Overcome the Challenge of Per- and Polyfluorinated Substances (PFAS) Removal in Aquatic Systems using Molecular Tailoring Technology

Overview/Abstract

Per- and Polyfluorinated substances (PFAS) are a family of toxic chemicals that have been widely used for over 70 years in industrial and consumer products including surfactants intermediates and non-stick cookware coating. In recent years, PFAS have been classified as "emerging contaminants" by the U.S. EPA and drawn great attention due to their high persistence and wide contamination in environment and harmful impact on human health. Currently, tap water has become one of the major sources for human exposure to PFAS, and about 45% of the nation's tap water is estimated to have at least one type of PFAS. While conventional adsorbents, such as granular activated carbon (GAC) and resins, show 50 - 90% removal efficiency for long-chain PFAS (>8C), they are typically poor removal efficiency and early breakthroughs for short-chain PFAS (<4C) from waters, largely due to the lack of selectivity to PFAS and the competition from dissolved organic matter (DOM) and ions in water matrix.

Covalent organic frameworks (COFs) are a class of highly ordered network polymers with extremely high surface area and exceptional stability and have shown 3-5 times higher adsorption capacity towards long-chain PFAS than conventional adsorbents. However, COFs adsorption capacity is also impacted by DOM in nature water due to the lack of selectivity. Molecular imprinting polymers (MIPs), also termed plastic antibody, is another class of promising polymers that can create highly selective binding sites for PFAS but their application as adsorbents is limited because porous skeletons of MIPS tend to deform and collapse, declining their selectivity with time due to a lack of strong frame support between the functional binding sites. The integration of these two promising technologies to make molecularly printed binding sites on the frame of COFs, can produce a new polymer MI-COFs with the combined outstanding features of high selectivity, stable rigid skeleton, and exceptional surface area. Currently, the research on MI-COFs is at the initial stage but has shown promising potential in the application of sensor technologies and organic compound extraction. The use of MI-COFs as adsorbents for PFAS removal has not been studied yet. In this project, we propose to explore the MI-COFs polymers for short-chain PFAS and advance their application on short-chain PFAS removal in aquatic contaminant remediations. We hypothesize that the new MI-COFs tailored using short-chain PFAS as template will show high selectivity, binding affinity, and capacity, and can efficiently eliminate the interference from DOM and foreign ions on PFAS removal. Functional monomers, crosslinkers, and organic building units that have high affinity to PFAS molecules will be screened and used to predesign and tailor the MI-COFs polymers. The performance of MI-COFs for PFAS adsorption will be systematically evaluated under equilibrium (batch experiments) and nonequilibrium (column experiments). The specific objectives of the proposed research include: 1) design and synthesize MIPs that show high selectivity to short-chain PFAS, 2) design and synthesize COFs which have high adsorption capacity, and 3) tailor MI-COFs composite adsorbents, and advance PFAS removal technology in real world natural water systems. The data of this project will be used to secure external funding from federal and state funding agencies.