

## High-throughput screening of properties of liquids — on the computer

Prof. Dr. Tristan Bereau

*Institut für Theoretische Physik, Universität Heidelberg*

Advanced statistical methods are rapidly permeating 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 comparatively little has happened in soft matter. I will describe how we use multiscale simulations to leverage data-driven methods in soft matter. We aim at establishing structure-property relationships for complex thermodynamic processes across the chemical space of small molecules. Akin to screening experiments, we devise a high-throughput coarse-grained simulation framework. Coarse-graining is an appealing screening strategy for two main reasons: it significantly reduces the size of chemical space and it can suggest a low-dimensional representation of the structure-property relationship. I will briefly outline several applications of our methodology, including the establishment of structure-property relationships and molecular discovery. Finally, I will mention a number of ways machine learning can help fulfil the promise of connecting models at different scales.