SFB 1078

Protonation Dynamics in Protein Function

Thu, **June 23th** 2022

16:15 Uhr

Hörsaal A, FUB

Arnimallee 14, 14195 Berlin

Colloquium

Prof. Ioan Andricioaei

Department of Chemistry, and Department of Physics and Astronomy, University of California, Irvine, US

Computer Simulations of the Interaction of Ions, DNA and Dendrimers with Protein Pores: Examples and Theoretical Models

Molecules pass through membrane pores one at a time, and therefore this process is to be fundamentally understood at the single-molecule level. In my talk, I will present computer simulation results obtained by my research team that showcase several examples of pore transport. Examples will include protein translocation through mitochondrial pores, DNA ejection from bacteriophage viruses, and dendrimer transport in the context of single-pore current measurements.

On the methodological side, two techniques developed for these simulations will be showcased. One uses molecular-dynamics derived parameters to scale up the dynamics on the micrometer-microsecond scale via the Kirchhoff theory for elastic rods. The other allows for the enhanced calculation of long-time kinetics in complex systems and is based on the Wiener stochastic path integral formalism: assigning weights to Langevin trajectories of artificially biased dynamics allows for the calculation of time correlation functions for the unbiased system of interest via re-weighting.

www.sfb1078.de