AKB 9 Chemical Bonds and Adsorption

Time: Tuesday 11:00–12:00   Room: ZEU 260

AKB 9.1 Tue 11:00 ZEU 260

Polymer and peptide adsorption to attractive substrates —
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Germany

The interest in understanding polymer adsorption at substrates has
grown quite recently with the development of high-resolution experi-
mental equipment allowing for studying the technologically important
problem of substrate-binding specificity of synthetic peptides. In our
study of simple hybrid models [1,2], we investigate how solubility of the
surrounding solvent and temperature influence the substrate-binding of
nongrafted polymers in a cavity with an attractive surface. Applying a
suitably adapted variant of the multicanonical chain-growth algorithm
[3] for self-avoiding walks, we performed simulations of lattice polymers
with up to 200 monomers and obtained the entire temperature-solubility
pseudo-phase diagram of the hybrid system within a single simulation.
We clearly separated expected thermodynamically stable phases domi-
nated by the respective adsorbed and desorbed collapsed and random-coil
conformations. Another central aspect of our study is the discussion of
pseudo-phases that specifically depend on finite-size properties such as
the precise number of monomers or, for peptides, the sequence of residues.
[1] M. Bachmann and W. Janke, Phys. Rev. Lett. **95**, 058102 (2005).
[2] M. Bachmann and W. Janke, to be published.
[3] M. Bachmann and W. Janke, Phys. Rev. Lett. **91**, 208105 (2003).

AKB 9.2 Tue 11:15 ZEU 260

Analysis of Adsorbed Protein Patterns at Surfaces — ●ARMIN
NAGEL[1], HUBERT MANTZ[1], CHRISTOF WEITENBERG[1], ANTHONY
QUINN[2], MARKUS BELLION[3], LUDGER SANTEN[3], and KARIN JACOBS[1]
— [1]FR 7.2 Experimental Physics - Soft Matter, Saarland University,
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The aim of this project is to identify the mechanisms for salivary pro-
tein adsorption at solid-liquid interfaces, with the intention of optimising
the biocompatibility of dental replacement materials.

The methodology involves the characterisation of protein adsorption on
surfaces that have been specifically tailored to have differing interaction
potentials by varying the short and long range forces. The composition
and topography of these tailored surfaces is carefully controlled and char-
acterised via AFM and wettability analysis, enabling the structural and
interfacial tension components to be identified.

AFM scans of the protein layers, both ex situ (in air) and in situ (in
a buffer solution) are compared to ellipsometry measurements of the ki-
netics. The resulting complex patterns were analysed by image analysis
methods (Minkowski Measures), so that tendencies during the adsorption
process could be identified.

We compare the experimental protein patterns with patterns obtained
by Monte-Carlo simulations of the protein adsorption process.

AKB 9.3 Tue 11:30 ZEU 260

Characteristics of Protein Adsorption at Solid-Liquid Interfaces
— ●HUBERT MANTZ[1], ARMIN NAGEL[1], ANTHONY QUINN[2], and KARIN
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Adsorption of proteins occurs instantly whenever a protein solution
(e.g. any body fluid) gets in touch with a surface (biomaterials or medi-
cal devices) and thereby is of crucial importance to all kinds of biomedical
technologies. Adsorption is a very complex process and is not yet fully
understood. The adsorbed amount and the structure of the adsorbed
layer depend on many factors including properties of the surface, the
surrounding medium and the protein itself.

In this study, the in situ adsorption kinetics of some selected saliva
proteins (amylase and lysozyme) in liquid environment has been stud-
ied by ellipsometry. Through judicious choice and modification of the
substrates, the influence of short- and long-range forces on the adsorp-
tion process could be separated. The ellipsometry measurements were
compared with AFM images of the resulting topographies.

The experimentally observed adsorption kinetics does not follow any
standard adsorption model. We compare our results with Monte-Carlo
simulations (cf. contribution of Bellion et al.), assuming conformational
changes of the proteins upon increasing surface coverage.

AKB 9.4 Tue 11:45 ZEU 260

**Kinetics of Protein Adsorption at liquid/solid interfaces: A
Monte Carlo study** — ●MARKUS BELLION and LUDGER SANTEN
— Fachrichtung Theoretische Physik, Universität des Saarlandes, 66041
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We investigate by means of extensive Monte Carlo simulations the
protein adsorption at liquid/solid interfaces. Proteins are modelled as
colloidal particles. The particle-particle and the particle-surface interac-
tions are described in the framework of the DLVO theory, which considers
steric repulsion, electrostatic and van der Waals interactions. In order
to investigate the time evolution of the surface coverage in agreement
with the experimental setup (see contribution of H. Mantz, A. Quinn,
A. Nagel and K. Jacobs for comparison), we use a layered three dimen-
sional simulation box. In the upper layer a grandcanonical ensemble is
applied, which controls the concentration of proteins in the solution. In
contrast, the particle number is conserved in proximity to the liquid/solid
interface.

In agreement with the experimental results we find the aggregation
of a protein monolayer. If we include the possibility of conformational
changes, we are able to reproduce the experimentally observed three
stepped kinetics: a fast linear increase of the adsorbed amount for low
coverages is followed by a second linear regime before saturation of the
surface coverage sets in. The second linear regime can be understood as
a collective transition from a conformation which is stable on the single-
particle level to a conformation that optimizes adsorbed amount at the
surface.