

Colloquium Dahlem Center for Complex Quantum Systems

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Conformational Transitions of Nucleic Acids under External Forces: Examples and a Stochastic Path Integral Theory for their Kinetics

Location: Hörsaal A (1.3.14)

Time: Tuesday, May 3rd, 2011, 14:00

Abstract:

I will present molecular dynamics simulations of several examples of conformational transitions that nucleic acids and their complexes undergo upon the application of external forces and/or torques:

- (1) DNA supercoil relaxation by topoisomerases,
- (2) the condensation of DNA by dendrimers and, time permitting,

(3) RNA unfolding.

Then I will showcase the use of the formalism of stochastic path integrals to deduce the kinetics of these transitions, from simulation trajectories or experimental single molecule recordings of the transition, under other conditions that those that are actually simulated or recorded.