Supplementary Information

Synthesis of modulator-driven highly stable zirconium-fumarate frameworks and their mechanistic investigations for the adsorption of arsenite and arsenate from aqueous solutions

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Figure S1. $^1$H NMR spectra of Zr-fum MOF of 0 eq BA and 5 eq BA as ferrocene as reference.
**Figure S2.** Nitrogen adsorption-desorption isotherms of the synthesized products under liquid nitrogen at 77 K.

**Table S1.** Physicochemical analysis of synthesized materials

<table>
<thead>
<tr>
<th>Materials</th>
<th>BET SSA (m²/g)</th>
<th>Pore volume (cm³/g)</th>
<th>Avg. Pore size (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zr-fum-0 eq BA</td>
<td>260.4</td>
<td>0.357</td>
<td>3.358</td>
</tr>
<tr>
<td>Zr-fum-1 eq BA</td>
<td>363.2</td>
<td>0.120</td>
<td>3.354</td>
</tr>
<tr>
<td>Zr-fum-3 eq BA</td>
<td>483.9</td>
<td>0.569</td>
<td>3.058</td>
</tr>
<tr>
<td>Zr-fum-5 eq BA</td>
<td>760.1</td>
<td>0.700</td>
<td>3.352</td>
</tr>
<tr>
<td>Zr-fum-10 eq BA</td>
<td>566.1</td>
<td>0.334</td>
<td>3.288</td>
</tr>
</tbody>
</table>
Figure S3. Pseudo-second-order kinetic models of (a) AsO$_4^{3-}$ and (b) AsO$_3^{3-}$ adsorption onto Zr-fum-0 eq BA, Zr-fum-1 eq BA, Zr-fum-3 eq BA, Zr-fum-5 eq BA and Zr-fum-10 eq BA. Experimental conditions: Initial conc. = 2 mM AsO$_4^{3-}$ and 1.6 mM AsO$_3^{3-}$, dose ratio = 1 g/L, agitation = 100 rpm, temp = 25 °C.
Figure S4. (a) Zeta potential at pH 6.8 and (b) Eh-pH diagram of the arsenic species and (c) residual ion concentration of Zr-fum-3 eq BA, Zr-fum-5 eq BA and Zr-fum-10 eq BA.
Figure S5. Effect of coexisting anions on synthesized Zr-fum-5 eq BA MOFs.
Figure S6. FTIR spectra of after adsorption of AsO$_4^{3-}$ and AsO$_3^{3-}$ using Zr-fum-5 eq BA and Zr-fum-10 eq BA.
Figure S7. XPS spectra of after adsorption of AsO$_4^{3-}$ and AsO$_3^{3-}$ on Zr-fum-5 eq BA
Figure S8. Langmuir adsorption isotherm for Zr-fum-5 eq BA MOF (a) AsO$_4^{3-}$ and (b) AsO$_3^{3-}$ adsorption.