ADVANCED MATERIALS

Supporting Information

for

Advanced Materials, adma.200602645

Supplementary Section

Table S1 : Crystal data for **MIL-53LP**.

Formula	***[Cr^{III}(OH)(OOC-C_6H_4-COO)].(CO_2)$_x$ (x~0.54)***
Chemical formula	$Cr_4O_{24.32}C_{34.16}H_{20}$
Molar weight (g.mol^{-1})	1020.3
Calculated density (g.cm^{-3})	1.57
Crystal system	Monoclinic
Space group	*C 2/c* (n°15)
a (Å)	19.713(1)
b (Å)	8.310(1)
c (Å)	6.806(1)
β (°)	105.85(1)
V (Å^3)	1072.48(2)
Z	1
Figures of merit	M_{19}/F_{19}=11/40
Radiation λ (Å)	0.71118
Temperature (K)	195
2θ range (°)	2-26.7
N. reflections	157
N. independent atoms	10
N. intensity parameters	26
N. profile parameters	9
N. soft distance constraints	24
R_P	4.5
R_F	12.1
Isotropic thermal factor	1.2(1)
Profile function	Pearson VII
Background	Experimental (36 points)
N. of asymmetry parameters	2

Table S2 : atomic positions of MIL-53LP at 195 K under 1 bar of CO_2:

(S.G. *C* 1 2/c 1 (no. 15), *a* = 19.716(1) Å, *b* = 8.310(1) Å, *c* = 6.805(1) Å, β = 105.85(1) °, V=1072.6(2) Å^3)

Atom	**Wyckoff**	**Site Occupation**	**x**	**y**	**z**
Cr	4*a*		0	0	0
O(1)	4*e*		0	-0.106(2)	3/4
O(2)	8*f*		0.0645(6)	0.165(1)	0.944(2)
O(3)	8*f*		0.0857(9)	0.120(1)	0.652(2)
C(1)	8*f*		0.1055(5)	0.169(3)	0.838(2)
C(2)	8*f*		0.2016(6)	-0.259(3)	0.621(2)
C(3)	8*f*		0.2756(6)	-0.295(2)	0.707(2)
C(4)	8*f*		0.179(1)	-0.219(2)	0.419(2)
C	4*e*	0.54(1)	0	0.557(6)	3/4
O	8*f*	0.54(1)	0.0469(7)	-0.442(3)	0.920(2)

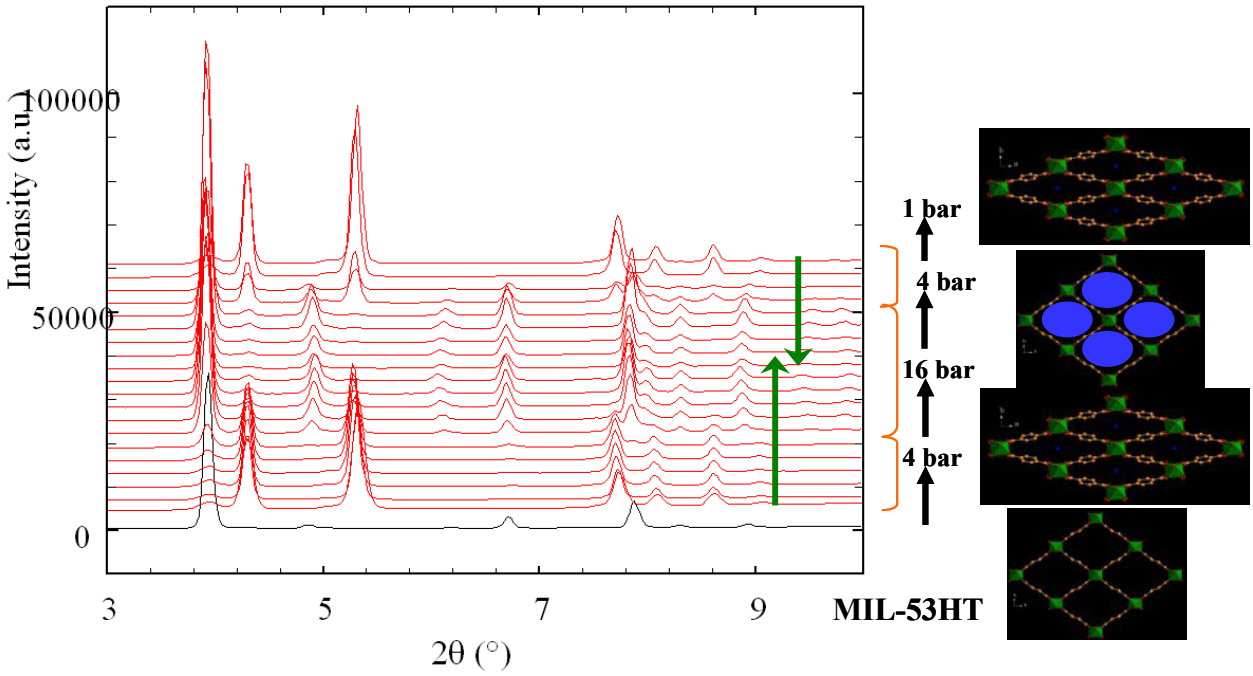

Figure S1: left : XRPD patterns of MIL-53(Cr) under CO_2 pressure at 298 K; (λ=0.71118 Å). A pattern of the outgassed sample, prior to the introduction of CO_2, is shown in black. Right: schematic view of the various structures of MIL-53 as a function of the pressure.

