Electronic Supplementary Material (ESI) for RSC Advances

Electronic Supporting Information

Polyethylenimine covalently grafted on mesostructured porous silica for CO_2 capture

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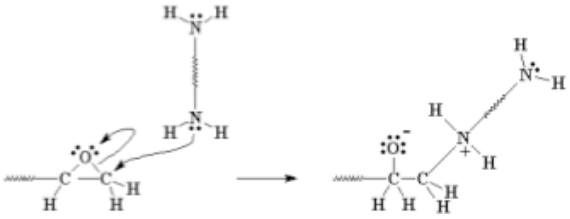
Appendix 1. LUS synthesis[28,29]

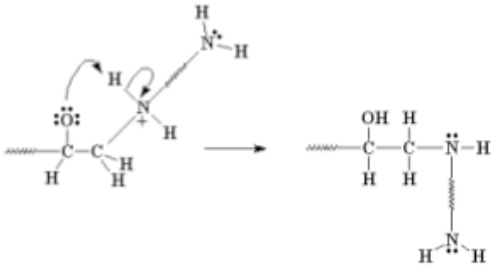
The composition of the initial gel was the following: 1 SiO_2 : 0.05 CTATos : 0.50 NaOH : 80 H_2O. Upon 2 hours aging treatment at 333 K followed by an hydrothermal step of 20 hours at 403 K a well-structured solid was obtained. Prior to the incorporation of the organic functions, the surfactant was extracted out of the as-made solid using a treatment with an acidic ethanol solution at 313 K (HCl, 1 M) followed by calcination at 823 K, obtaining the solid **LUS-C**. A weigth loss of 44% was observed at 1373 K for the as-made **LUS-A** according to the thermogravimetric analysis (TGA), 33% weight loss corresponding to the decomposition of the template CTA^+ between 393 and 673 K and 11 % to water desorption from both adsorbed molecular water (303-393 K) and silanol condensation (673-1373 K). After HCl treatment, the weight loss diminished to 9% (**LUS-H**), which can be attributed to decomposition of traces of template and water desorption as above. Finally, after calcination (**LUS-C**), a weight loss of 3.4% was observed at 1373 K, assigned only to water desorption.

Scheme S1. Oxacyclopropane ring opening by reaction with PEI[29,30]

The reaction between primary amine groups belonging to PEI with the epoxyde generates an alcohol-amine sequence in β position resembling the structure of a monoethanolamine used in solution for CO_2 capture. This reaction begins by the S_N2 nucleophilic attack of the primary amine on the less substituted carbon of the epoxyde followed by opening of the cycle according to the following scheme



The hydroxyl group is further generated by proton displacement from the ammonium group to the oxygen atom as follows



Figures

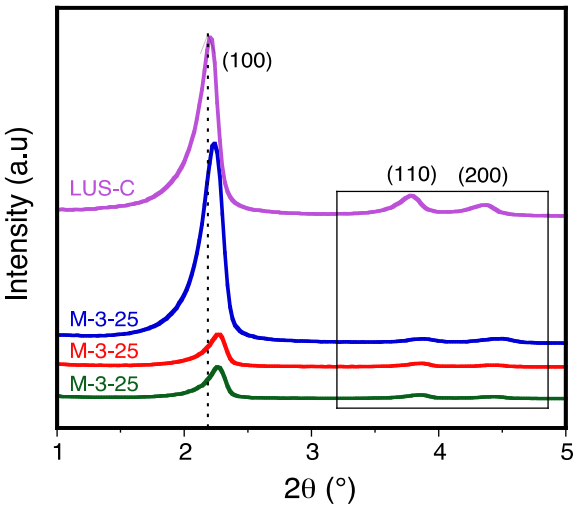


Figure S1. XRD patterns of **LUS-C**, **M-3-25**, **M-3-50** and **M-3-75**.

