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« Something fast... something slow... »

Using state-of-the-art molecular dynamics simulation methods to study diverse dynamic processes in bio-molecules.

Bio-molecular systems exhibit a broad range of dynamics over a hierarchy of time-scales ranging from femto-seconds to seconds. The study of such diverse dynamic events over different time-scales requires a variety of molecular dynamics simulation methods and techniques.

In this seminar, I shall present the results of two projects concerning the simulation of two very different dynamic processes: The first project involves the use of excited state Car-Parrinello molecular dynamics to study irradiation induced DNA damage and repair mechanisms, a process that occurs on a time-scale of femto-seconds. The second project concentrates on the simulation of NMR Residual Dipolar Coupling (RDC) order parameters, which probe protein dynamics up to milli-second time-scales, using biased potential classical molecular dynamics. Both projects provide a detailed and interesting insight into these dynamic processes, which are separated by a time-scale factor of 1.D12, and demonstrate the power of contemporary simulation methods for the study of bio-molecular systems.