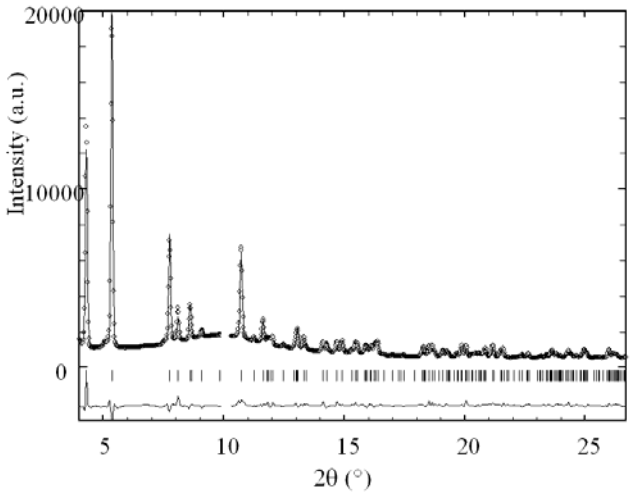

Figure S2: Rietveld fit for MIL-53LP measured at 195 K under1 bar of CO_2, λ=0.71118 Å.

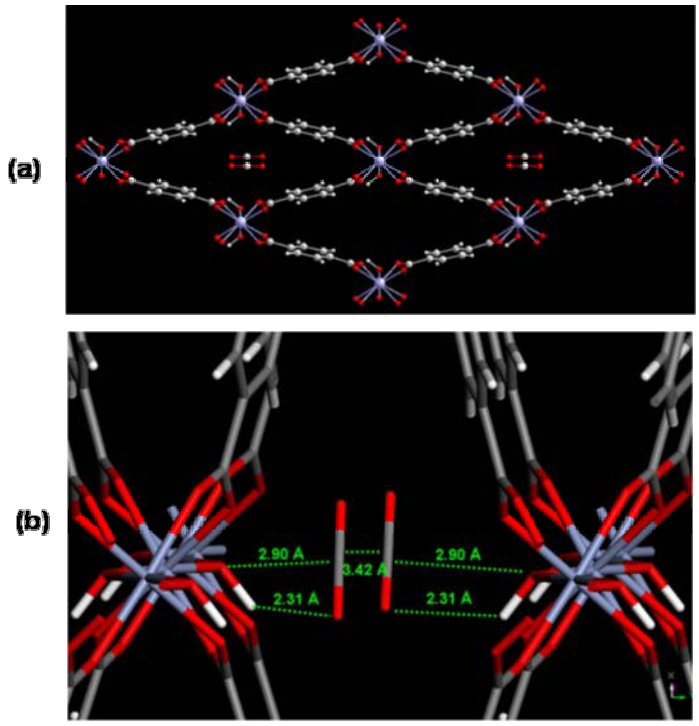

Figure S3: Top: view of the DFT optimised MIL-53LP structure along the c axis; bottom : view of the •straight-on and direct interactions between CO_2 and the hydroxyl group in the DFT optimised MIL-53LP solid (red circles: oxygen, gray circles: carbon, white circle : hydrogen, blue circle : chromium).

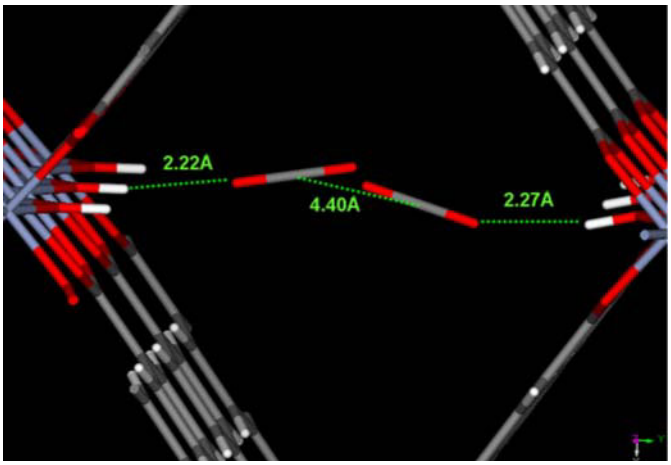

Figure S4: view of the •straight-on and direct interactions between CO_2 and the hydroxyl group in the DFT optimised MIL-53HP solid (red circles: oxygen, gray circles: carbon, white circle : hydrogen, blue circle : chromium)

figS5.pps

Figure S5: "movie" of the variation of the MIL53 structure (bands at 1017 and 1022 cm^{-1}) and of the ν_2 CO_2 absorption band during a cycle of CO_2 adsorption-desorption. 45 spectra recorded in the 0-10 bars pressure range are presented.