

Molecular Level Insights into the Adsorption of Perfluorooctanoic Acid on Clay Surfaces

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Abstract : Perfluorooctanoic acid (PFOA), a persistent and hazardous member of the per- and polyfluoroalkyl substances (PFAS) family, presents significant environmental challenges due to its exceptional durability, potential for bioaccumulation, and mobility in natural systems. As a "forever chemical," PFOA resists degradation, resulting in widespread contamination of soils and sediments. This study investigates the molecular-level mechanisms governing the adsorption of PFOA on two negatively charged clay minerals, kaolinite, and montmorillonite, under the influence of humic acid. Adsorption behavior is analyzed using the Langmuir isotherm model under two conditions: humic acid-coated clay to mimic organic substances and non-coated clay. The study also examines the effects of pH levels of 2 and 7, focusing on the role of protonation states, clay surface characteristics, and solution chemistry in influencing adsorption dynamics. Humic acid, an organic substance formed from the decomposition of plant and animal matter, significantly influences the surface properties of clay particles. By altering surface charge, increasing hydrophobicity, and providing additional binding sites, it enhances the clays' ability to interact with PFOA. Typically, the negatively charged surfaces of kaolinite and montmorillonite repel the equally negatively charged PFOA molecules, creating electrostatic repulsion that limits direct adsorption. However, the cation exchange capacity (CEC) of these clays is a pivotal factor that allows them to retain positively charged species, such as metal ions or functional groups introduced by humic acid coatings. These positively charged components act as intermediaries, bridging electrostatic interactions and facilitating hydrophobic partitioning, ultimately increasing the adsorption efficiency of PFOA onto the clay surfaces. At pH 2, increased protonation of the clay surfaces reduces electrostatic repulsion, enhancing PFOA adsorption, while humic acid coatings provide additional binding sites due to hydrophobicity. Conversely, at pH 7, adsorption is reduced due to dominant electrostatic repulsion, lower surface protonation, and competition between PFOA and humic acid components for available adsorption sites. This study provides molecular-level insights into the critical roles of clay chemistry, CEC, organic matter, and interfacial dynamics in overcoming electrostatic barriers to PFOA adsorption. By highlighting the essential role of organic matter in overcoming electrostatic repulsion, this work contributes to the development of more effective strategies for mitigating PFAS contamination in soils and water systems, offering valuable guidance for environmental remediation efforts.

Keywords : adsorption, clay surface, humic acid, Langmuir isotherm, prfluorooctanoic acid, PFAS

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