Mesoscopic modeling of PFAS aggregation and adsorption on model mineral surfaces

PhD position at IFP Energies nouvelles (IFPEN)

Thousands of per- and polyfluoroalkyl substances (PFAS) have been synthesized since the mid-20th century. These compounds, selected for their exceptional properties, find many applications in our daily lives, including waterproofing textiles, food packaging, firefighting foams, and non-stick coatings for kitchen utensils. However, the strength of the C-F bonds gives PFAS a very high stability, making these compounds highly resistant to degradation in the environment, earning them the nickname "forever chemicals." These chemicals accumulate in water, soil, and even in the tissues of living organisms, infiltrating food and water supplies. Due to their amphiphilic nature—possessing both hydrophobic and hydrophilic properties—PFAS adsorb onto organic matter, soil particles, and diverse surfaces, thereby complicating their removal from contaminated sites. While long chain PFAS strongly absorb onto activated carbon materials commonly used in water filtration systems, shorter-chain PFAS exhibit weaker affinity, posing greater challenges for capture and removal. Although solutions such as advanced filtration systems and adsorption techniques have been proposed to address PFAS contamination, these technologies remain imperfect. Significant research efforts are needed to develop more effective and sustainable technologies for PFAS remediation. This includes a deeper understanding of the molecular-level interactions of these substances and the exploration of innovative approaches for their capture, ensuring a healthier and cleaner environment for future generations.

In this context, we propose a thesis topic focused on the use of molecular modeling techniques, in particular Dissipative Particle Dynamics (DPD), to simulate the adsorption of PFAS in aqueous solution on porous materials and mineral surfaces representative of real materials. A coarse-grained model, already available in the laboratory, makes it possible to describe the behavior of PFAS in solution and to predict the critical micellar concentration values for fluorocarboned surfactants. The thesis work will therefore consist in developing a methodology to model the adsorbent material using a coarse-grained approach. Numerical simulations of adsorption will then be performed for different systems and conditions in order to better understand the role of the variables involved, such as the size of the molecules, the chemistry and topology of the surface, the competitions between PFAS, etc.

Your Qualifications

You should have a university master's degree in chemical sciences with strong motivation in scientific research and innovation and team collaboration spirit. You have good academic ethics, rigorous scientific attitude and general knowledge in physical chemistry with basic notions in the following fields: adsorption, molecular modeling, programming (Python) &/or machine learning. Fluency in English, and in French or willingness to learn French. The starting date will be in November 2025.

We Offer

3 year position at IFP Energies nouvelles (Rueil-Malmaison, France). Our institution is a leading research institute that is globally recognized for its research, innovation, and scientific value.

Application procedure on the IFP Energies Nouvelles website

Applications must be submitted to Dr. Carlos Nieto-Draghi (carlos.nieto@ifpen.fr, ORCID: 0000-0001-5956-9259), Dr. Benoit Creton (benoit.creton@ifpen.fr, ORCID: 0000-0002-3287-877X) with the following elements: 1) motivation letter stating your research interests, 2) CV.