**PFAS SURFACTANT BINDING TO FUNCTIONAL POLYMERS FOR ENVIRONMENTAL SEPARATIONS**

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**ABSTRACT**

Surface active per- and polyfluoroalkyl substances (PFAS) find niche applications because of their high chemical and thermal stability, their incompatibility with both water and hydrocarbons, and their unique ability to render surfaces non-stick. However, several widely used PFAS surfactants have been found extremely resistant to degradation, accumulate in the environment, and have long half-lives in humans, consequently causing great concern [1-3].

In the context of developing materials and processes for sequestering PFAS surfactants from aqueous media, we research how such surfactants associate with (bind to) other molecules or particles/surfaces. To this end, we utilize complementary experiments (small-angle neutron scattering, SANS, with contrast variation) and modeling (molecular dynamics, MD), and present here examples on how the structure of micelles formed in water by the notorious PFAS surfactant perfluorooctanoate (PFOA) responds to the presence of various additives (salt [4], urea [5], ethanol [6]) and polymers (homopolymer poly(ethylene oxide) (PEO), PEO-based amphiphilic block copolymers [7]) across a wide range of compositions. A detailed description emerges on how the additives or polymer segments distribute at the outer surface of the micelles and in their interior, which is used to rationalize the macroscopic behavior and various properties of the mixtures.

Fundamental knowledge on PFAS surfactant–polymer interactions supports the design of new materials to selectively capture and remove such surfactants from aqueous media. Self-assembly into micelles is a key feature of surfactants in aqueous solution, and reveals how PFAS surfactants interact with themselves and with solvent (water) and other molecules present in solution. The capability established in our study to predict from first principles micelle formation and structure confirms that such multiple and often competing interactions have been properly accounted for. Micelles are relevant to environment and health in that PFAS surfactants, while typically found in very low bulk solution concentrations, they tend to concentrate a lot (partition) in the vicinity of surfaces in the context of separations (activated carbon, ion exchange resins) and in the context of biointerfaces (proteins, lipid membranes).

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