

Supplementary Information

Clean Chlorination of Silica Surfaces by a Single-site Substitution Approach

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1. Microelemental analysis of 1-3, 1a and 1b

Table S1. Elemental analysis data^a

Compound	Element (%)			
	Cl	C	P	S
1 (SiO ₂₍₇₀₀₎ -Cl)	1.02	ND ^b	ND ^b	NA ^c
1a (SiO ₂₍₇₀₀₎ -Cl)	0.65	NA ^c	NA ^c	0.01
1b (SiO ₂₍₇₀₀₎ -Cl)	0.67 ^d	nd ^e	nd ^e	NA ^c
2 (SiO ₂₍₅₀₀₎ -Cl)	1.29	ND ^b	ND ^b	NA ^c
3 (SiO ₂₍₂₀₀₎ -Cl)	0.23	ND ^b	ND ^b	NA ^c

^a Calculated from micro analysis of the compounds. ^b Non detectable. ^c Not applicable. ^d Estimated by titration with AgNO₃ according to reference 1. ^e Not determined

2. IR spectra

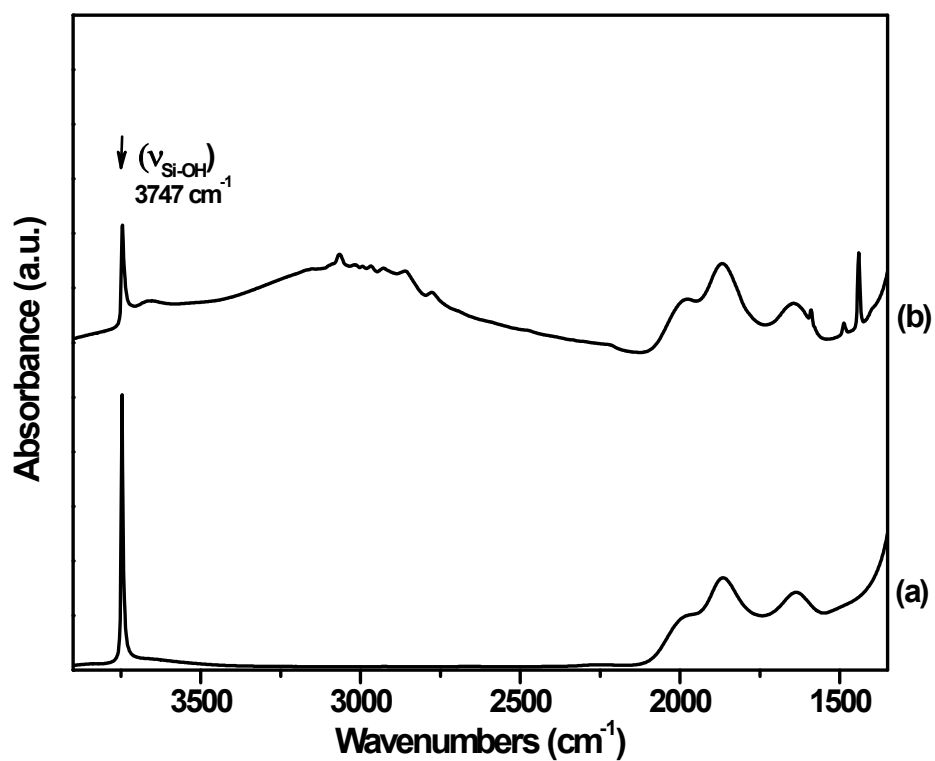


Figure S1. IR spectra of SiO₂₍₇₀₀₎ (a) and **1b** (b), the chlorinated silica prepared by treating SiO₂₍₇₀₀₎ with CCl₄/PPh₃ in CH₂Cl₂.

