Al-modified mesoporous silica for efficient conversion of methanol to dimethyl ether

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I) Supplementary data for X-ray diffraction

Fig. S1 X-ray diffractograms obtained for the Al-TMPS solids.
II) Supplementary data for N$_2$ physisorption

**Fig. S2** Nitrogen physisorption isotherms and pore size distributions for the Al-TMPS solids.
III) Supplementary data for ammonia thermo-desorption

Fig. S3 Ammonia temperature programmed desorption profiles for the TMPS solids.

The NH$_3$-TPD profiles of the aluminium-containing samples were fitted using the Origin 8.5 software. Four components were taken into account:

- weak sites, at ~446 K (peak 1),
- medium sites, at ~528 K (peak 2)
- strong sites with 2 components at 820-830 K (peak 3) and ~878 K (peak 4).

The obtained curves are presented in Figure S4 and the peaks positions and relative area summarized in Table S1.

Table S1. NH$_3$-TPD profiles decomposition peaks properties for the Al-containing catalysts.

<table>
<thead>
<tr>
<th>Peak 1</th>
<th>Peak 2</th>
<th>Peak 3</th>
<th>Peak 4</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Temp. (K)</td>
<td>Area</td>
<td>Fraction (%)</td>
</tr>
<tr>
<td>Al-TMPS-58</td>
<td>446</td>
<td>43</td>
<td>25</td>
</tr>
<tr>
<td>Al-TMPS-40</td>
<td>447</td>
<td>71</td>
<td>27</td>
</tr>
<tr>
<td>Al-TMPS-27</td>
<td>449</td>
<td>107</td>
<td>28</td>
</tr>
</tbody>
</table>

Fig. S4 Curve fitting of the NH$_3$-TPD.
**IV) Catalytic activity in methanol conversion to dimethyl ether**

the turn-over frequency (TOF), was calculated using the following formula:

\[
\text{TOF} = \frac{r_{\text{MeOH}} \times \text{SSA}}{\text{TPD}}
\]

with
- **TOF**: turn-over frequency (s\(^{-1}\))
- **\(r_{\text{MeOH}}\)**: rate of methanol conversion (mol.s\(^{-1}\).m\(^{-2}\))
- **SSA**: specific surface area (m\(^2\))
- **TPD**: acid site content (mol), determined by NH\(_3\)-TPD

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**Fig. S5** Catalytic activity of the silica and aluminosilicates: turnover frequencies as a function of temperature over A) TMPS solids, B) Al-TMPS solids, and associated Arrhenius plots in presence of C) TMPS solids and D) Al-TMPS solids.