

Electronic Supplementary Information (ESI)

Soft-Pillared@Magadiite: Influence of the interlayer space and amine type on CO₂ adsorption

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Determination of the nitrogen concentration of 3N@MAG and Gy@3N@MAG

$$X \left(\frac{C}{N} \right)_{CTA} + Y \left(\frac{C}{N} \right)_{amine} = \left(\frac{C}{N} \right)_{CHN}$$

$$X + Y = 1$$

wherein (C/N)_{CTA} is 19 (CTA⁺ ions), (C/N)_{amine} is the carbon/nitrogen ratio, to 3N@MAG is in the range of 2.3-3.0, to Gy@3N@MAG 4.3-5.7 and can be determined from ²⁹Si NMR results calculating the percentage of the T^m (m: 1,2 or 3) sites, (C/N)_{CHN} is the ration obtained by CHN results. The concentration of N from 3N@MAG and Gy@3N@MAG can be calculated as follow:

$$N_{CTA} = X \cdot N_{total}$$

$$N_{amine} = Y \cdot N_{total}$$

wherein X is the percentage of N from CTA⁺ ions and Y is the percentage of N from organosilanes.

Table S1. Carbon, hydrogen and nitrogen (CHN) elemental analysis for the synthesized materials.

Materials	C / %	N / %	N _{total} / mmol g ⁻¹	N _{CTA} / mmol g ⁻¹	N _{silane} / mmol g ⁻¹	Pending ^a / mmol g ⁻¹
CTA-MAG	34.5	2.1	1.5	1.5	-	-
Gy@MAG	10.8	0.1	0.0	0.0	-	1.3
3N@MAG	11.3	4.1	2.9	0.2	2.7	0.9
Gy@3N@MAG	15.9	3.6	2.6	0.2	2.4	0.8

^a Obtained by dividing the total carbon of the organosilane (C_{silane}) and a factor which was determined by the integration of T¹⁻³ sites peaks area from ²⁹Si HPDEC-MAS NMR spectra. This factor is in the range of 6-8, 7-9 and 13-17 for Gy@MAG, 3N@AG and Gy@3N@MAG, respectively.

Table S2. Pseudo-second order modelling parameters fitted to 3N@MAG and Gy@3N@MAG, at different adsorption temperature.

Adsorbent	q _e / mmol g ⁻¹	k ₂ / g mmol ⁻¹ min ⁻¹	RSS / %	R ²
3N@MAG 25 °C	0.0982	1.6306	0.2773	0.9972
3N@MAG 50 °C	0.2310	0.1975	1.2204	0.9878
3N@MAG 75 °C	0.3865	0.2205	0.4808	0.9952
3N@MAG 90 °C	0.2931	0.2978	0.4210	0.9958
Gy@3N@MAG 25 °C	0.3820	0.1445	0.5814	0.9942
Gy@3N@MAG 50 °C	0.2828	0.5789	0.6988	0.9930
Gy@3N@MAG 75 °C	0.1612	0.6571	0.1520	0.9985
Gy@3N@MAG 90 °C	0.1112	0.8781	0.2274	0.9977

Table S3. Fractional order modeling parameters fitted to 3N@MAG and Gy@3N@MAG, at different adsorption temperature.

Adsorbent	q _e / mmol g ⁻¹	k _n / mmol ^{1-m} g ^{m-1} min ⁻ⁿ	m	n	RSS / %	R ²
3N@MAG 25 °C	0.1010	1427.9416	1.6799	1.0098	0.3200	0.9968
3N@MAG 50 °C	0.2214	0.1670	0.4873	1.3019	0.1772	0.9982
3N@MAG 75 °C	0.3791	34.7029	2.3754	1.0401	0.5488	0.9945
3N@MAG 90 °C	0.2892	143.2788	3.7912	1.0175	0.5843	0.9942
Gy@3N@MAG 25 °C	0.3602	4.3191	1.2817	1.0824	0.3912	0.9961
Gy@3N@MAG 50 °C	0.2931	414.5918	2.5840	1.0227	1.9034	0.9810
Gy@3N@MAG 75 °C	0.1614	116.4740	2.4315	1.0298	0.4338	0.9957
Gy@3N@MAG 90 °C	0.1111	444.2569	2.1475	1.0099	0.2425	0.9976

Table S4. Avrami modeling parameters fitted to 3N@MAG and Gy@3N@MAG, at different adsorption temperature.

Adsorbent	$q_e / \text{mmol g}^{-1}$	k_A / min^{-1}	n_A	RSS / %	R^2
3N@MAG 25 °C	0.0958	0.0834	0.5681	0.0744	0.9993
3N@MAG 50 °C	0.2213	0.0043	0.4611	0.1952	0.9980
3N@MAG 75 °C	0.3615	0.0519	0.6901	0.7611	0.9924
3N@MAG 90 °C	0.2734	0.0544	0.7045	0.7083	0.9929
Gy@3N@MAG 25 °C	0.3613	0.0334	0.6870	0.2991	0.9970
Gy@3N@MAG 50 °C	0.2652	0.1109	0.8611	0.3321	0.9967
Gy@3N@MAG 75 °C	0.1523	0.0653	0.6922	0.2570	0.9974
Gy@3N@MAG 90 °C	0.1075	0.0541	0.6313	0.2061	0.9979