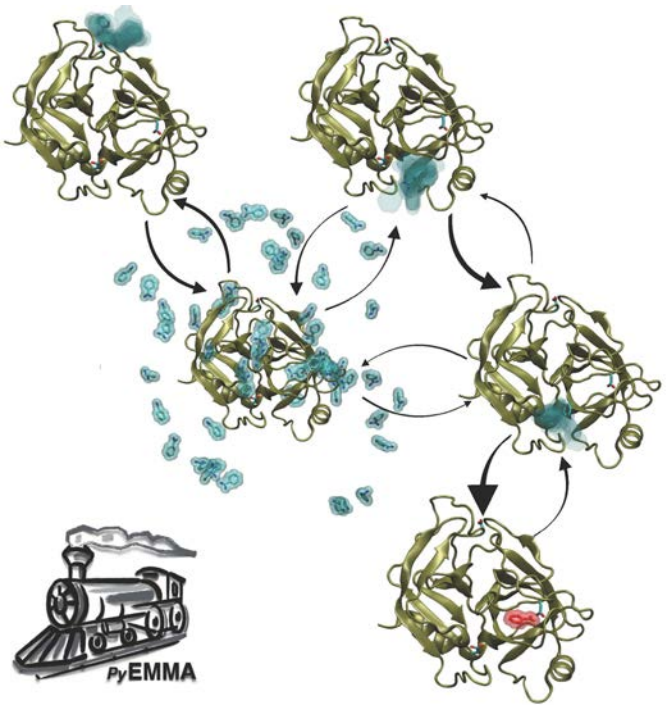
ulm university universität
uulm

Einladung
zum
Physikalischen Kolloquium
Montag, 02.11.2015
16:15 Uhr in N24/H13

Professor Dr. Frank Noé
Computational Molecular Biology
Freie Universität Berlin

Beating the sampling problem in molecular dynamics simulation

Molecular dynamics (MD) simulations are incredibly versatile and allow us to inspect molecular system at great time- and space resolution.
However, a key limitation of MD is that the efficient calculation of ensemble averages by time-averaging is challenging due to the long correlation times in many molecular systems. This well-known sampling problem has limited progress in many fields where molecular dynamics are relevent, for example in the study of protein structure, dynamics and function. I will describe recent techniques in the area of Markov state modeling developed by us and other groups, and sketch how we can reach out to simulate processes at hundreds of milliseconds and beyond without sacrificing atomistic resolution.



Ab 16.00 Kaffee, Tee und Kekse vor dem Hörsaal H13
Organisation: **Prof. Dr. F. Jelezko, Tel. 23750**
Host: **Prof. Dr. J. Michaelis, Tel. 23050, off.: 23051**