Analyzing Per- and Polyfluoroalkyl Substances (PFAS) Through Atomistic Simulations

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Per- and polyfluoroalkyl substances (PFAS), a class of highly fluorinated hydrocarbons, pose global contamination and pollution concerns due to both their toxicity and their potential to increase risks of reproductive disorders, endocrine disruption, and cancer. The resistance of such substances to degradation in the environment has earned them the title of “forever chemicals.” Two of the most abundant PFAS species, Perfluorooctanoic Acid (PFOA) and Perfluorooctane Sulfonate (PFOS), have been associated with tens of thousands of deaths annually. Despite extensive recent efforts, analysis of the molecular-level behavior of PFOA and PFOS has remained elusive. To address this knowledge gap, we conduct extensive investigation of the properties of PFOA and PFOS through first-principles electronic structure and molecular mechanics calculations. Utilizing both classical Molecular Dynamics (MD) and quantum Density Functional Theory (DFT) techniques, we perform structural optimization of PFOA and PFOS molecules in simulation cells; such structures are utilized to characterize time-evolution of molecular systems. We also study chemical properties of PFOA and PFOS when placed in larger systems, such as diffusion in aqueous environments and hydrophobicity. Our MD and DFT results align closely with experimental results and contribute the first detailed atomic-level studies of PFAS substances. Moreover, we discover atomic-scale reductive defluorination of PFOA catalyzed by Cobalt-containing Vitamin B12 complexes, furthering our understanding of PFOA degradation mechanisms. Thus, our study provides a molecular-level basis for mitigating the toxic effects of PFAS substances, potentially offering protections for 200 million exposed individuals within the U.S. – and far more globally.