

Supporting information

An Efficient Hybrid Adsorbent Based on Silica-Supported Amino *Penta*-Carboxylic Acid for Water Purification

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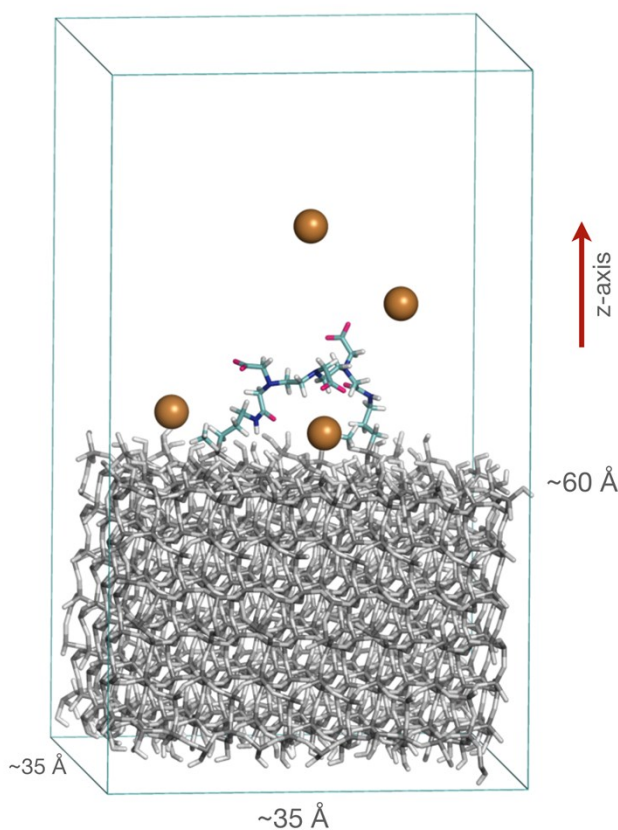


Figure S1. General aspect of the SiDTPA simulation box, comprising the silica substrate (grey-scale sticks), the DTPA bridge (coloured sticks) and the Cu²⁺ cations (orange spheres). The water molecules, filling the remaining empty space, were removed for the sake of clarity. Scaling of the simulation box during pressure control was restricted to the z-axis (red arrow)

