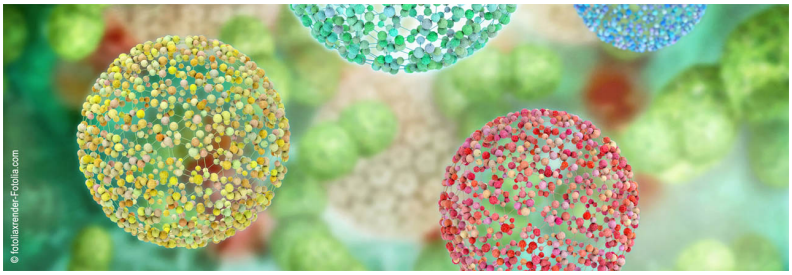

Contribution ID: **5** Type: **not specified**

Lecture 3: Computer simulation of molecular systems - Principles and example applications

Wednesday, 5 July 2023 09:00 (1h 30m)

Computer simulations are widely used in the natural sciences to get insight into the behaviour of molecular systems at a microscopie level. ln this lecture, we will introduce the basic principles of Monte Carlo (MC) and Molecular Dynamics (MD) simulations based on a classical description of the energy of the system. We will get to know the basics of a molecu lar mechan ics force field, have a look at how molecular configurations are generated in MC sampling and MD simulation and learn about how to analyse the simulations to extract, for example, structural and thermodynamic properties of interest. For instance, how can we characterize the structure of a salt solution or how can we calculate the free energy of binding of a drug molecule to a receptor protein?

Presenter: Dr REIF, Maria