



"Soft-Matter Seminar"

Molecular simulations of peptides and membranes

Dr. Volker Knecht

Department of Theory and Bio-Systems
Max Planck Institute of Colloids and Interfaces, Potsdam

Abstract:

My talk will consist of two parts on biomolecular systems both involving polypeptides. The first part will be about peptide folding and self-assembly, highly relevant from a fundamental point of view as well as due to potential applications for medicine and nanotechnology. The second part will concern the important biological process of membrane fusion, and how merger of two lipid membranes in close proximity can be induced by fusion peptides. As the underlying molecular details are difficult to study experimentally, we are using molecular dynamics (MD) simulation techniques to provide a microscopic understanding of these processes. I will show how MD simulations have been used to refine the structure of a beta-sheet peptide monolayer at a water/air interface and give examples for conformational transitions in peptides induced by aggregation or interfacial adsorption. A mechanism by which fusion peptides may induce membrane fusion is proposed. Finally, atomistic studies of the fusion-relevant lamellar-nonlamellar phase behavior of a lipid mixture and lipid vesicle fusion will be presented.

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16:00 Uhr
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Prof. Dr. Roland Netz
Physik-Department T 37, Technische Universität München, Theoretische Physik
85747 Garching