Symposium Data-driven Methods in Molecular Simulations of Soft-Matter Systems (SYMS)

jointly organized by
the Chemical and Polymer Physics Division (CPP),
the Biological Physics Division (BP),
the Dynamics and Statistical Physics Division (DY), and
the Metal and Material Physics Division (MM)

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Multiscale simulations offer an appealing framework to approach many soft-matter systems. Recently, the advancement of data-driven methods, pushed forward by the statistics and computer-science communities, has started making significant impact in various fields of condensed-matter physics, however mostly hard condensed matter. In contrast to hard matter, for soft matter intra- and intermolecular molecular entropy is as relevant as are interaction energies. This symposium will present and discuss early developments of data-driven methods applied to soft matter. It will provide a forum to help illustrate how these methods can help solve or ease problems in the field, e.g., force-field parametrization and adequate conformational sampling.

Overview of Invited Talks and Sessions

(Lecture room H 0105)

Invited Talks

SYMS 1.1	Mon	15:00–15:30	H 0105	**Stochastic numerical algorithms: from molecular dynamics to big data analytics** — •Benedict Leimkuhler
SYMS 1.2	Mon	15:30–16:00	H 0105	**A Generally-Applicable Machine-Learning Scheme for Materials and Molecules** — •Michele Ceriotti
SYMS 1.3	Mon	16:00–16:30	H 0105	**Girsanov reweighting for path ensembles and Markov state models** — •Bettina G. Keller, Luca Donati, Carsten Hartmann
SYMS 1.4	Mon	16:45–17:15	H 0105	**Liquid State Theory Meets Deep Learning and Molecular Informatics** — •Alpha Lee
SYMS 1.5	Mon	17:15–17:45	H 0105	**Computational high-throuhgput screening of drug-membrane thermodynamics** — •Tristan Bereau

Sessions

SYMS 1.1–1.5	Mon	15:00–17:45	H 0105	**Data-driven Methods in Molecular Simulations of Soft-Matter Systems**