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Multiscale simulations of soft matter augmented by data-driven methods

Multiscale simulations, all the way from quantum chemistry to continuum mechanics, probe a variety of length and time scales relevant to soft-matter systems. In this talk, I will describe different strategies to help improve physics-based simulations with recently-developed data-driven methods and concepts. Applications discussed will include Bayesian inference for molecular kinetics; machine learning to vastly improve force-field transferability; and high-throughput screening of drug-membrane thermodynamics.

Dr. Tristan Bereau
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room P 603, Mo. 29.10.2018, 13:30 h

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