Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Institute for Molecular Physical Science (IMPS)

Einladung zu einem Kolloquium

Datum/Zeit:	**Dienstag, 10.12.2024, 16.45 Uhr**
Referent:	**Prof. Gerhard Hummer (Doktorandenwahlsprecher IMPS)** Max-Planck-Institut für Biophysik, Frankfurt am Main, Deutschland
Titel:	*Learning from molecular simulations*
Ort:	**HCI G7**

Molecular dynamics (MD) simulations allow us to probe complex molecular processes, from the nucleation of crystals to the function of the molecular machineries of life. In my presentation, I will showcase the power of traditional and emerging ways of using MD simulations through the combination with AI. I will first illustrate how we can use MD simulations to go from structure to mechanism by showing how the electrochemical potential across the inner mitochondrial membrane drives the rotation of the ATP synthase motor as the machine central to all life. I will then use our recent work on the mechanics and physicochemical characterization of the nuclear pore complex and its condensate-like permeability barrier to show how MD simulations allow us to integrate rich experimental data into concise models of cellular processes. I will conclude my presentation by outlining an AI-driven MD simulation algorithm that autonomously and simultaneously builds quantitative mechanistic models of complex molecular events, validates the models on the fly and in turn uses the models to accelerate the sampling.

Gäste sind willkommen