Contribution ID: **96** Type: **Poster**

Nonequilibrium biomolecular simulations

Nonequilibrium effects can be found at the core of biomolecular functions, such as signal and energy transport. Investigating these nonequilibrium effects in molecular dynamics simulations requires extensive computational hardware, such as provided by NEMO and BinAC: as the simulated processes are non-ergodic, observables of interest do not converge over time, and thus a large number of simulations (up to 1500 independent runs) is needed to observe statistically significant effects. Using a broad range of molecular test systems, we are interested in nonequilibrium effects as vibrational energy transfer within proteins, allosteric communication between ligand binding and effector sites, protein/ligand unbinding and conformational changes of proteins. We give an overview of the methods that we employ for investigating these nonequilibrium aspects of biomolecular function such as constant energy, excited state relaxation, and dissipation-corrected targeted molecular dynamics simulations.

Abstract (optional)

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Session Classification: Lunch / Poster Session 1

Track Classification: Scientific Track