

Introduction to Molecular Dynamics Simulation

Overview:

Molecular dynamics (MD) simulation is a powerful tool for studying the behavior of biological systems, such as proteins, DNA, and cell membranes. MD simulation allows us to simulate the movement of atoms over time and provides atomistic insights into biological processes that are difficult or impossible to study experimentally. This day-long workshop is designed to provide an introduction to MD simulations.

Course Content:

The workshop will begin with an overview of the basic principles of MD simulations, including force fields, integration algorithms, and analysis methods. Following the introduction, participants will be guided through a series of basic and general tutorials on simulations and analyzing the results. The course does not require any specific prerequisites, and the goal is to enable students to learn more complex tutorials in the future.

Venue: University of Duisburg-Essen, Faculty of Physics, AG Kuiper,
Lotharstr. 1
47057 Duisburg
Germany
Office: MF 245
Closest Tram Station: Zoo/Uni Duisburg

Duration of the course: 2 June 2023, from 10:00am-4:00pm.

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