

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 N₂ adsorption isotherms determined at 77K.

Specific surface area (m ² g ⁻¹)	Microporous surface area (m ² g ⁻¹)	Micropore volume (cm ³ g ⁻¹)	Mesopore volume (cm ³ g ⁻¹)	Total pore volume (cm ³ g ⁻¹)
1950	1935	0.8447	0.0473	0.8920

*The textural characterization of the AC was based on N₂ 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.

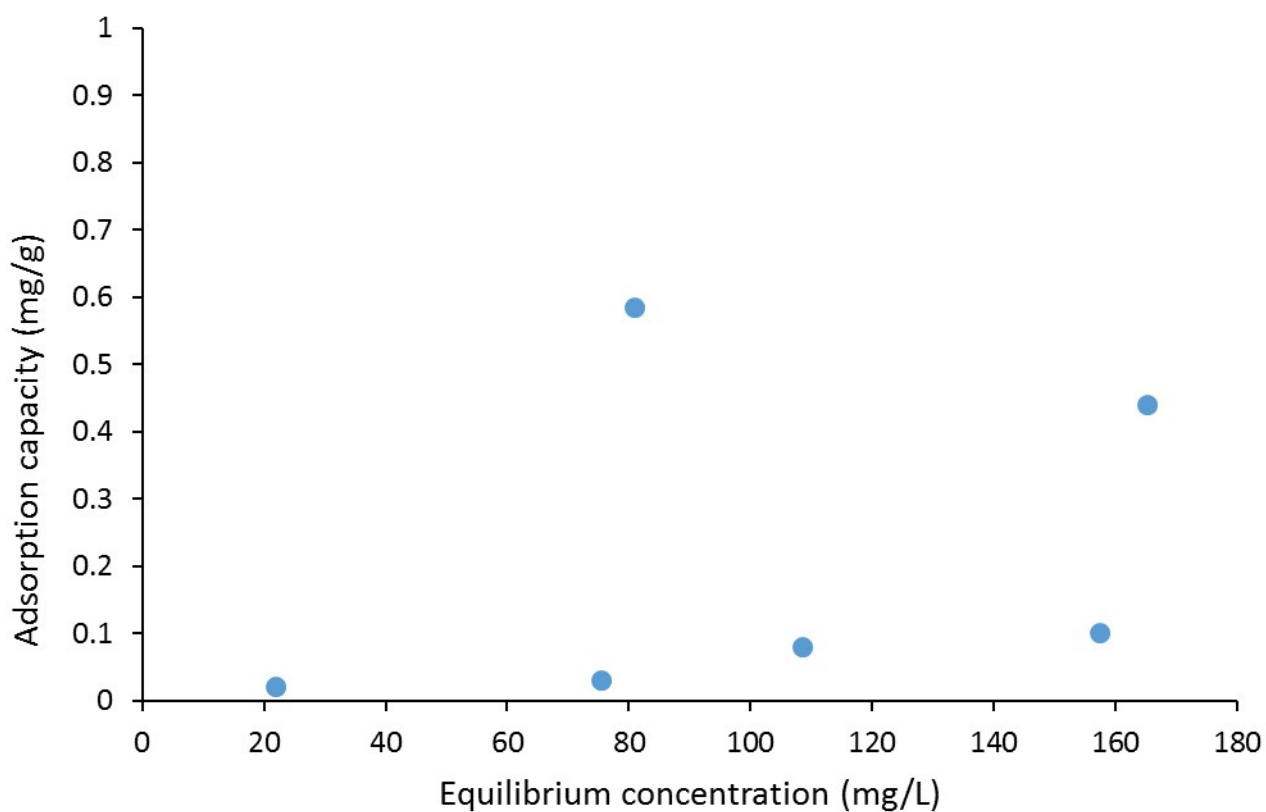


Figure S1. Adsorption capacity data of As(V) on AC at 303K.