SFB 1078

Protonation Dynamics in Protein Function

Mon, **May 30th** 2022

15:30 Uhr

Freie Universität Berlin

Hörsaal B

Colloquium

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Modelling Membrane Transport and Protein Binding

The modeling of drug/protein and drug/lipid membrane interactions is fundamental to get insight into many relevant biological pathways. The simulation of such complex situations requires the application of different quantum and classical mechanical techniques. Moreover, these hybrid calculations are often performed within a dynamic framework in combination with enhanced-sampling approaches, such as umbrella sampling and accelerated molecular dynamics, to account for long time scale events. In this contribution, the application of many of these approaches will be illustrated by discussing the mechanisms of some biological events recently investigated by our research group, including the permeation of the antitumoral drug cisplatin though a lipid bilayer, the binding of different inhibitors to the RNA- dependent RNA polymerase protein of SARS-CoV-2, and the binding of photoswitches to a voltage-gated ion channel.

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