The effect of GME topology on the multicomponent adsorption in ZIFs

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Supporting Information

Table 1: atom atom interaction parameters

<table>
<thead>
<tr>
<th>ZIF atoms</th>
<th>adsorbate atoms</th>
<th>atom</th>
<th>σ(A)</th>
<th>ε/k_B(K)</th>
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<tbody>
<tr>
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<td>Carbon CO_2^a</td>
<td>Carbon</td>
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<td>Oxygen</td>
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<tr>
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<td>Nitrogen N_2^b</td>
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<td>Nitrogen</td>
<td>Oxygen O_2^c</td>
<td>Nitrogen</td>
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<tr>
<td>Zinc</td>
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<td>Zinc</td>
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<tr>
<td>Cl</td>
<td>O(H_2O)^d</td>
<td>Cl</td>
<td>3.52</td>
<td>99.23</td>
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<tr>
<td>Br</td>
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<td>Br</td>
<td>3.73</td>
<td>126.31</td>
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<tr>
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<td>Carbon CO_2^a</td>
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<tr>
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<td>O(H_2O)^d</td>
<td>O(H_2O)</td>
<td>3.15</td>
<td>76.58</td>
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</table>

^a C-O distance (Å): 1.18; ^b N-N distance (Å): 1.1; ^c O-O distance (Å): 1.21;
^d O-H distance (Å): 0.9572, H-O-H angle 104.52°; ^com center of mass charge;
^H hydrogen atom charge;

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*To whom correspondence should be addressed
Table 2: Atomic charges ($e$) on $Im – Zn – nIm$ fragments for ZIFs 68-78

<table>
<thead>
<tr>
<th></th>
<th>ZIF68</th>
<th>ZIF69</th>
<th>ZIF70</th>
<th>ZIF78</th>
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<tbody>
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<td>Zn1</td>
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<td>C3</td>
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<td>N8</td>
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<tr>
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<td>-0.417138</td>
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Table 3: Atomic charges (e) on \( Im - Zn - nIm \) fragments for ZIFs 79-82

<table>
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<th>ZIF81</th>
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Figure 1: $CO_2$ adsorption isotherms computed at 298K in this work, compared with a set of experimental and simulated isotherms provided in the literature. The citing articles are included in the reference list of the manuscript.
Figure 2: $CH_4$ and $N_2$ adsorption isotherms computed at 298K in this work, for ZIF68, ZIF69, ZIF78 and ZIF79, compared with a set of experimental and simulated isotherms provided in the literature. The citing articles are included in the reference list of the manuscript.
Figure 3: \( CO_2 \) adsorption in the unit cell, the \textit{kno} and \textit{gme} channels of ZIF70, for single and multicomponent systems.
Figure 4: $CO_2$ adsorption in the unit cell, the *kno* and *gme* channels of ZIF80, for single and multicomponent systems.
Figure 5: CO$_2$ adsorption in the unit cell, the $kno$ and $gme$ channels of ZIF82, for single and multicomponent systems.