Supporting information

Exploring the role of V$_2$O$_5$ in the reactivity of NH$_4$HSO$_4$ with NO on V$_2$O$_5$/TiO$_2$ SCR catalysts

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Figure captions

Fig. S1. XRD patterns of the series V/Ti catalysts

Fig. S2. FTIR spectra of the series V/Ti catalysts

Fig. S3. *In situ* DRIFTS study of the NH₄HSO₄ decomposition behavior over the V4/Ti catalyst surface
The XRD patterns of the series catalysts are presented in Fig. S1. All the diffraction peaks of the samples with V content lower than 8 wt% could be indexed to anatase TiO$_2$ and rutile TiO$_2$ phases. The absence of V$_2$O$_5$ and NH$_4$HSO$_4$ crystallites suggests that vanadium and sulfate species are highly dispersed, which exist in an amorphous state on the TiO$_2$ surface. Given increases in V$_2$O$_5$ content to 8 wt%, new diffraction peaks indexed to V$_2$O$_5$ phase appear, indicating that V loading is beyond the theoretical monolayer coverage on the TiO$_2$ support.$^1$
In the case of the NH$_4$HSO$_4$-deposited samples, the characteristic peaks attributed to bidentate SO$_4^{2-}$ at 1214, 1128, 1050 cm$^{-1}$ are generated, which are assigned to the $v_3$ vibrations of bidentate SO$_4^{2-}$ in $C_{2v}$ symmetry (Fig. S2). The bands at 1214 and 1128 cm$^{-1}$ appear because of asymmetric and symmetric stretching of the S=O vibrations. In the meantime, the peak at 1050 cm$^{-1}$ is related to the asymmetric S-O stretching vibrations. Given an increase in V$_2$O$_5$ content, new bands centered at 1088 and 1025 cm$^{-1}$, which could be related to the stretching of the S-O vibrations in pure NH$_4$HSO$_4$, appear. The presence of vanadium species leads to a deficit in TiO$_2$ surface basic sites, thereby allowing the appearance of pure NH$_4$HSO$_4$ phase. Combined with the XRD patterns in Fig. S1, NH$_4$HSO$_4$ might exist in the amorphous state.
In situ DRIFTS was conducted to investigate the detailed NH$_4$HSO$_4$ decomposition behavior on the catalyst surface. As is shown in Fig. S3, characteristic IR peaks centered at 1242 and 1433 cm$^{-1}$ attributed to bidentate SO$_4^{2-}$ and NH$_4^+$ appear when the temperature is 100 °C.$^6,7$ In the meantime, the bands at 2834, 3050, 3262 cm$^{-1}$, assigned to the stretching vibrations of N-H in NH$_4^+$ also come out.$^8$ With increasing temperature, the peak related to bidentate SO$_4^{2-}$ undergoes a blue shift, together with the occurrence of a decrease in the intensity of the bands attributed to sulfate and ammonium species. In addition, characteristic IR peak centered at 1378 cm$^{-1}$ attributed to tridentate SO$_4^{2-}$ comes out at a temperature of 450 °C, which might be due to the transformation of sulfate species from (M$_2$SO$_4$)H structure to (M-O)$_3$=O one.$^9$
### Tables

**Table S1**

N$_2$ adsorption results of the series V/Ti catalysts

<table>
<thead>
<tr>
<th>Samples</th>
<th>BET (m$^2$ g$^{-1}$)</th>
<th>Pore volume (cm$^3$ g$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>ABS-Ti</td>
<td>30</td>
<td>0.22</td>
</tr>
<tr>
<td>ABS-V1/Ti</td>
<td>30</td>
<td>0.23</td>
</tr>
<tr>
<td>ABS-V2/Ti</td>
<td>28</td>
<td>0.23</td>
</tr>
<tr>
<td>ABS-V4/Ti</td>
<td>24</td>
<td>0.22</td>
</tr>
<tr>
<td>ABS-V8/Ti</td>
<td>28</td>
<td>0.19</td>
</tr>
</tbody>
</table>
Reference