SFB/TRR 21 - Colloquium

27. April 2012, Ulm

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Protein dynamics I (Tutorial): a general introduction

Cellular life is based on protein activity. The traditional structure-function paradigm, "to know function study structure" which goes back to Watson and Crick, have guided our interpretation of protein function for decades. It is only rather recently that the role of dynamics has been recognized, supporting the idea that structural analysis is not sufficient to fully understand protein function. It is very difficult to study protein dynamics experimentally at an atomic level of detail, although techniques such as single-molecule FRET, X-ray crystallography, and NMR supply useful, but limited, information. Consequently, molecular dynamics simulations are playing an increasing role in determining the mechanism, as a supplement to the experimental studies. A general discussion of the field is presented, with special emphasis on molecular dynamics simulations.

27. April 2012, 14:00 Uhr

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