National Training School in Theoretical Chemistry

Intermolecular Potentials and Methods of Computer Simulation

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Molecular simulations have become an increasingly important research tool in the physical sciences. Realistic atomistic simulations can provide a direct visualization of processes occurring at the molecular level, and simulations of model systems can allow theories to be tested, and the origins of complex behaviour to be unravelled.

These lectures will focus on the two basics methods of molecular simulation, namely molecular dynamics and Monte Carlo, as well as providing an overview of what can be achieved through more advanced techniques. A prerequisite for any simulation is a means to calculate the energy of the system, and the lectures will also provide an introduction to field of intermolecular potentials, focussing on the forms commonly used in simulations and their drawbacks.

The aim of the lectures is to provide students with a better appreciation of how simulations work and what they can achieve, and to be a starting point for those wishing to write their own simulation codes.