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

Adsorption of CO_2 and CH_4 on amine-functionalised MCM-41: experimental and theoretical studies

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Supplementary data

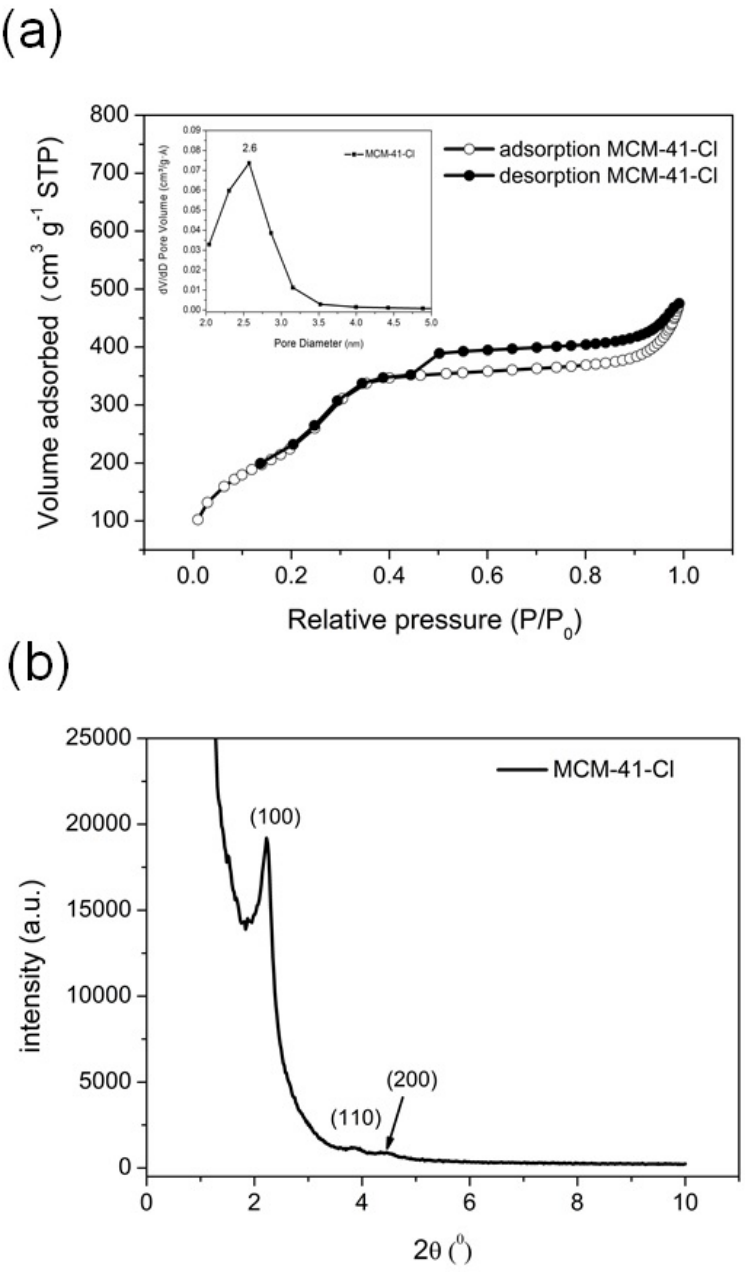


Fig. S1: (a) N_2 adsorption/desorption isotherms of MCM-41-Cl and BJH pore distribution (inset) obtained from the adsorption branch of the isotherm. (b) Powder X-ray diffraction pattern for MCM-41-Cl.

