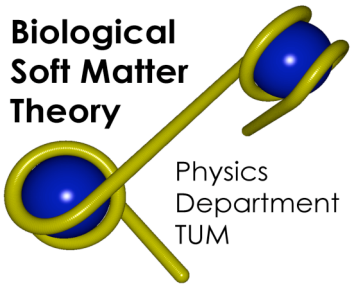

"Soft-Matter Seminar"

Hydrophobic effect in proteins

Cristiano L. Dias

Department of Biochemistry and Department of Physics, University of Toronto

Abstract:
The hydrophobic interaction between non-polar residues plays an important role in protein structure and stability. A lot of effort has been spent in studying this interaction due to ist importance and implications. However, only recently have we started to understand this multi-faceted interaction at the molecular level. I will talk about my efforts to model water molecules and the hydrophobic effect using a coarse grained model known as Mercedes-Benz model. The temperature dependence of the hydrophobic interaction will be discussed within the scope of this model and shown to be responsible for the unfolding of proteins at low temperature, a phenomena known as cold denaturation. If time permits, I will also talk about the role of the hydrophobic interaction in the formation of secondary structures in small poly-peptides.

On aggregates and nanopumps

Markus S. Miettinen

Institute of Biochemistry and Biology, University of Potsdam

Abstract:
Detailed information on the structure and dynamics of biomolecules can be difficult to obtain experimentally. In such cases computer simulations can help to assess the feasibility of suggested models. In the first part of the talk I estimate the feasibility of three different conformations of a polyglutamine peptide to be the disease-initiating conformation in the inherited neurodegenerative polyglutamine-diseases. I find simulations to support one of the conformations strongly.
In the second part I discuss simulation artefacts that can lead to pumping of water molecules through a carbon nanotube without any external driving force [Gong]. I present two possible mechanisms of creating the flux. One of these (the charge groups) explains the strong flux in [Gong]. The other one (temperature gradient created by the thermostat) gives a hint on how the nanopump could, in fact, be actualized in a real system.

Dienstag, den 9.11.2010
16:15 Uhr
Raum PH 3024

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