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High-Performance Electrosorption, Desorption and Oxidation of Perfluoroalkyl Carboxylic Acids (PFCAs, C4&C8) using MXene-based Membrane Filtration

Per- and Polyfluoroalkyl Substances (PFASs) are a group of anthropogenic chemicals that have been produced and used for over 60 years in a broad spectrum of industrial products or processes and result in prevalent environmental pollution. Many conventional treatment processes are not effective for PFAS separation or degradation due to the low concentrations and the stable covalent C−F bond. Advanced oxidation processes like electrochemical oxidation and photocatalytic oxidation are more effective for perfluoroalkyl carboxylic acids (PFCA) than perfluoroalkyl sulfonic acids (PFSA). Besides, these technologies are expensive and have high energy footprints. Adsorption using granular carbon or anionic ion exchange is commonly used to separate PFAS from water but requires further disposal and destruction of the concentrated PFAS. Electrosorption has proven effective towards separation of many water pollutants (e.g., fluoride, ammonium, nitrate, arsenic, and uranium) with low energy and chemical consumption. Carbonaceous materials such as activated carbon, carbon nanotubes (CNTs), and reduced graphene oxide (rGO) have been used for electrochemical adsorption to separate the low concentration PFAS (often at sub ppb levels) from water and also achieve controlled desorption process. However, the lack of reactivity of carbonous materials lead to the low efficiency of PFAS destruction. This project aims to develop and evaluate electrically assisted adsorption of both short and long chained PFCAs using externally charged electrically conducting membranes (ECMs) made of selected carbonaceous nanomaterials (CNMs) or transition metal carbides (MXenes). We evaluated the adsorption and desorption kinetics and capacity under variations of DC charges/currents. Herein, an MXene-based membrane filtration process was used for the PFOA and PFBA adsorption and destruction. Specifically, Ti3C2Tx for different surface terminations (T=F, O and Cl) were prepared and the results show that the oxygen terminated MXene-based membrane has significantly higher adsorption capacity (215 mg·g−1) and a degradation rate constant (2.8×10−2 min−1) compared to those with the F and Cl terminations. Electrochemical oxidation treatment with an applied +6 V potential in the 0.1 M Na2SO4 solution yielded >99 % reduction of the PFOA or PFBA (1 ppm) in 3 hours. The density functional theory (DFT) calculations revel the O-terminated MXene surface on Ti3C2O2 yielded the highest PFOA/PFBA adsorption energy. Bader charge analysis shows that when interacting with PFOA, Ti3C2O2 with surface defects (e.g., missing of O, Cl, or F atoms) donates 0.19 |e| and 0.28 |e| more electrons to PFOA relative to Ti3C2F2 and Ti3C2Cl2, respectively. Moreover, the reaction pathway of PFOA on Ti3C2O2 is most favorable among these three MXene structures as indicated by the greater negative free energies. Thus, synthesizing MXene with O-terminated surface could be critical to efficient PFAS adsorption and degradation. The collaboration team for this NJIT-BGU seed grant project also consists of Dr. Joshua Young (NJIT), Dr. Mengqiang Zhao (NJIT), Dr. Avner Ronen (BGU) and Dr. Chris Arnousch (BGU).

Wen Zhang is currently an associate professor of NJIT's Newark College of Engineering in the Department of Civil and Environmental Engineering with a second appointment in the Department of Chemical and Material Engineering. Wen is a licensed Professional Engineer (P.E.) registered in the States of New Jersey and Delaware. He is an American Academy of Environmental Engineers and Scientists (AAEES) Board Certified Environmental Engineer (BCEE). Dr. Wen Zhang's research focuses on colloidal interfaces and processes that are crucial for environmental and chemical engineering applications. His research embraces environmental behavior and interfacial processes for nanomaterials, microplastics and soft particles such as microbes and bubbles, catalytic/reactive membrane filtration systems for desalination, resource recovery and emerging contaminant removal, photocatalysis, microalgal removal and harvesting. His latest research also expands from agricultural applications of nanobubbles to lithium recovery from spent lithium-ion batteries.