Computational and experimental study on the adsorption of short- and long-chain PFAS by using MXene/MOF based material

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are persistent, mobile fluorinated contaminants of growing concern. We developed a polydopamine-modified MXene/MIL-100(Fe) nanocomposite (PDA-MXene@MIL-100(Fe)) and evaluated its adsorption for three PFAS both long- and short-chain. Morphology, stability, and surface chemistry were confirmed by SEM, TGA, ζ-potential, XRD, and FTIR. Batch studies across pH showed excellent uptake in acidic conditions; equilibrium studies showed the Freundlich isotherm model, indicating heterogeneous, multi-site adsorption, while kinetics followed a pseudo-second-order model. . The composite showed good removal in real municipal wastewater matrices as well. Computational modeling with DFT (Density Functional Theory) and COSMO-RS (conductor-like screening model for real solvents) were used to describe the adsorption mechanism.

Methodology:

The adsorption experiments were carried out in batch mode. Each experiment was performed for PFAS mixture composed of PFOA, PFHpA, and PFHxA. To evaluate the effect of pH on adsorption performance, the pH of the PFAS solution was adjusted to values of 3, 5, 7, and 9. Subsequently, 30 mg of sorbent, was added individually to the PFAS solutions. For kinetic studies, same mixtures and amount of sorbent were added to the flask at pH 3 conditions. Subsamples were withdrawn at predetermined time intervals: 2, 10, 20, 30, 60, 120, 180, 360, and 1440 mins, to monitor adsorption kinetics. PFOA, PFHpA, PFHxA, MXene, PDA-MX(Ti)), MIL100(Fe), and the composite PDA-MX(Ti)@MIL100 were optimized by using geometry optimization module from DMol3 of Material Studio 2020. The output files from Materials Studio were converted into the *cosmo* format, which is required for applying the conductor-like screening model for real solvents (COSMO-RS) .

References

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Figures

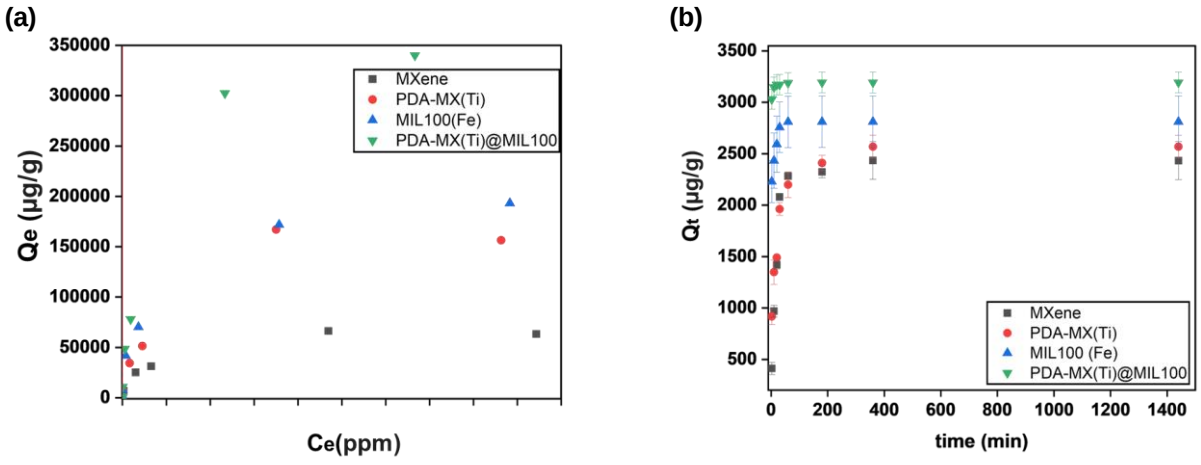

Figure 1: (a) Isotherm data for PFAS adsorption taken at different initial concentration, 60 min and 25 ˚C (b) Kinetics data for PFAS adsorption taken at 1 ppm initial concentration , 60 min and 25 ˚C.