

# Molecular Modelling for use in Multi-Scale Simulation Tools

## Background

Our group are working on the development of a new modelling tool. A key aspect of the success of the tool is to combine simulations on different scales, combining large-scale simulations determined by properties on the molecular scale.

## Description

The purpose of the project is twofold, firstly to learn more about molecular modelling and molecular modelling tools, e.g. GROMACS and LAMPS. Secondly, how to use such tools in connection with process models.

The project has no prerequisites, but the student should have an interest in learning about molecular modelling techniques and modern simulation technologies.

## Supervision

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