Physikalisches Institut

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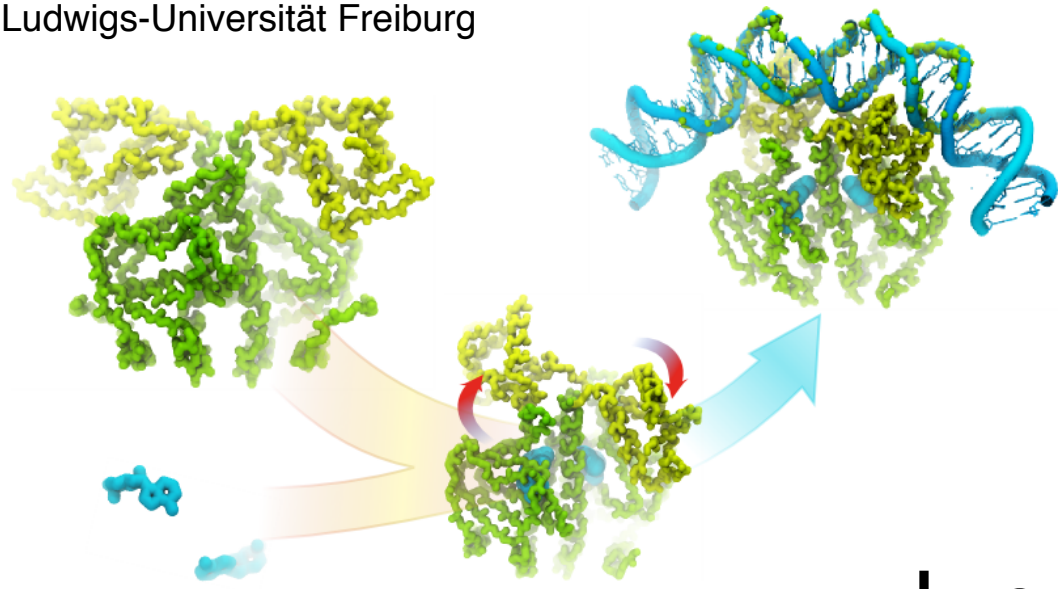

June 6

Exploring the energy landscape of amyloid peptide aggregation

Birgit Strodel

Forschungzentrum Jülich

In this talk I will present results for the amyloidogenic heptapeptide GNNQQNY from the yeast protein Sup35 and the heptapeptide KLVFFAE comprising residues 16 to 22 of the Alzheimer amyloid-beta peptide. Using an all-atom model for GNNQQNY and a combination of replica exchange molecular dynamics and discrete path sampling, a detailed picture about the thermodynamics and kinetics of dimerization for the GNNQQNY peptide is provided. The formation of larger oligomers is studied employing a coarse-grained force field, revealing different aggregation pathways for GNNQQNY and KLVFFAE as a result of their different amino acid composition. I will conclude my talk with an outlook on how to tackle the aggregation of larger peptides, such as the 42-residue long amyloid-beta peptide, and how the cellular environment can be taken into account. This is required as proteins experience a significantly different environment in vivo than in the context of the idealized dilute environment commonly studied in experiments and simulations.

Molecular Dynamics Seminars 2012

Seminar Room of Gustav Mie Haus, Ground Floor, 16:15

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