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

<table>
<thead>
<tr>
<th>Compound</th>
<th>Element (%)</th>
<th>Cl</th>
<th>C</th>
<th>P</th>
<th>S</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (SiO$_2$(700)-Cl)</td>
<td>1.02</td>
<td>ND $^b$</td>
<td>ND $^b$</td>
<td>NA $^c$</td>
<td></td>
</tr>
<tr>
<td>1a (SiO$_2$(700)-Cl)</td>
<td>0.65</td>
<td>NA $^c$</td>
<td>NA $^c$</td>
<td>0.01</td>
<td></td>
</tr>
<tr>
<td>1b (SiO$_2$(700)-Cl)</td>
<td>0.67$^d$</td>
<td>nd $^e$</td>
<td>nd $^e$</td>
<td>NA $^c$</td>
<td></td>
</tr>
<tr>
<td>2 (SiO$_2$(500)-Cl)</td>
<td>1.29</td>
<td>ND $^b$</td>
<td>ND $^b$</td>
<td>NA $^c$</td>
<td></td>
</tr>
<tr>
<td>3 (SiO$_2$(200)-Cl)</td>
<td>0.23</td>
<td>ND $^b$</td>
<td>ND $^b$</td>
<td>NA $^c$</td>
<td></td>
</tr>
</tbody>
</table>

$^a$ Calculated from micro analysis of the compounds. $^b$ Non detectable. $^c$ Not applicable. $^d$ Estimated by titration with AgNO$_3$ according to reference 1. $^e$ Not determined
2. IR spectra

Figure S1. IR spectra of SiO$_2$(700) (a) and 1b (b), the chlorinated silica prepared by treating SiO$_2$(700) with CCl$_4$/PPh$_3$ in CH$_2$Cl$_2$. 

$v_{\text{Si-OH}}$ 3747 cm$^{-1}$
3. BET isotherms for SiO$_2$(700) and SiO$_2$(700)-Cl

Figure S2. N$_2$ adsorption/desorption isotherm plot for SiO$_2$(700) measured at 77 K. Connecting traces are guides for the eye.
Figure S3. N$_2$ adsorption/desorption isotherm plot for SiO$_2$(700)-Cl measured at 77 K. Connecting traces are guides for the eye.

4. Supporting references: