Design of sustainable fluids using machine learning and molecular simulation

Professor Erich Muller

We are seeking highly motivated candidates for fully funded PhD projects at the exciting interface of molecular simulation and machine learning to design the next generation of sustainable fluids. This pioneering research focuses on creating environmentally benign lubricants, solvents, and refrigerants from the ground up by computationally predicting their physical, chemical, and environmental properties. In this project, you will employ state-of-the-art molecular dynamics and Monte Carlo simulations to generate vast datasets of molecular behaviour, which you will then use to train sophisticated machine learning models. The ultimate goal is to develop an innovative in silico framework that rapidly screens and optimises novel chemical structures, accelerating the discovery of high-performance, non-toxic, and biodegradable fluids to solve critical industrial and environmental challenges. Ideal applicants will have a strong background in chemistry, physics, chemical engineering, or a related discipline, with a keen interest in computational science and a passion for sustainability.