

Functionalized nanocomposites via eutectic solvent for environmentally sustainable applications

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Per- and polyfluoroalkyl substances (PFAS) are persistent organic pollutants of global concern due to their exceptional chemical stability, bioaccumulative potential, and toxicity. Conventional adsorbents struggle to effectively remove PFAS or function across diverse pH and ionic strength conditions. Herein, we propose the use of MXene-based composites intercalated with deep eutectic solvents (DESs) as a novel hybrid membrane for PFAS removal from wastewater. In this study, we introduce a greener modified method to synthesize 2D MXene integrated with intercalation mechanism using a low-cost DES. The selection of the desired DES was based on screening over 200 compounds optimized through density functional theory (DFT) towards Perfluoropropionic acid (PFPrA) and Perfluorooctanoic acid (PFOA). Besides, best performing compounds molecular interaction with different PFAS types was further investigated using classical molecular dynamics. The intercalation of DESs within $Ti_3C_2T_x$ layers enhances surface accessibility and tailors electrostatic and hydrophobic interactions toward PFAS molecules. The tunability of DES composition offers a promising strategy for tailoring MXene–DES hybrids toward specific PFAS targets and environmental matrices.

References

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