Our team focuses on the theoretical modelling of biochemical and biophysical processes at a molecular, atomic, and electronic level of detail. We place emphasis both on development of methods and on their application to specific systems. Particular areas of interest include: protein engineering, drug design and software development.

Objectives

Main objectives include:

- Developing our in-house code Monte Carlo (PELE) for better sampling of protein/DNA-ligand interactions
- Improving the user experience in interactive molecular modelling by combining biophysics/biochemistry software with state-of-the-art graphics, High Performance Computing and Artificial Intelligence.
- Develop new approaches for mapping in silico protein engineering focusing on: protein mutation, substrate migration and chemical process.
- Application studies of our (and others') modelling techniques for addressing specific biomedicine and biotechnology problems. Here we aim to establish collaboration with top experimental labs and industries.