Molecular modeling of solvent/polymer interactions in the context of PVC recycling

Postdoctoral position at IFP Energies nouvelles (IFPEN)

Recycling plastic waste, particularly PVC, necessitates tailored regeneration processes due to the presence of harmful additives such as lead metal stabilizers and phthalate-based plasticizers. The deformulation method, which can involve dissolving PVC to isolate and purify the polymer fraction, is highlighted as a promising solution. This technique enables the recovery of polymers free from additives, potentially reformable as virgin polymers, while minimizing environmental impacts. However, our understanding of the physicochemical phenomena involved in PVC deformulation remains limited, despite extensive prior research on polymer dissolution. Molecular Dynamics (MD) simulations play a crucial role in developing recycling strategies for PVC waste, offering a molecular-level perspective that enhances our understanding of polymer-solvent interactions. Nevertheless, the complexity of polymer systems necessitates multi-scale simulation approaches, from quantum chemistry to continuum methods, to encompass the various relevant time and length scales. The coarse-grained (CG) approach is particularly effective for modeling polymers, despite the fact that it sacrifices atomistic details to access larger time and length scales unattainable with all-atom-based simulations.

In this postdoctoral project, we will focus on predicting molecular solvent-polymer interaction energies using a mesoscopic approach to better understand the solvation phenomena of PVC polymer matrix's models, that realistically reflects the structure of polymers with entanglements and long chains, with the inclusion of most common additives. The initial phase of the postdoctoral activity will involve a focused literature review on molecular simulations applied to the dissolution mechanisms of PVC, aiming to identify the most effective coarse-grained simulation methods for estimating characteristics and properties such as the radius of gyration, end-to-end distance, and solvation free energy. The study will also explore the potential of using mixed solvents and to predict additive selectivity. The findings are intended to be valorised through scientific publications.

Your Qualifications

You should have a PhD in the application of coarse-grained simulation of polymer solutions 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 notions in the following fields: polymer science, molecular modeling, programming (Python) & machine learning. A B2 level in English (CEFR) is compulsory. The starting date will be in May 2025.

We Offer

18-month postdoctoral 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. This postdoctoral project is part of the French PEPR recycling initiative.

Application procedure

Applications must be submitted to Dr. Carlos Nieto-Draghi (carlos.nieto@ifpen.fr, ORCID: 0000-0001-5956-9259), Dr. Alexandra Chaumonnot (alexandra.chaumonnot@ifpen.fr) or Dr. Benoit Creton (benoit.creton@ifpen.fr, ORCID: 0000-0002-3287-877X) with the following elements: 1) Application (motivation letter stating your research interests), 2) CV, 3) Copy of PhD diploma/certificate, 4) 2 Letters of recommendations.