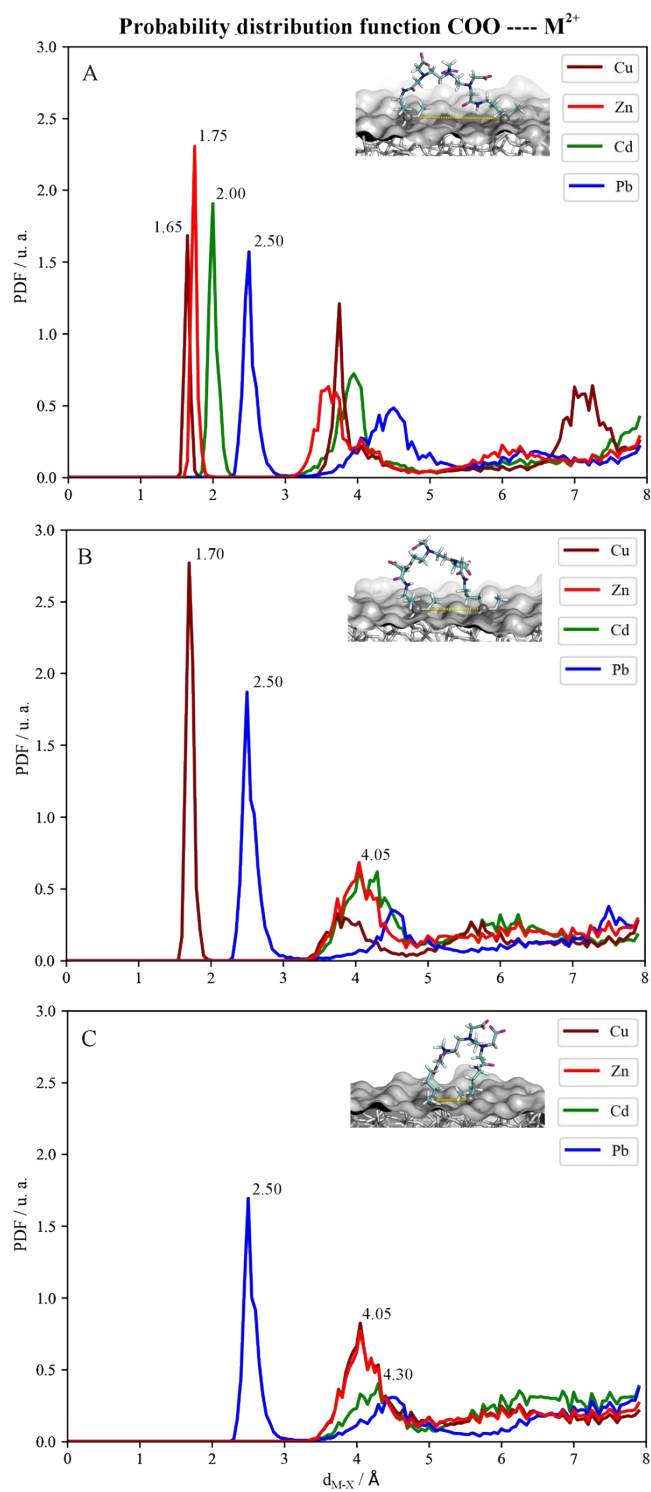


Figure S2. Probability distribution functions for the CO₂⁻ ... M²⁺ distance in structures S1, S2 and S3 (top, middle and bottom, respectively)

