Molecular Docking and Adsorption of 'forever molecules': Per- and Polyfluoroalkyl onto 2D Carbon Nanomaterials

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Per- and polyfluoroalkyl substances (PFAS) have emerged as a significant environmental threat due to their persistence, bioaccumulative nature, and potential toxicity [1]. These synthetic compounds, extensively utilized in various industrial and consumer products, have now become widespread in water, air, soil, and even within living organisms on a global scale. Their pervasive presence raises serious concerns, as once released, PFAS can contaminate groundwater, surface water, and drinking water supplies, posing considerable risks to both human health and aquatic ecosystems [2]. This research explores the application of graphene oxide (GO) and graphene (G) for the adsorptive removal of PFAS from aqueous environments. GO, along with its derivatives, has garnered significant attention due to its excellent dispersibility in water, enhanced chemical functionality, and robust three-dimensional structure [3]. These attributes position it as a promising material for solid-liquid separation processes, enabling effective PFAS adsorption while also reducing operational costs in water treatment systems. To unravel the adsorption mechanisms involved, computational methods such as Density Functional Theory (DFT), Monte Carlo (MC) simulations, and Molecular Dynamics (MD) simulations were employed. These approaches provided critical insights into the interactions between GO and four specific PFAS molecules: GenX, ADONA, perfluorooctanoic acid (PFOA), and perfluorooctanesulfonic acid (PFOS). The results from this study are crucial in advancing the development of sustainable, environmentally friendly solutions for PFAS removal. By elucidating the fundamental principles governing the adsorption of PFAS onto GO, this research lays the groundwork for designing innovative materials and processes to tackle the growing issue of PFAS pollution. The findings offer promising potential for the development of more efficient water treatment technologies to address this urgent environmental concern. Furthermore, molecular docking of PFAS with human proteins, such as serum albumin, plays a pivotal role in unravelling their transport mechanisms within the human body. By providing detailed insights into how these highly persistent chemicals interact and bind with proteins, docking studies reveal key factors that influence their systemic distribution, bioaccumulation, and associated toxic effects. This deeper understanding is essential for accurately assessing the risks PFAS pose to human health and for developing targeted strategies to mitigate exposure and contamination.

References

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