Supporting Information to

CO_2 adsorption on different organo-modified SBA-15 silicas: effects of content of basic surface groups.

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Results

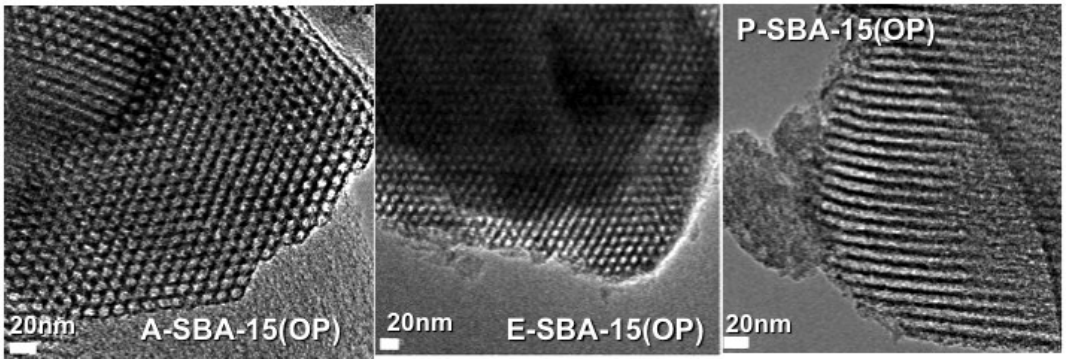

Fig. S1. TEM measurements of one-pot prepared SBA-15 related sample.

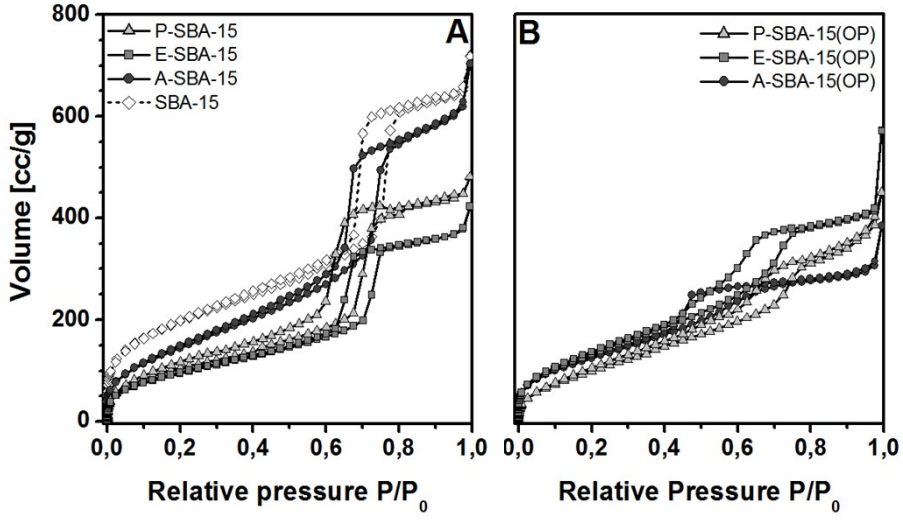

Fig. S2. N_2 adsorption–desorption isotherms at 77 K of functionalized SBA-15 samples prepared by grafting procedure (frame A) and one-pot synthesis (frame B).

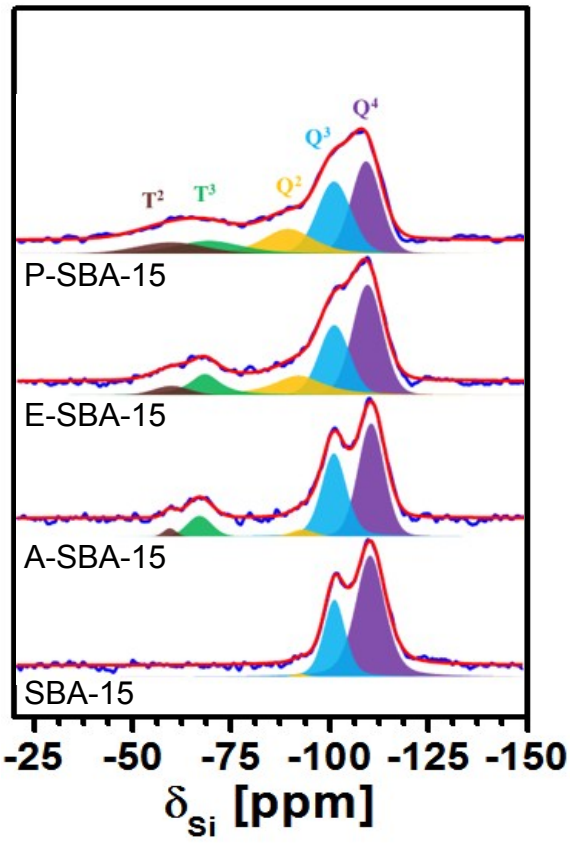

Fig. S3. ^{29}Si MAS NMR spectra of SBA-15 (a), A-SBA-15 (b), E-SBA-15 (c) and P-SBA-15 (d) recorded at a MAS rate of 10 kHz. Each curve includes experimental and its deconvoluted spectrum with individual contribution from each ^{29}Si sites.

