

# nanoSeminar Series 2020

Institute for Materials Science

**Prof. Dr. Tristan Bereau**

*MPI for Polymer research, Mainz, Germany*

**“Soft-matter materials modeling in the data-driven era”**

**Thursday, December 10<sup>th</sup> 2020**

**13:00 – 14:00**

Normal: Seminar Room 115, Hallwachsstr. 3 (HAL)

Pandemic version: <https://tinyurl.com/nanoSeminar-GA>

Advanced statistical methods are rapidly impregnating many scientific fields, offering new perspectives on long-standing problems. In materials science, data-driven methods are already bearing fruit in various disciplines, such as hard condensed matter or inorganic chemistry, while much less has happened in soft matter.

I will describe how we use data-driven methods to better understand structure-property relationships and move toward material/compound design in soft matter. The first example will consist of the design of polymer membranes with improved gas-separation properties. The training of kernel-based ML model on a relatively small experimental dataset led to the identification and experimental verification of exceptional CO<sub>2</sub>/CH<sub>4</sub> separation performance.

Moving to multiscale computer simulations, we explore the use of coarse-grained models in the context of compound screening. Modeling the passive permeation of drugs across a phospholipid membrane, we generate predictions for more than 1 million compounds, and connect key functional groups to the thermodynamic process. Finally, I will describe how we further connect back to an atomistic resolution using deep generative adversarial networks.

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## Prof. Dr. Tristan Bereau

Van 't Hoff Institute for Molecular Sciences and Informatics Institute  
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research Mainz, Germany*



Tristan Bereau is an assistant professor at the Van 't Hoff Institute for Molecular Sciences and the Informatics Institute of the University of Amsterdam. He completed a Ph.D. in Physics at Carnegie Mellon University, Pittsburgh, PA, USA. In 2012, Tristan moved to the University of Basel as a postdoctoral researcher. He was a group leader at the Max Planck Institute for Polymer Research from 2014, leading an Emmy Noether group from 2016 to 2019. His work focuses on the interface between multiscale modeling and machine learning for soft matter.