3. BET isotherms for $\text{SiO}_{2(700)}$ and $\text{SiO}_{2(700)}\text{-Cl}$

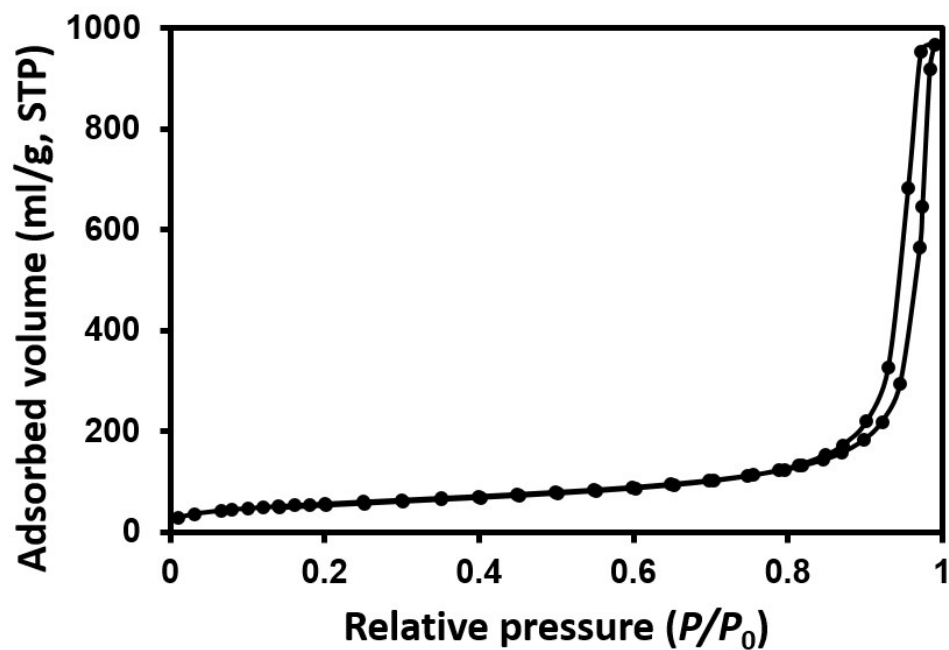


Figure S2. N_2 adsorption/desorption isotherm plot for $\text{SiO}_{2(700)}$ measured at 77 K. Connecting traces are guides for the eye

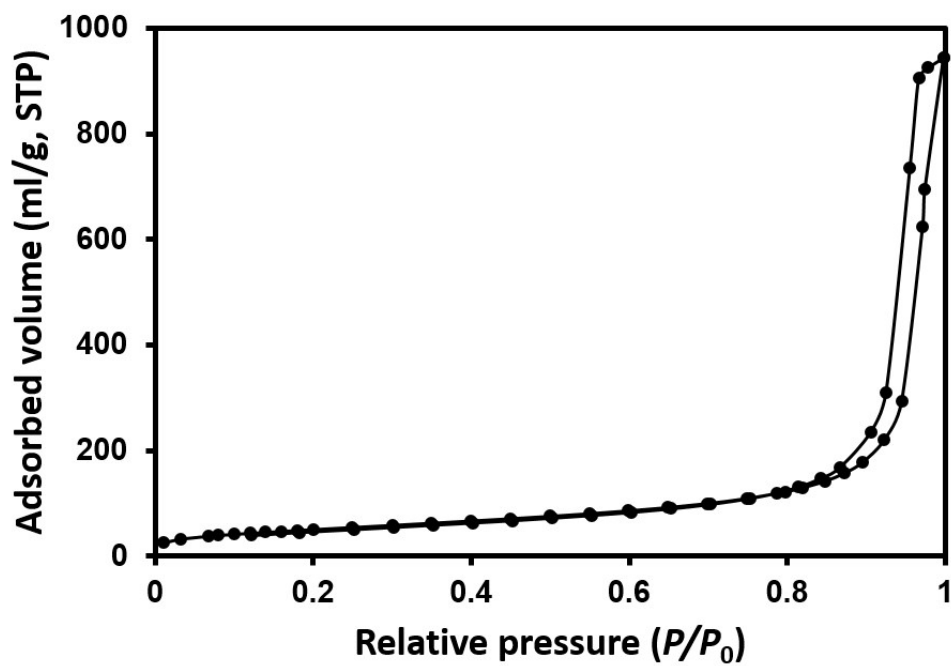


Figure S3. N₂ adsorption/desorption isotherm plot for SiO₂₍₇₀₀₎-Cl measured at 77 K.
Connecting traces are guides for the eye

4. Supporting references:

(1) F. Mohanazadeh and H. Amini, *Bull. Korean Chem. Soc.*, 2010, **31**, 3038-3040.