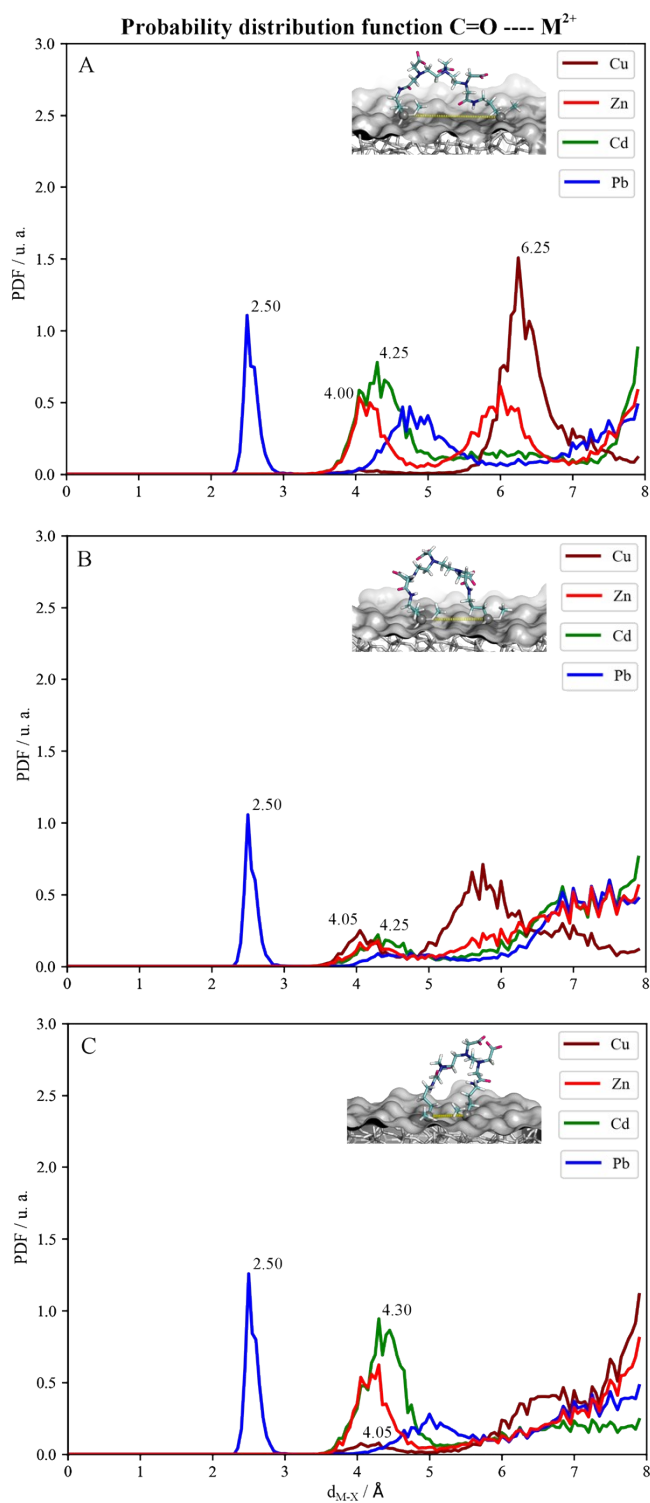


Figure S3. Probability distribution functions for the C=O ... M²⁺ distance in structures S1, S2 and S3 (top, middle and bottom, respectively). Only Pb mildly interacts with the carbonylic oxygens in structure S3 (shorter distance between anchoring points).

