PFAS removal from water using hydrotalcite and hydrotalcite nanoparticles

Poly- and perfluoroalkyl substances (PFAS) are human-made chemicals that are often used in household products, industrial products, and firefighting foams. They are called “Forever chemicals” because they don’t break down easily and can stay in the environment for a very long time. PFAS can cause harmful health effects like cancer, hormone disruption, and liver damage. To remove PFAS from the environment, conventional methods like activated carbon and ion exchange resins have limitations.

This project aims to find better ways to remove PFAS from water using hydrotalcite minerals. Hydrotalcite can adsorb and eliminate PFAS from water, but its performance can be improved by modifying it. Computational methods will be used to study how PFAS and hydrotalcite interact at the molecular level and how to optimize their adsorption. This research will help develop more effective solutions for cleaning PFAS-contaminated water.

Abstract

Poly- and perfluoroalkyl substances (PFAS) are anthropogenic chemicals, which are a class of highly fluorinated synthetic chemicals known as “Forever chemicals” due to their persistence in the environment. They are frequently used in many households, industrial products, and firefighting foams. PFAS are persistent in nature, highly soluble in aquatic environment, and associated with damaging health effects such as carcinogenicity, endocrine disruption, and liver damage. Hence, effective techniques are needed to remove the PFAS present in the environment.

Conventional methods like activated carbon and ion exchange resins have limitations, including reduced efficiency in the presence of dissolved organic matter and lack of selectivity for PFAS removal.

This project will investigate the efficient removal of perfluoroalkyl acids (PFAAs) such as PFOA and PFOS from the water using different hydrotalcite (HT) types. These are also known as anionic clays and are a family of layered minerals. HT generally exhibit positive surface charges over a range of environmentally relevant pH conditions, making them suitable for the adsorptive removal of anionic pollutants. It will be synthesized by tailoring its surface properties to check the sorption of PFAS commercially available HTs. Computational methods such as molecular dynamics simulation and density functional theory will be used to understand the surface interaction of PFAS and hydrotalcite. MD simulations will help understand the adsorption behaviour of PFAS on the hydrotalcite surface, providing insights into the adsorption mechanism and factors that influence the adsorption behaviour.