The result of the reaction between the surface of SBA-15 silica and the silane species was evaluated by solid state NMR spectroscopy. The local environment of Si atoms were determined by ^{29}Si MAS NMR spectra and are shown in Fig. S3, together with the corresponding deconvoluted spectra and their individual components from each silicon site. All samples showed resonances at around -111, -102 and -93 ppm due to Q^4 (**Si**$(OSi)_4$), Q^3 (**Si**$(OSi)_3OH$) and Q^2 (**Si**$(OSi)_2(OH)_2$) species, respectively. Figure S3 (a) shows the ^{29}Si MAS NMR spectra of pristine SBA-15, where both Q^3 and Q^4 sites are partially resolved. While similar resolution was also observed in A-SBA-15, broader contributions were found in E-SBA-15 and P-SBA-15. Grafted SBA-15 samples A-SBA-15, E-SBA-15 and P-SBA-15 show resonances at -66 and -58 ppm due to T^3 and T^2 Si sites, respectively. A successful grafting process has been confirmed by the presence of T^3 (**Si**$(OSi)_3C$) and T^2 ($Si(OSi)_2(OH)C$) silicon sites in organically modified SBA-15. [1] Standard CPMAS conditions were used to acquire the ^{13}C CPMAS NMR spectra of organically modified SBA-15 at room temperature in order to confirm the surface functionalization as well as to distinguish ^{13}C sites. Figure S3 displays ^{13}C CPMAS spectra of pristine A-SBA-15, E-SBA-15 and P-SBA-15 recorded with a MAS rate of 10kHz and a cross polarization contact time of 2 ms. Well-defined resonances at around 8, 24 and 42 ppm for carbon atoms C1, C2 and C3, respectively are visible in the spectra of pristine A-SBA-15. Equally, similar carbons in E-SBA-15 and P-SBA-15 exhibit resonance at around 9 and 22 ppm. However, carbon atoms bind to NH group display a separate resonance at around 50 ppm in E-SBA-15 and P-SBA-15 besides the resonance at 40 ppm for NH_2 bound carbon. Therefore, it can be concluded that, organic surface functionalization in SBA-15 by grafting has been successful in all the three systems.

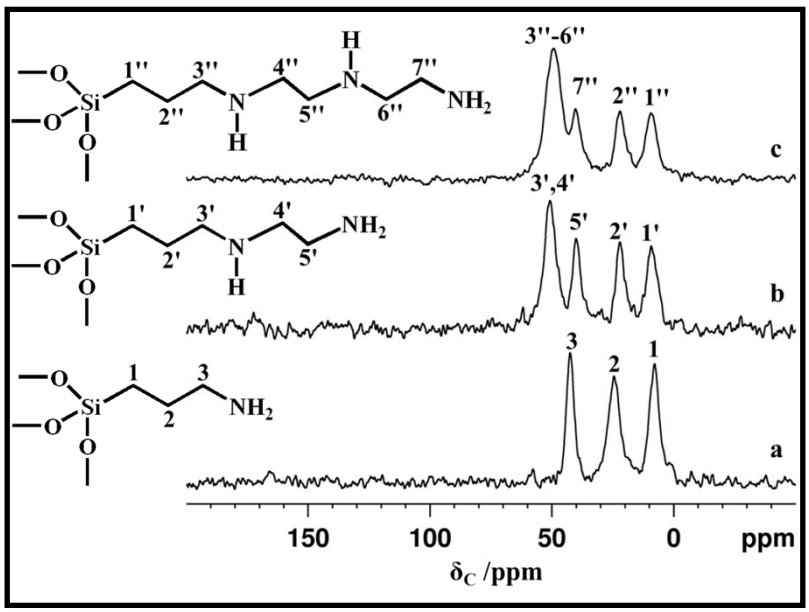

Fig. S4. ^{13}C CPMAS NMR spectra of pristine A-SBA-15 (a), E-SBA-15 (b) and P-SBA-15 (c). A cross polarization contact time of 2 ms and a MAS rate of 10 kHz were used in all the experiments.

