Modifications induced by pretreatments on Au/SBA-15 and their influence on the catalytic activity for low temperature CO oxidation

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Experimental

Characterization

XRD. Scherrer equation: D_{XRD} = Kλ/βcosθ, where K is a constant related to the crystallite shape (0.9) and β is the pure breath of the powder reflection free of the broadening due to instrumental contributions. A Pseudo-Voigt function was used to fit the most intense peak and extrapolate θ and β_{exp}, from which β was obtained by means of the Warren correction $\beta = (\beta_{exp}^2-\beta_{std}^2)^{1/2}$ using a standard Si sample.

TEM. Distribution function used for fitting the hystogram: $P(D) = \frac{1}{D_{TEM}\sigma_{TEM}(2\pi)^{1/2}}\exp\left(-\frac{\ln^2(D/D_{TEM})}{2\sigma_{TEM}^2}\right)$, where σ_{TEM} and D_{TEM} are the standard deviation and the mean particle size value, respectively.

XPS. Data analysis involved non-linear Shirley-type background subtraction and curve-fitting by Esca Tools 4.2 software (Surface Interface Inc., Mountain View, California). Changes in the Au(4f) signal shape were analyzed by curve-fitting procedures with Au(4f) doublets endowed with fixed spectroscopic parameters ($Au(4f_{7/2}-4f_{5/2})$ spin-orbit separation, 3.6 eV and intensity ratio R = 0.75) but using variable position, full width at half maximum (FWHM) and intensities.

EPR. Samples were placed in a silica reactor provided with an isolation stopcock and equipped with a side tube for EPR measurements. The reactor was connected *via* a ground joint to all-glass vacuum apparatus, equipped with a pressure transducer (10^{-2} to 10^3 Torr, MKS Baratron) and a trap placed downstream from the reactor and kept at 77 K, to condense the gases desorbed from the samples surface (mostly H_2O and CO_2).

Results

Characterization of SBA-15

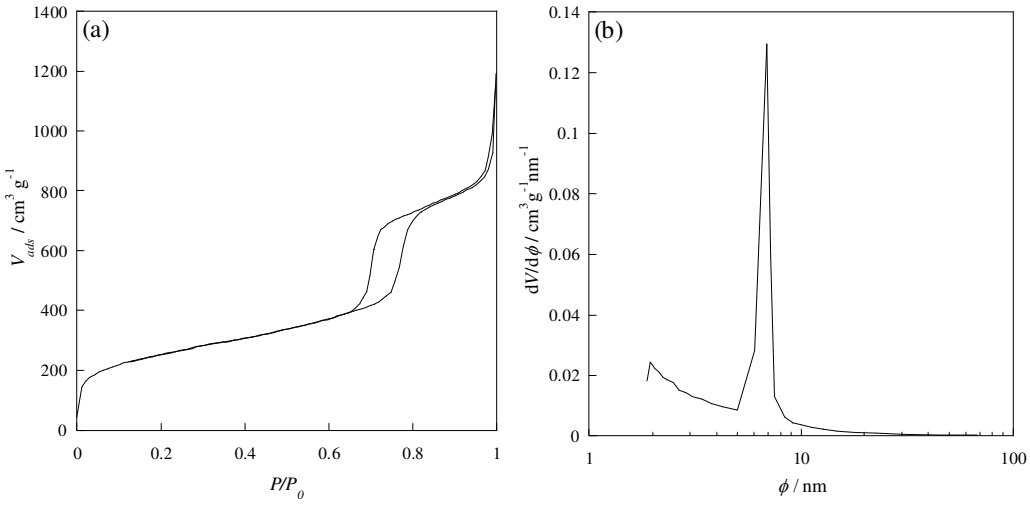

Figure S1. N_2 adsorption-desorption isotherms at 77 K (a) and pore size distribution curve (b) for SBA-15 support.

Characterization of functionalized SBA-15

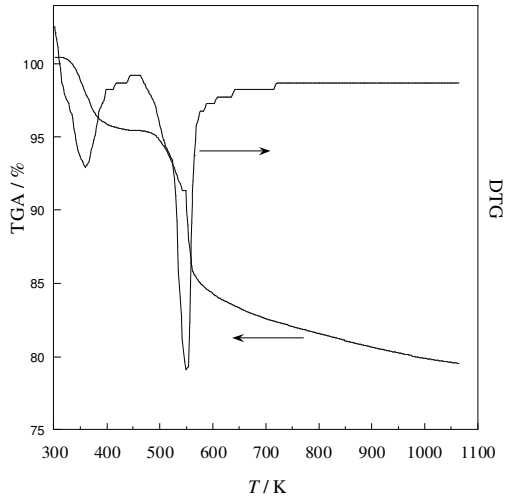

Figure S2. TGA and DTG curves for the SBA-15-SHcc sample.

NMR. The Q^n notation refers to the tetrahedral units of the amorphous silica network defined as $Si(OSi)_n(OH)_{4-n}$, in which each unit forms n bonds with neighbouring tetrahedra. The T^m notation refers to the peaks of the silane organic moieties incorporated as a part of the silica wall structure as $R\text{-}Si(OSi)_m(OH)_{3-m}$ (m = 1-3).