Supporting Information

Impact of Crystal Orientation on the Adsorption Kinetics of a Porous Coordination Polymer/Quartz Crystal Microbalance Hybrid Sensor

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S1. Effect of Temperature on Synthesis of Zn-CID-5

Fig. S1 XRD patterns of compounds under various temperatures: (a) 120, (b) 110, (c) 100, (d) 90, (e) 80, (f) 70, (g) 60, (h) 50, (i) 40, (j) 30 °C and simulation of Zn-CID-5 (open form). The red circles indicate the unknown peaks.
S2. Effect of Temperature on the Yield of Zn-CID-5

Table S1 The yield of Zn-CID-5 at various temperatures.

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Time</th>
<th>Yield</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>30 °C</td>
<td>5 min</td>
<td>9.81 mg</td>
<td>-</td>
</tr>
<tr>
<td>40 °C</td>
<td>5 min</td>
<td>17.7 mg</td>
<td>-</td>
</tr>
<tr>
<td>50 °C</td>
<td>5 min</td>
<td>12.0 mg</td>
<td>15.0 %</td>
</tr>
<tr>
<td>60 °C</td>
<td>5 min</td>
<td>11.7 mg</td>
<td>14.6 %</td>
</tr>
<tr>
<td>70 °C</td>
<td>5 min</td>
<td>10.4 mg</td>
<td>13.0 %</td>
</tr>
<tr>
<td>80 °C</td>
<td>5 min</td>
<td>10.2 mg</td>
<td>12.7 %</td>
</tr>
<tr>
<td>90 °C</td>
<td>5 min</td>
<td>10.4 mg</td>
<td>13.0 %</td>
</tr>
<tr>
<td>100 °C</td>
<td>5 min</td>
<td>17.3 mg</td>
<td>21.2 %</td>
</tr>
<tr>
<td>110 °C</td>
<td>5 min</td>
<td>18.4 mg</td>
<td>23.0 %</td>
</tr>
<tr>
<td>120 °C</td>
<td>5 min</td>
<td>30.2 mg</td>
<td>37.6 %</td>
</tr>
</tbody>
</table>
S3. Effect of Reaction Time on Synthesis of Zn-CID-5

Fig. S2 XRD patterns of compounds under various reaction time: (a) 30, (b) 25, (c) 20, (d) 15, (e) 10, (f) 5 min, (g) and simulation of Zn-CID-5 (open form).
S4. Effect of Reaction Time on the Yield of Zn-CID-5

Table S2 The yield of Zn-CID-5 at various reaction time

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Time</th>
<th>Yield</th>
<th>Product</th>
</tr>
</thead>
<tbody>
<tr>
<td>120 °C</td>
<td>5 min</td>
<td>30.19 mg</td>
<td>37.6 % Zn-CID-5</td>
</tr>
<tr>
<td>120 °C</td>
<td>10 min</td>
<td>43.80 mg</td>
<td>54.6 % Zn-CID-5</td>
</tr>
<tr>
<td>120 °C</td>
<td>15 min</td>
<td>46.23 mg</td>
<td>57.6 % Zn-CID-5</td>
</tr>
<tr>
<td>120 °C</td>
<td>20 min</td>
<td>54.18 mg</td>
<td>67.5 % Zn-CID-5</td>
</tr>
<tr>
<td>120 °C</td>
<td>25 min</td>
<td>55.09 mg</td>
<td>68.7 % Zn-CID-5</td>
</tr>
<tr>
<td>120 °C</td>
<td>30 min</td>
<td>57.56 mg</td>
<td>71.7 % Zn-CID-5</td>
</tr>
</tbody>
</table>
S5. Size Distribution of Zn-CID-5

