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## Structural changes in ZIFs upon gas and liquid phase adsorption

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Chemical contamination in water and air streams requires the design of novel adsorbents able to retain/concentrate these pollutants selectively and with a high adsorption capacity. Activated carbons, zeolites, silicas, and metal-organic frameworks are among the most frequently used adsorbents to this end. Utilizing MOFs for this purpose offers a significant advantage in terms of customization, as the pore structure and surface chemistry of these materials can be tailored to match specific applications, rendering them as highly versatile tools for adsorption processes. Among them, ZIFs, a sub-class of MOFs, are characterized by a high specific surface area, a flexible and ultra-hydrophobic pore structure and a high chemical and thermal stability [1]. These properties and the simpleness of the synthesis protocols make them ideal adsorbents for gas and liquid-phase adsorption processes. Compared to conventional adsorbents, ZIFs can suffer structural changes upon adsorption. Gate-opening, phase transition, breathing, etc., have been widely reported in the literature for ZIFs upon an external stimulus [2,3]. Despite their relevance for the adsorption performance and the selectivity of the process, structural changes in liquid-phase adsorption processes are less described. Based on these premises, the aim of this study is to identify potential structural changes in ZIFs upon liquid-phase adsorption, preferentially for aromatic contaminants, and to perform a comparative analysis with similar structural phenomena upon gas adsorption. This comparison will be achieved through the integration of adsorption studies, chemical and structural characterization techniques, modeling, as well as synchrotron-based measurements conducted prior and post-adsorption.

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