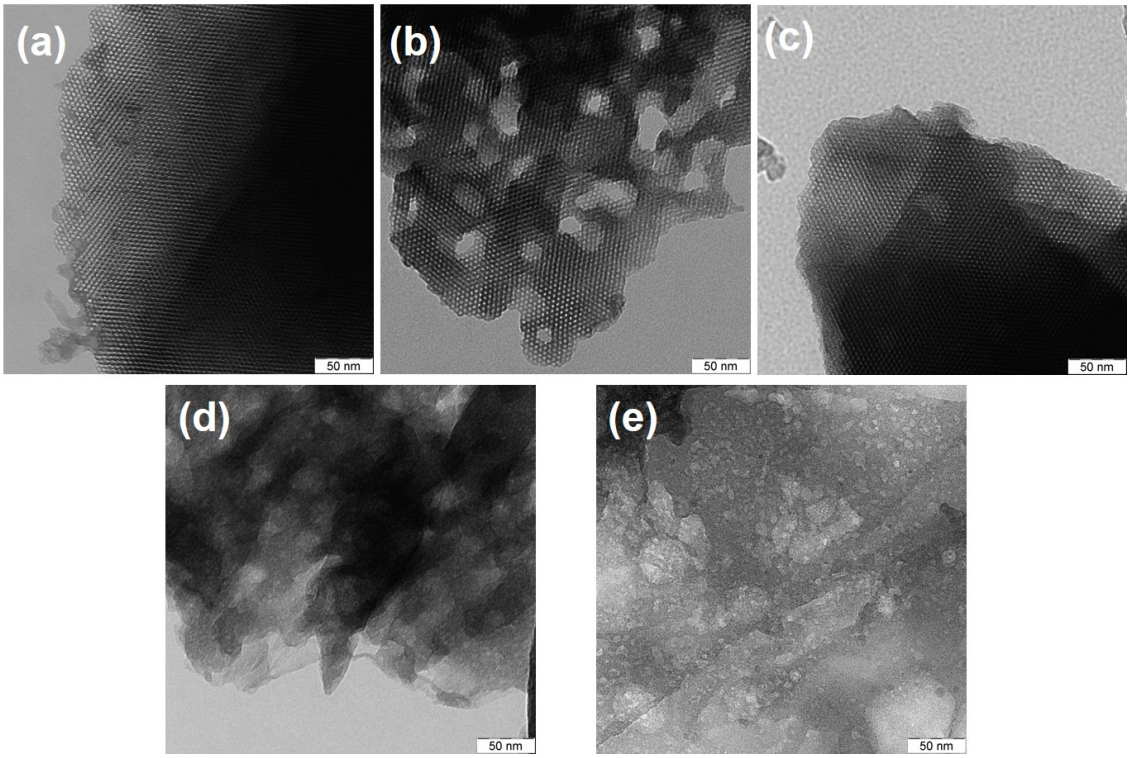
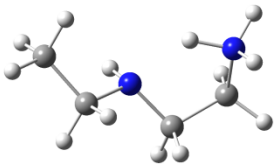
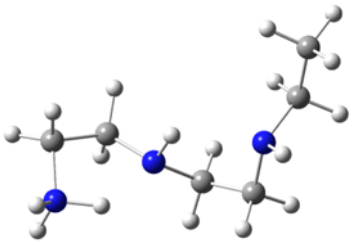


Fig. S2: Transmission electron microscopies of (a) MCM-41, (b) **MCM-41N2**, (c) **MCM-41-N3**, (d) **MCM-41-methylaminopyridine** and (e) **MCM-41-guanidine.**

Table S1. wB97x-D/6-311++G(d,p) relative energies of the protonated amines. Relative energy is the electronic energy at 0 K (without correction for zero-point vibrational energy). Relative Gibbs free energy includes thermal correction to 298 K

	Relative energy (kJ mol^{-1})	**Relative Gibbs free energy at 298 K (kJ mol^{-1})**
Protonated N^1-ethylethane-1,2-diamine		
	0.0	0.0
	-30.0	-26.7
Protonated N^1-(2-aminoethyl)-N^2-ethylethane-1,2-diamine		
	0.0	0.0

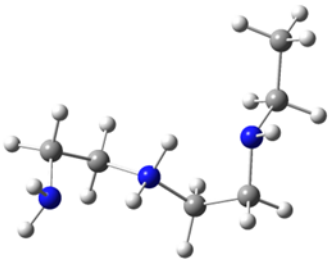
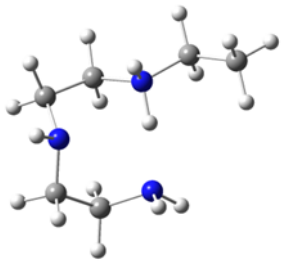
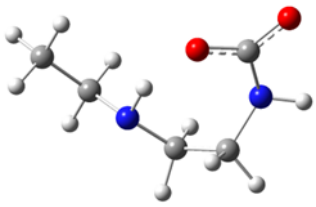
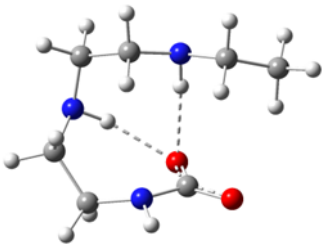
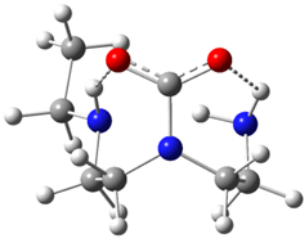
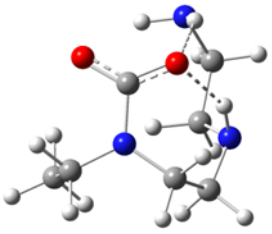
	-46.2	-43.2
	-61.8	-53.0

Table S2. wB97x-D/6-311++G(d,p) relative energies of the protonated amines. Relative energy is the electronic energy at 0 K (without correction for zero-point vibrational energy). Relative Gibbs free energy includes thermal correction to 298 K

	Relative energy (kJ mol^{-1})	**Relative Gibbs free energy at 298 K (kJ mol^{-1})**
Carbamates from N^1-ethylethane-1,2-diamine		
	0.0	0.0
	-2.2	-1.8

Carbamates from N^1-(2-aminoethyl)-N^2-ethylethane-1,2-diamine

	0.0	0.0
	7.0	4.1
	5.7	3.6