Electronic Supplementary Information

Understanding the adsorptive interactions of arsenate—iron nanoparticles with curved fullerene-like sheets in activated carbon using a quantum mechanics/molecular mechanics computational approach

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Table S1. Textural characteristics of AC based on the N$_2$ adsorption isotherms determined at 77K.

<table>
<thead>
<tr>
<th>Specific surface area (m$^2$ g$^{-1}$)</th>
<th>Microporous surface area (m$^2$ g$^{-1}$)</th>
<th>Micropore volume (cm$^3$ g$^{-1}$)</th>
<th>Mesopore volume (cm$^3$ g$^{-1}$)</th>
<th>Total pore volume (cm$^3$ g$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1950</td>
<td>1935</td>
<td>0.8447</td>
<td>0.0473</td>
<td>0.8920</td>
</tr>
</tbody>
</table>

*The textural characterization of the AC was based on N$_2$ adsorption isotherms determined at 77K using a TriStar 3000 analyzer (Micromeritics). The AC samples were de-gassed for 24h at 573K to remove any moisture or adsorbed contaminants.

Figure S1. Adsorption capacity data of As(V) on AC at 303K.