The influence of particle size of amino-functionalized MCM-41 silicas on CO₂ adsorption

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Supporting Information



Figure S.I.1. XRD patterns between 2 and 7 °2θ of MCM-41 micro (a), MCM-41 nano (b), P_MCM-41 micro (a') and P_MCM-41 nano (b').



Figure S.I.2. TGA curves of MCM-41 micro (a), MCM-41 nano (b). The measurements were done under Argon flow (20 ml/min) from 20 to 1100°C (1°C min⁻¹ heating rate).



Figure S.I.3. FTIR spectra of CO₂ adsorbed (Pmax = 60 mbar) at 35°C on P_MCM-41 micro (a-a^{IV}) and P_MCM-41 nano (b- b^{IV}). The arrows indicate decreasing CO₂ pressure until vacuum. Spectra are reported after subtraction of the spectrum recorded before CO₂ interaction, used as a background.



Figure S.I.4. Heat Flow from DSC-TGA Analysis for MCM-41 micro (Frame A) and MCM-41 nano (Frame B) samples.



Figure S.I.5. TPD curves for P_MCM-41 micro and P_MCM-41 nano sample at 2 ml/min flow rates. CO₂ partial pressure: 0.1 bar.

Integrating the area under the TPD curves, the value of irreversible chemisorbed fraction can be achieved. The obtained values of irreversible fractions respectively for P_MCM-41 micro and P_MCM-41 nano samples are 0.16 and 0.06 mmol·g⁻¹.

Sample	TPD	TGA	Volumetry	
	irreversible fraction	irreversible fraction	irreversible fraction	
	[mmol/g]	[mmol/g]	[mmol/g]	
P_MCM-41 micro	0.16	0.16	0.16	
P_MCM-41 nano	0.06	0.07	0.10	

Table 1. Irreversible fractions obtained with TPD, TGA and Volumetric Analysis for the grafted MCM-41 materials.

Sample / Temperature	CO ₂ Adsorption	reversible fraction	irreversible fraction
	Capacity [mmol/g]	[%]	[%]
P_MCM-41 micro / 20°C	0.63	64.9	35.1
P_MCM-41 micro / 35°C	0.60	72.8	27.2
P_MCM-41 micro / 50°C	0.58	78.6	21.4
P_MCM-41 micro / 70°C	0.55	86.6	13.4
P_MCM-41 micro / 90°C	0.49	93.3	6.7
P_MCM-41 nano / 20°C	0.96	87.4	12.6
P_MCM-41 nano / 35°C	0.79	90.7	9.3
P_MCM-41 nano / 50°C	0.60	95.4	4.6
P_MCM-41 nano / 70°C	0.38	96.0	4.0
P_MCM-41 nano / 90°C	0.21	99.1	0.9

Table 2. CO ₂ Adsorption Capacity,	reversible and irreversible	fractions obtained	with TGA analysi	S
for the grafted MCM-41 materials.				