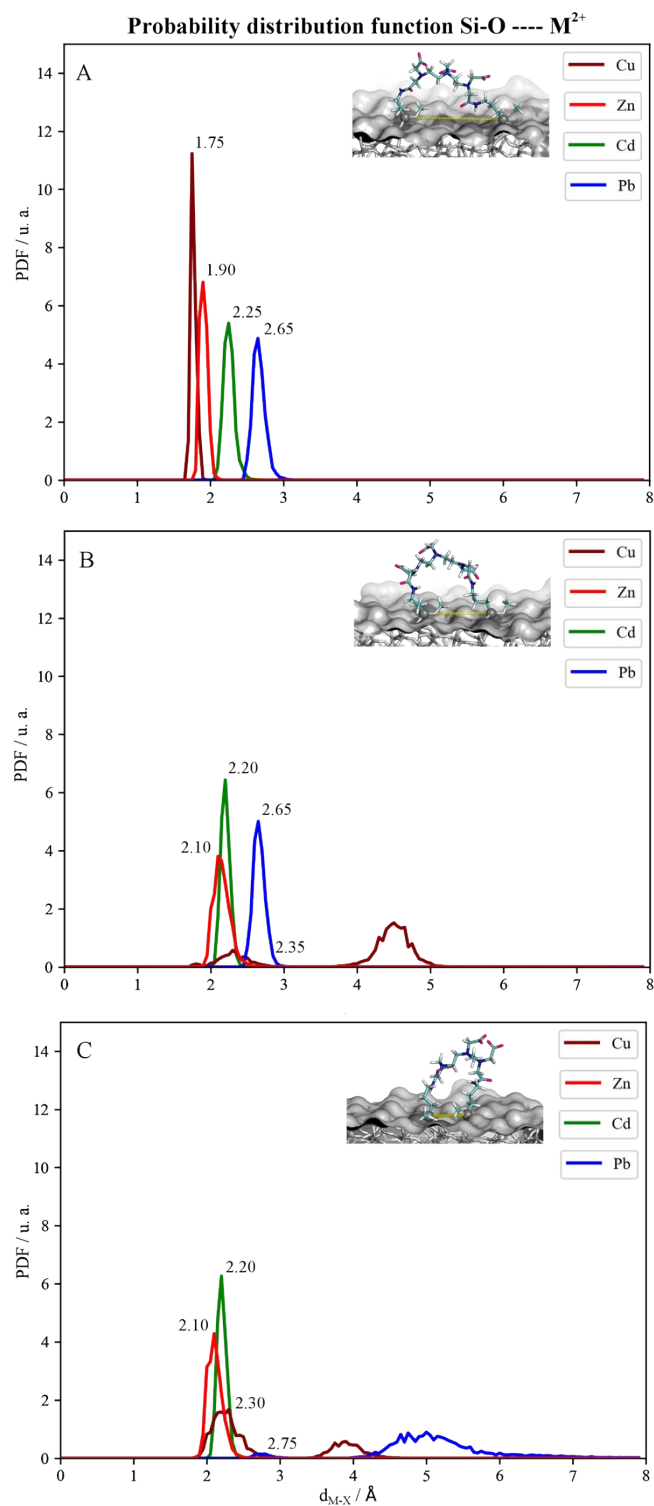


Figure S4. Probability distribution functions for the Si-O⁻ ... M²⁺ distance in structures S1, S2 and S3 (top, middle and bottom, respectively). The position of the Si-O⁻ site under analysis is depicted in Figure S5.

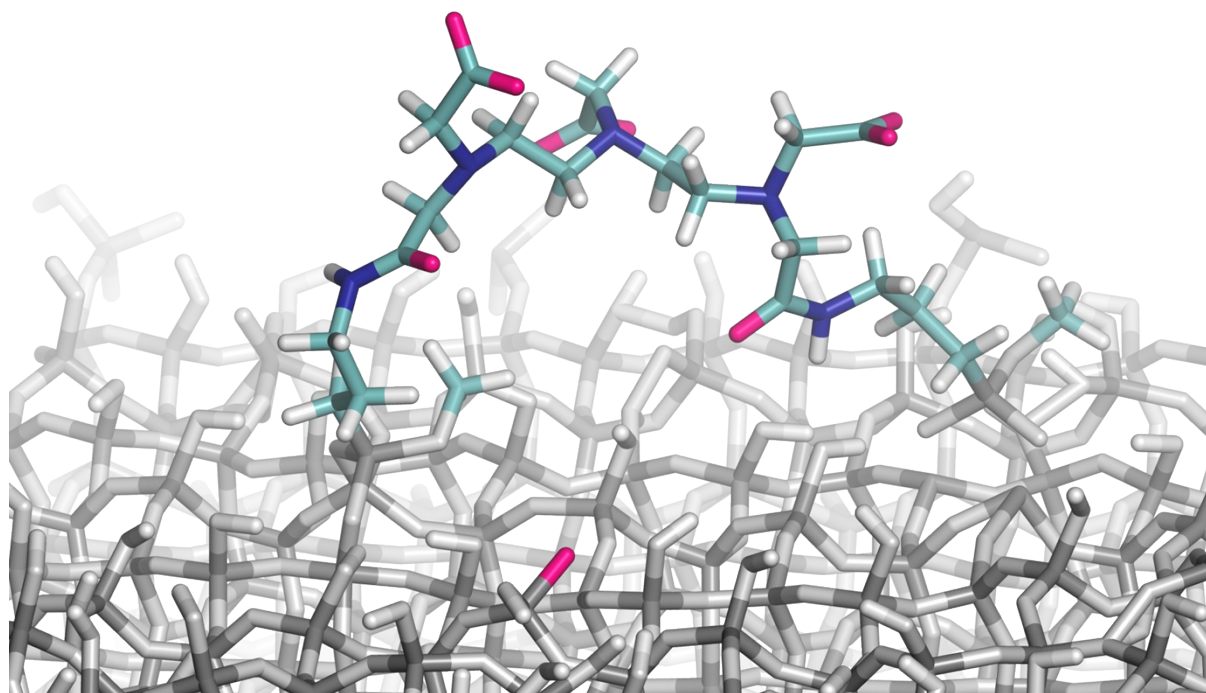


Figure S5. Location of the Si-O⁻ binding site (bottom pink stick) relative to the anchoring position of DTPA in structure S1 (relative location in structures S2 and S3 is similar).