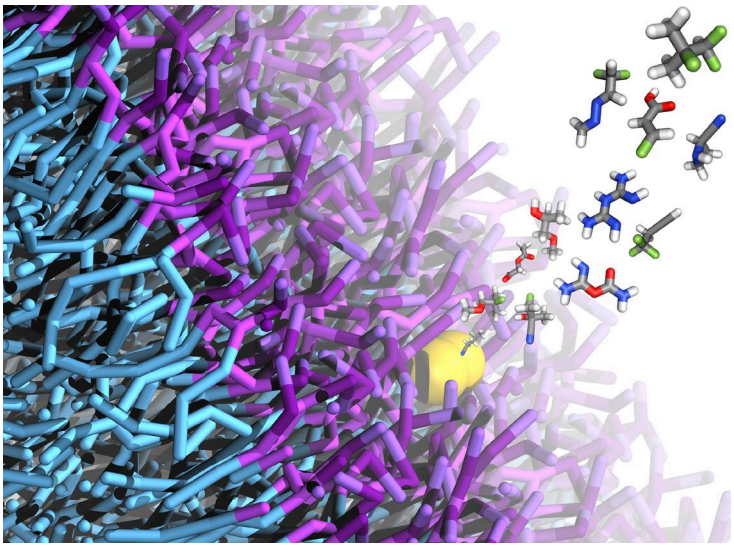
Physikalisches Institut
Fakultät für Mathematik und Physik
Albert-Ludwigs-Universität Freiburg

PHYSIKALISCHES KOLLOQUIUM

AM 05. FEBRUAR 2024 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



THE ROLE OF MULTISCALE MODELING IN MOLECULAR DISCOVERY

TRISTAN BEREAU

UNIVERSITÄT HEIDELBERG

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 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 mention a biological application of our methodology that led to the discovery of in vivo active compounds. Finally, I will mention a number of ways machine learning can help fulfill the promise of connecting models at different scales.