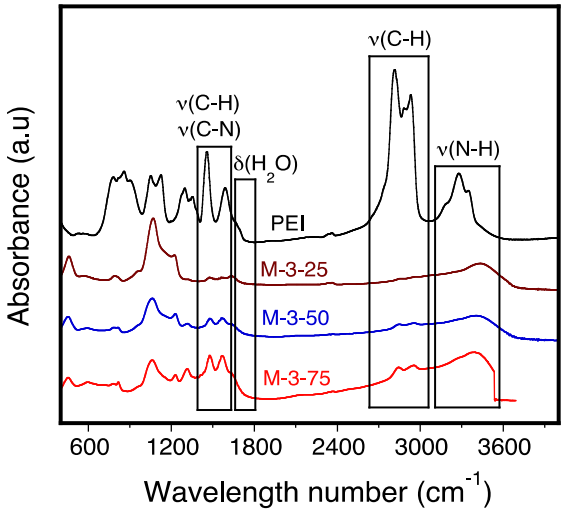


Figure S2. FT-IR spectra of **PEI** and samples **M-3-25**, **M-3-50** and **M-3-75**.

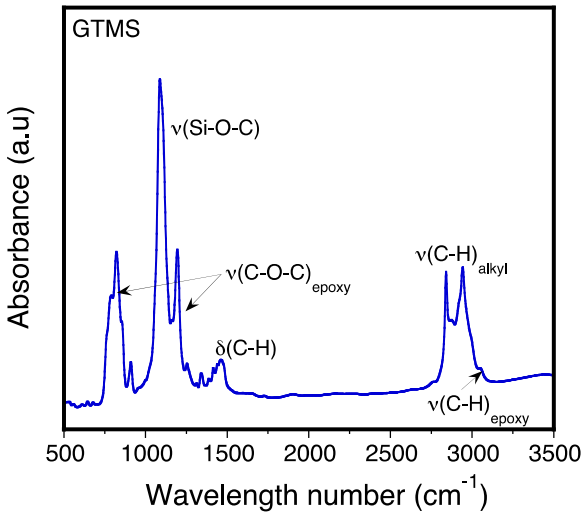


Figure S3. FT-IR spectrum of **GTMS**.

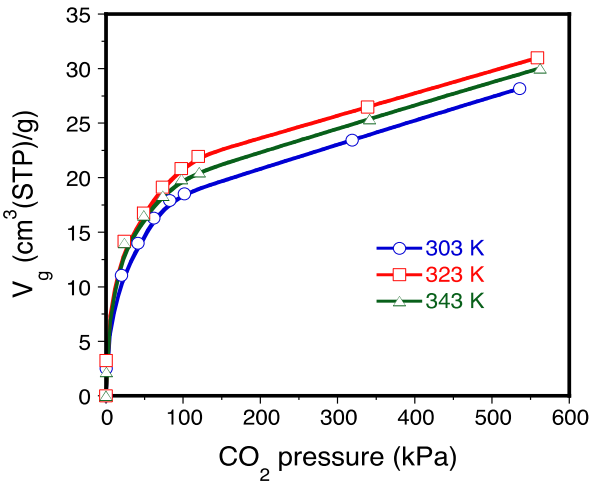


Figure S4. CO_2 adsorption isotherms as a function of temperature for sample **M-1**.

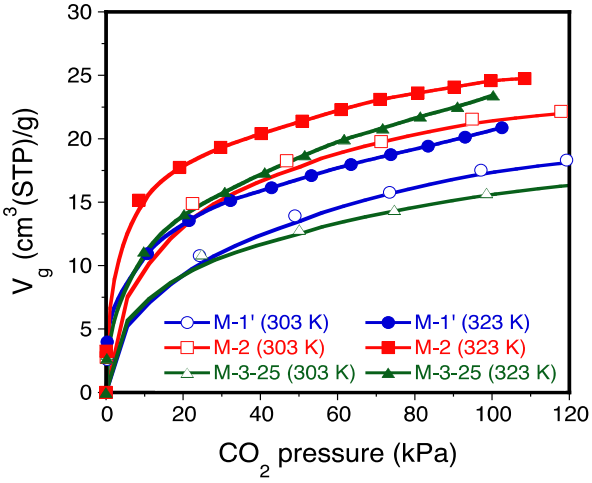


Figure S5. CO_2 adsorption isotherms as a function of temperature for materials **M-1'**, **M-2** and **M-3-25**. Straight and dashed lines correspond to data obtained, respectively, at 303 and 323 K.