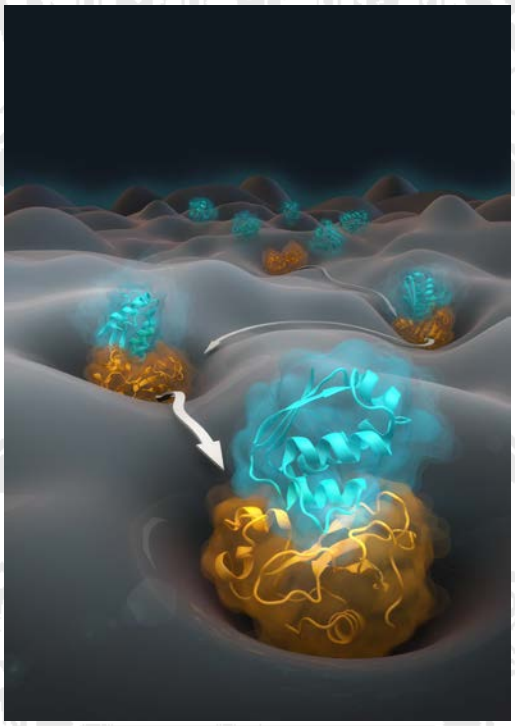
PHYSIKALISCHES KOLLOQUIUM

AM 18. DEZEMBER 2017 UM 17 UHR C.T.

IM GROßEN HÖRSAAL



MOLECULAR KINETICS AND MACHINE LEARNING

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Computing the molecular kinetics of biomolecular processes, such as protein folding or protein-protein association, is an extremely challenging problem as these dynamics are very high-dimensional and governed by rare event processes. I will show that the problem can be formulated as a variational problem where, similar as in quantum mechanics, the eigenfunctions of the underlying dynamical operator provide a subspace that contains the relevant rare-event processes. With such a dimension reduction technique - and a variety of other algorithmic tools such as Markov state models - we can reach beyond the seconds timescale with atomistic protein models and thus, for the first time, probe very rare event processes such as protein-protein dissociation in full spatiotemporal detail. Finally, I will elude to new deep learning techniques that are able to estimate highly accurate and robust models of molecular kinetics.