum of BOs (SBOs) of ~ 1

Other irons in Fe55@C240		
$Fe_{\#}$	Bond to $C_{\#}$	BO $>$ 0.1 (Sum of BOs)
$Fe_{3rdshell,Facet}$ (30 Fe)		
Fe13	-	-
Fe14	227	0.1035
Fe15	220	0.1424
Fe16	-	-
Fe17	233/234	0.1255/0.1188 (0.24)
Fe18	-	-
Fe19	-	-
Fe20	-	-
Fe21	-	-
Fe22	131	0.1882
Fe23	176	0.1507
Fe24	158/179	0.1101/0.1112 (0.22)
Fe25	-	-
Fe26	142	0.1027
Fe27	133/126/211/248	0.1118/0.1529/0.1241/0.1014 (0.49)
Fe28	-	-
Fe29	-	-
Fe30	-	-
Fe31	-	-
Fe32	-	-
Fe33	201	0.1164
Fe34	-	-
Fe35	167	0.1463
Fe36	-	-
Fe37	-	-
Fe38	204/274	0.1342/0.1006 (0.23)
Fe39	-	-
Fe40	-	-
Fe41	194	0.1572
Fe42	-	-
$Fe_{central}$ (1 Fe)		
Fe43	-	-
$Fe_{2nd,Layer}$ (12 Fe)		
Fe44 to Fe55	-	-

Table S2 DDEC6 bond orders (BOs) calculated from the method of Manz et al. [1] and reported for the other iron layers of Fe55@C240, i.e. $Fe_{3rdshell,facet}$, $Fe_{central}$ and $Fe_{2nd\ Layer}$

Atom & Atom number	BO
C_{156}	0.983
C_{157}	0.989
O_{297}	1.818

Table S3 DDEC6 bond orders calculated from the method of Manz et al. [1] for CO bound to Fe55@C240. The most favorable adsorption site ($Bh_{156,157}$, see Table 1, Manuscript) was taken as an example for the BO calculations.

Atom & Atom number	BO
C_{137}	0.8937
C_{138}	0.8899
O_{297}	1.9854

Table S4 DDEC6 bond orders calculated from the method of Manz et al. [1] for CO bound to Fe55@C240 in a less favorable adsorption site ($Bh_{137,138}$, see Table 1, Manuscript)

References

1 Manz, T. A. *RSC Advances* 2017, **72**, 45552-45581.