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CIVIL & ENVIRONMENTAL ENGINEERING SEMINAR SERIES

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Computational Modeling of Materials for Perfluoroalkyl Substance Removal from Water

Recently, a large family of molecules called perfluoroalkyl substances (PFAS) have garnered attention as emerging contaminants of major concern as they can cause health problems in humans. These compounds were extensively used because of their water-resistant properties, but this same fact means that they do not degrade in aqueous environments. Furthermore, their low concentration means that traditional separation technology cannot efficiently remove them; as such, new materials and technologies are urgently needed for remediation by capturing PFAS molecules from the environment. First, adsorptive removal has been found to be a promising method for PFAS remediation because of its low energy requirements, low cost, and ability to concentrate the PFAS in a waste stream for more efficient destruction. Two promising family of materials for adsorption of aqueous pollutants are the metal organic frameworks (MOFs, which consist of metal or metal-oxide centers connected by organic linkers) and covalent organic frameworks (COFs, which consist only of organic molecules ("linkers") covalently bonded together. In this work, we investigated the adsorption of PFAS molecules in a wide variety of these compounds, including the M-MOF-74 (M = transition metal) family, and COF-300, BF-COF1, and BF-COF2. We found that (a) changing the transition metal in M-MOF-74 can dramatically improve PFAS adsorption and (b) the COFs may be able to strongly adsorb small chain PFAS. Second, we investigated destruction of PFAS on the 2D family of Ti3C2X2 (X = O, F, Cl) MXenes. Density functional theory results demonstrate that O-termination of these MXenes can result in strong PFAS adsorption and effective degradation. These results were compared with those of our experimental collaborators and demonstrate good agreement in observed trends, demonstrating synthesis of these materials and their integration into membranes is a good route to PFAS remediation. Our collaborators for these projects are Dr. Roni Kasher (BGU), Dr. Wen Zhang (NJIT), Dr. Meng-Qiang Zhao (NJIT), Dr. Sagnik Basuray (NJIT), and Dr. Avner Ronen (BGU).

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