Interdisciplinary Center for Scientific Computing

UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

IWR COLLOQUIUM WINTER SEMESTER 2024/25

Prof. Tristan Bereau

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Generative Machine Learning for Molecular Simulations

Generative machine learning is offering new ways of tackling complex scientific problems. I will describe recent efforts in the context of multiscale molecular simulations of soft-matter systems: a combination of free-energy calculations, representation learning, and Bayesian optimization to design small molecules; a backmapping strategy that learns the atomistic distribution of atoms conditional on the coarse-grained degrees of freedom; and finally a denoising diffusion model to efficiently compute free energies.

Also streamed via Zoom

November 6, 2024 • 16:15

Mathematikon • Conference Room / 5th Floor
Im Neuenheimer Feld 205 • 69120 Heidelberg
www.iwr.uni-heidelberg.de/events/iwr-colloquium

HGS MathComp Mixer
Prior to the IWR-Colloquium: Get-together for all members of the HGS MathComp
15:45 · Mathematikon · Common Room / 5th Floor