

# **PFAS adsorption via novel amphiphilic silane functionalized membranes and subsequent destruction utilizing magnetite nanoparticle catalyzed UV-Fenton chemistry**

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Novel technologies for capture and destruction of PFAS are becoming increasingly important as PFAS contamination increases in drinking water throughout the globe. A number of physical adsorption techniques have been implemented on large-scale for PFAS removal, however, these techniques are limited by their high cost and low adsorption efficiency, especially for short and ultra-short chain PFAS. A novel filtration membrane was developed by functionalization of an Al-O(OH) membrane with amphiphilic silanes. Under dynamic filtration conditions, >99% removal was achieved for 11 out of 18 PFAS listed in the EPA 537.1. Comparison with GAC indicated that the amphiphilic coating improved capture efficiency with breakthrough performance 30 to 80 times greater for PFOA, and even greater for PFOS. Enhanced sampling metadynamics simulations to compute binding free energies of PFAS with the membrane surface were implemented to study the influence of chemical design on capture of difficult to remove PFAS. Modification of the amphiphilic chain based on computational results improved performance to >90% removal for 18 out of 18 PFAS listed in the EPA 537.1. This alteration simultaneously achieved >95% removal for PFBA and >80% removal for PFPrA, two ultra-short chain PFAS.

Following concentration of PFAS via adsorption membranes or other wastewater treatment processes, UV-Fenton chemistry catalyzed by nanosize magnetite ( $\text{Fe}_3\text{O}_4$ ) particles and hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) can be utilized as a promising method for disrupting PFAS carbon-fluorine bonds. We observe greater than 90% degradation efficiency for 14 out of 18 PFAS compounds defined by the EPA 537.1 by UV-Fenton reaction. PFAS destruction efficiency is enhanced at elevated pH levels; however, by varying both the  $\text{Fe}_3\text{O}_4$  mineral form and  $\text{H}_2\text{O}_2$  concentration in solution, improved efficiency can be achieved for difficult to destroy short chain PFAS at neutral pH conditions, such as those found in drinking water. High resolution mass spectrometry (HRMS) was utilized to demonstrate destruction efficiency and to identify degradation products. Throughout the process,  $\text{Fe}_3\text{O}_4$  retained its oxidation state and catalytic efficiency after multiple cycles of PFAS destruction, indicating the material is reusable, and showed no drop in degradation efficiency after multiple uses and may be an