

# IWR Colloquium

## Winter Semester 2024 / 2025

November 6, 2024 • 16:15

Mathematikon • Conference Room / 5th Floor

**Speaker:**

Prof. Tristan Bereau

Institute for Theoretical Physics, Heidelberg University

**Title:**

“Generative Machine Learning for Molecular Simulations”

**Abstract:**

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.

**Website Prof. Bereau:**

<https://tristanbereau.com/>

**Website IWR Colloquium:**

[www.iwr.uni-heidelberg.de/events/iwr-colloquium](http://www.iwr.uni-heidelberg.de/events/iwr-colloquium)