**r = 0**

**Width distribution**

- Size (nm)
- Trend

Length distribution

2026.87 x 3468.48 nm

**r = 15**

**Width distribution**

- Size (nm)
- Trend

Length distribution

373.53 x 535.80 nm

**Fig. S3** Size distribution of Zn-CID-5 obtained at r = 0 and 15.
**Fig. S4** XRD patterns of compounds under various reaction conditions: (a) $r = 15$, (b) $r = 12.5$, (c) $r = 10$, (d) $r = 7.5$, (e) $r = 5$, (f) $r = 1$, (g) $r = 0$, (h) and simulation of **Zn-CID-5** (open form).
S7. Environmentally-Controlled XRD

**Fig. S5** Experimental apparatus of XRD measurement under methanol humidity control
S8. XRD under MeOH Atmosphere ($r = 0$)

**Fig. S6** XRD patterns of Zn-CID-5 ($r = 0$) under various methanol humidity in adsorption and desorption process.
S9. XRD under MeOH Atmosphere \((r = 15)\)

**Fig. S7** XRD patterns of Zn-CID-5 \((r = 15)\) under various methanol humidity in adsorption and desorption process.
S10. Adsorption Isotherms for Chloroform

![Graph showing adsorption isotherms](image)

**Fig. S8** Adsorption isotherms of Zn-CID-5 obtained under various conditions for chloroform: \( r = 0 \) (blue), \( r = 1 \) (green), \( r = 5 \) (orange), \( r = 12.5 \) (brown) and \( r = 15 \) (red). Closed and open symbols show adsorption and desorption, respectively.
S11. Crystal Structure of Zn-CID-5 along 1D Sheet

**Fig. S9** The crystal structures of **Zn-CID-5** along 1D sheet. 1 D chain is nearly perpendicular to (100), but tilted to (1-1-1).
S12. Crystal Structure of Zn-CID-5 along Pillar Ligand

Fig. S10 The crystal structures of Zn-CID-5 along pillar ligand.
S13. DE Model Fitting of the [100] Oriented Sample

\[ \frac{M_t}{M_e} = A_1 \{1 - \exp(-k_1 t)\} + A_2 \{1 - \exp(-k_2 t)\} \]

\[ A_1 = 0.850 \]
\[ A_2 = 0.150 \]
\[ k_1 = 3.901 \times 10^{-1} \]
\[ k_2 = 3.729 \times 10^{-2} \]
\[ R^2 = 0.901 \]

**Fig. S11** Time dependent mass uptake of the [100] oriented sample at \( P/P_0 = 40\% \) for MeOH. The red line represents the fitting curve by a double exponential function.
S14. DE Model Fitting of the [1-1-1] Oriented Sample

Fig. S12 Time dependent mass uptake of the [1-1-1] oriented sample at $P/P_0 = 40\%$ for MeOH. The red line represents the fitting curve by a double exponential function.
S15. DE Model Fitting of the Non-Oriented Sample

![Graph showing time dependent mass uptake of the non-oriented sample](image)

\[ \frac{M_t}{M_e} = A_1 \{1 - \exp(-k_1t)\} + A_2 \{1 - \exp(-k_2t)\} \]

- \( A_1 = 0.646 \)
- \( A_2 = 0.354 \)
- \( k_1 = 3.901 \times 10^{-1} \)
- \( k_2 = 3.729 \times 10^{-2} \)
- \( R^2 = 0.991 \)

**Fig. S13** Time dependent mass uptake of the non-oriented sample at \( P/P_0 = 40 \% \) for MeOH. The red line represents the fitting curve by a double exponential function.
S16. DE Model Fitting of the [010] Oriented Sample

\[
\frac{M_t}{M_e} = A_1 \{1 - \exp(-k_1 t)\} + A_2 \{1 - \exp(-k_2 t)\}
\]

- \(A_1 = 0.950\)
- \(A_2 = 0.050\)
- \(k_1 = 3.901 \times 10^{-1}\)
- \(k_2 = 3.729 \times 10^{-2}\)
- \(R^2 = 0.831\)

Fig. S14 Time dependent mass uptake of the [010] oriented sample at \(P/P_0 = 40\%\) for MeOH. The red line represents the fitting curve by a double exponential function.