PHYSIKALISCHES KOLLOQUIUM

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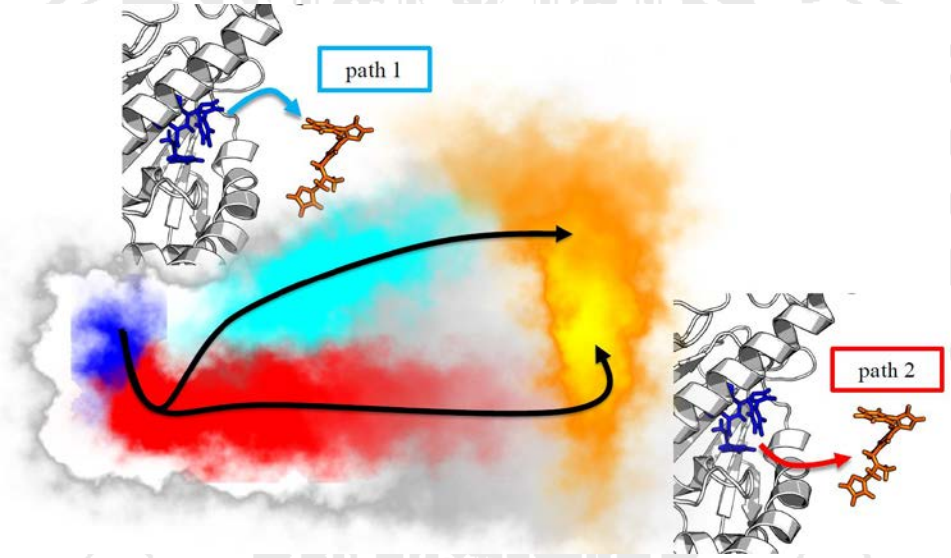
IM GROßEN HÖRSAAL



NON-EQUILIBRIUM DYNAMICS OF LIVING SOFT MATTER ON ATOMIC SCALES

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Biomolecular soft matter forms the nano-machinery of life. Its main players, i.e., proteins, DNA and RNA, display a complex pattern of self-organization that emerges from first principles of Physics. To understand these phenomena and the associated function of biomolecules, a microscopic description of their multiscale motions is essential. Molecular dynamics simulations provide a powerful approach to predict such dynamics directly from atomistic interactions. However, the necessity of integrating atomistic equations of motion on a femtosecond timescale contrast sharply with biologically relevant timescales of milliseconds to minutes. In this presentation, I will describe new methods to coarse-grain dynamics and accelerate simulations with the help of principles from non-equilibrium statistical mechanics. Using Jarzynski's equality, we derive a friction term that allows for an on-the-fly calculated dissipation correction. The application to realistic soft matter systems requires further theoretical developments such as a non-equilibrium extension of principal component analysis and machine learning of pathway separation. Langevin equation simulations in combination with temperature rescaling allows to access molecular dynamics on real timescales up to minutes with affordable computational cost. Furthermore, methods developed here are of interest for the prediction of velocity-dependent properties, such as friction in non-Newtonian liquids.