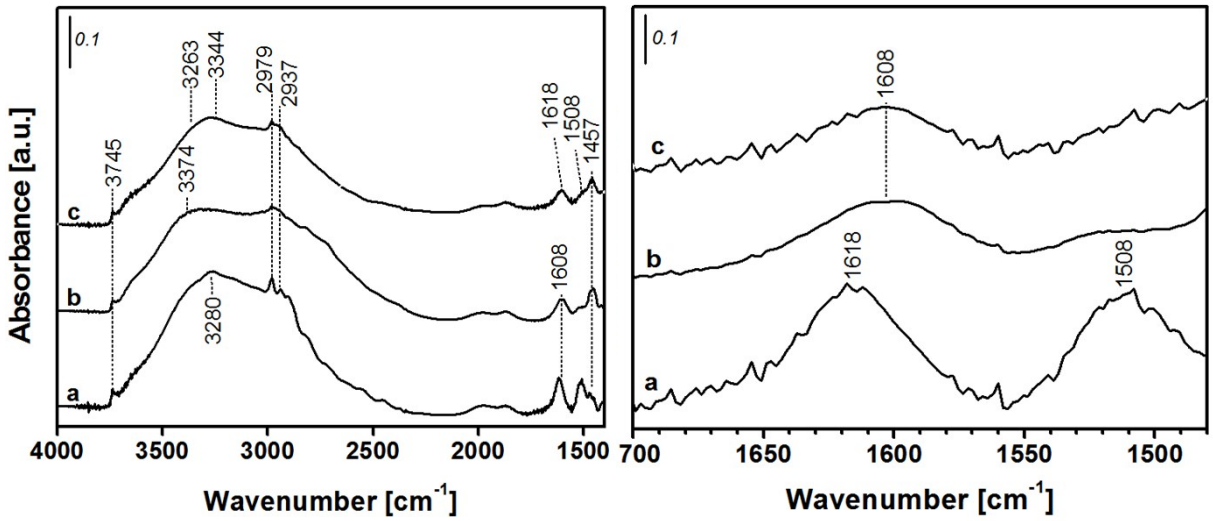

Fig. S5. FT-IR spectra of functionalized SBA-15 samples prepared by one-pot procedure (frame A). Enlargement of the FT-IR spectra in the 1800-1300 cm^{-1} range (frame B). Spectra were recorded outgassing the samples at r.t. for 30 minutes.

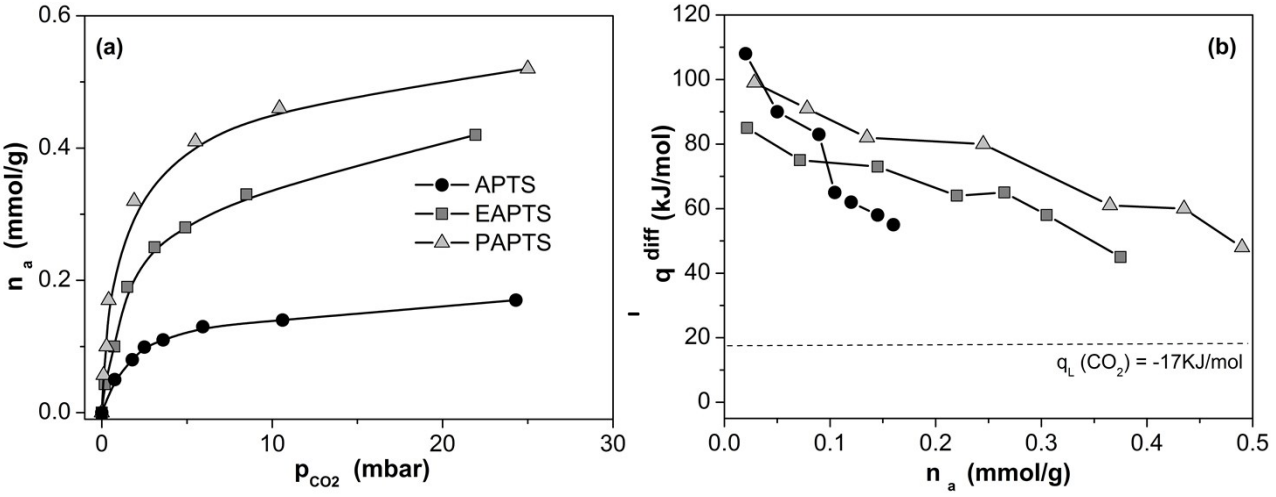

Fig. S6. Frame A) Quantitative isotherms related to the adsorption at 30°C of CO_2 at low equilibrium pressures on A-SBA-15 (circle), E-SBA-15 (square) and P-SBA-15 (triangle) samples. Frame B) Differential molar adsorption heats related to the adsorption of CO_2 at low coverages on grafted SBA-15 samples. The dashed horizontal line represents the standard molar enthalpy of liquefaction of CO_2 at 298K.

References

1 S.H. Kim, O.C. Han, J.K. Kim, K.H. Lee, *Bull. Korean Chem. Soc*., 2011, **32** (10), 3644.