Supporting Information

DFT Insights into the Adsorption of NH$_3$-SCR Related Small Gases in Mn-MOF-74

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Fig. S1 Comparison between experimental and calculated PXRD patterns of Mn-MOF-74 and Co-MOF-74
**Table S1.** Comparison of lattice parameters of Co-MOF-74 between experimental results and DFT optimization

<table>
<thead>
<tr>
<th>Co-MOF-74 lattice constant (Å)</th>
<th>Experimental data$^1$</th>
<th>Experimental data$^2$</th>
<th>Our Calculated data</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>26.132</td>
<td>25.948</td>
<td>25.877</td>
</tr>
<tr>
<td>b</td>
<td>26.132</td>
<td>25.948</td>
<td>25.877</td>
</tr>
<tr>
<td>c</td>
<td>6.722</td>
<td>6.838</td>
<td>6.866</td>
</tr>
</tbody>
</table>

**References**


Table S2. Optimized geometries of adsorbed NH$_3$-SCR related small gases in Mn-MOF-74

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Bond name</th>
<th>Bond length(Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>NH$_3$</td>
<td>Mn-N</td>
<td>2.059</td>
</tr>
<tr>
<td></td>
<td>N-H1*</td>
<td>1.032</td>
</tr>
<tr>
<td></td>
<td>N-H2*</td>
<td>1.028</td>
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<tr>
<td></td>
<td>N-H3*</td>
<td>1.030</td>
</tr>
<tr>
<td>NO</td>
<td>Mn-N</td>
<td>2.011</td>
</tr>
<tr>
<td></td>
<td>N-O*</td>
<td>1.207</td>
</tr>
<tr>
<td>O$_2$</td>
<td>Mn-O</td>
<td>2.053</td>
</tr>
<tr>
<td></td>
<td>O-O*</td>
<td>1.319</td>
</tr>
<tr>
<td>NO$_2$</td>
<td>Mn-N</td>
<td>2.064</td>
</tr>
<tr>
<td></td>
<td>N-O1*</td>
<td>1.364</td>
</tr>
<tr>
<td></td>
<td>N-O2*</td>
<td>1.374</td>
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<tr>
<td>H$_2$O</td>
<td>Mn-O</td>
<td>2.200</td>
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<tr>
<td></td>
<td>O-H1*</td>
<td>0.994</td>
</tr>
<tr>
<td></td>
<td>O-H2*</td>
<td>0.995</td>
</tr>
<tr>
<td>SO$_2(1)^a$</td>
<td>Mn-O</td>
<td>2.014</td>
</tr>
<tr>
<td></td>
<td>S-O1*</td>
<td>1.618</td>
</tr>
<tr>
<td></td>
<td>S-O2*</td>
<td>1.553</td>
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<tr>
<td>SO$_2(2)^b$</td>
<td>Mn-S</td>
<td>2.547</td>
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<tr>
<td></td>
<td>S-O1*</td>
<td>1.559</td>
</tr>
<tr>
<td></td>
<td>S-O2*</td>
<td>1.556</td>
</tr>
</tbody>
</table>

* means the intramolecule bond lengths of the adsorbed gas molecules;  
$^a$SO$_2(1)$ refers to the configuration when SO$_2$ adsorbs in the Mn-MOF-74 in the form of O end adsorption, while $^b$SO$_2(2)$ is the case of S end adsorption.