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(Dr. Thomas Gruhn)

Abstracts for Talks and Posters

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NOTES:

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Poster

Organic Field-Effect Transistors

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The work is part of a few national and European research projects and cooperations with industrial partners and is mainly focused on the following fields:

- Polymers for Optoelectronics and Nanoelectronics
- Organic Field-Effect Transistors
- Supramolecular Chemistry and Liquid-Crystalline Materials
- Modern Methods of Polymer Processing and Analytic

The projects are influenced by a strongly interdisciplinary character and include a broad spectrum of modern characterization techniques like x-ray diffraction, electron microscopy, atomic force microscopy, etc.

Actually I am mainly focused on the processing and optimization of thin film transistors. The devices are fabricated in top or bottom contact configuration by utilize modern techniques like e.g. photolithography. Fused thiophene-phenylene oligomers like benzo-bis-benzothiophenes are actually used as semiconductors. All state-of-the-art deposition methods both solution-processing like e.g. zone-casting and in the future sublimation are and/or will be used to reach highly ordered semiconductor films. To optimize the overall device performance different silanes and thiols are applied to the dielectric and/or the electrodes. At present charge carrier mobilities of up to 0.1 cm2V-1s-1 and transistor on/off-ratios of up to 107 are achieved, which are respectable results in comparison to the literature.

Poster

Generic coarse-grained model for protein folding and aggregation

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Alhzeimer's disease is associated with aggregation events: proteins change conformation and form amyloid oligomers. Little is known about their structure and effects on membranes. Aggregation is likely a slow process, and currently out of reach of all-atomistic simulations. We approach the problem at a coarse-grained level.

In this work, we concentrate on the protein part of the project by presenting a generic four-bead peptide model with implicit solvent. The level of resolution is chosen as a balance between the requirements of computer efficiency and accurate sampling of local conformations. This top-down model is based on a small number of interactions and parameters making it easily tunable, while keeping enough specificity in the different amino acids to catch important features of peptide interactions.

We show that our model can successfully fold simple helical proteins and reproduce aggregation events of small peptides. The nature of our project required a model that would be able to handle both features.

Poster

EAI minimal energy states

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Complex systems such as spin glasses simulated with local update schemes in the framework of Monte Carlo Simulations exhibit strong autocorrelations resulting in a slow dynamics especially pronounced in the temperature regime below the glass transition.

Due to the rough energy landscape, trappings in local energy minima have to be handled with (combinations of) different techniques such as parallel tempering and multi-canonical simulations lowering relaxation times and autocorrelations.

Our poster contains a short glimpse on these methods with special attention to autocorrelation (ac) times giving a measure for assessing the goodness of a random walk. Further it includes a survey on the highly degenerate configurations with minimal energy. Both issues concentrate on the 3d Edwards-Anderson Ising (EAI) spin glass model with bimodal interactions. For the minimal energy configurations it also captures the 2d version for the possibility of visual testing.

Poster

Assessing different mapping schemes for coarse grained simulations of peptide systems.

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The study of organic/inorganic interfaces using theoretical methods became in the last years of central importance in many fields of condensed matter, material science, and chemistry due to the large number of applications in current technology.

In most cases rather idealized and simple methods (e.g. scaling theories) have been treated from a theoretical and simulation point of view. However, while they provide a reasonable picture of the generic properties, system specific aspects can alter the properties significantly.

For a better understanding of the relevant aspects of the adsorption process, different simulation methods (such as quantum calculation, classical atomistic simulation, coarse-grained (CG) model) must be used in a consistent sequential way because of the multiscale nature of the problem.

In this respective the development of coarse grained models of large (bio) molecules in solution and the simulation study of these systems near specific surfaces must be developed in order to reach size and time scales comparable with experiments.

At first, it’s necessary to create CG system with right potentials. At this moment we try to find all of them and make test simulations. For getting potentials we use Boltzmann inversion which is one of the most popular methods.

When all potentials will be found and comparison with atomistic distributions will give close result we begin to simulate this system in water and make the chain longer.

Poster

Structural dynamics in recombinant light-harvesting chlorophyll a/b complex as monitored by EPR

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Light-harvesting chlorophyll a/b complex (LHCIIb) is a major component of the photosynthetic apparatus in green plants. Its 232-amino acid apoprotein noncovalently binds 8 chlorophyll (Chl) a and 6 Chl b molecules as well as four carotinoids. An astonishing feature of this protein is that it spontaneously folds into its three-dimensional structure in vitro upon mixing the denatured protein with its cofactors in detergent solution. In order to study the structural dynamics of LHCIIb, we combine site-directed spin labeling with electron paramagnetic resonance spectroscopy (EPR), specifically CW, ESE and DEER (double electron electron resonance), a pulse EPR technique that allows to measure distances in the range from 2 to 6 nm. By using these techniques we were able to assess local mobilities and accessibilities to hydrophilic or hydrophobic quenchers of individual protein domains in LHCIIb and changes in the distance distribution between two spin labels attached to selected amino acid residues. Moreover, in this work we combine pulse EPR methods for the first time with freezequench techniques to gather structural and kinetic information during the folding of LHCIIb in the time range from ms to min. The results will contribute to a better understanding of the dynamics and the folding mechanism of membrane proteins and of the self-organisation of supramolecular assemblies.

Poster

Spectroscopy of polypyrole bulk and core shell particle

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Conducting, insulating and semiconducting functional inks have attracted considerable attention due to their possible use as low-end printable electronics. [1] Intrinsic conducting polymers (ICP), have been developed combining favorable properties of polymers and metals. During the past decades, they where developed from laboratory materials to mature industrial products. A variety of applications such as OLEDs, capacitors, transistors and solar cells are based on commercially available poly (3, 4-ethylenedioxythiophene) (PEDOT)/polystyrene sulfonate (PSS).[2] PEDOT/PSS, however, has some particular problems, i.e. high acidity is needed to maintain its conductivity and dried particles are non-redispersable, thus limiting its applications. In contrast, polypyrrole (PPy), when doped with octanesulfonate, dodecylsulfonate, and polystyrenesulfonate, retains its rather high conductivity at neutral pH conditions.[3]
Therefore, a novel synthetic strategy that yields pyrroles with increased redispersibility facilitating technical use was proposed.[4] Induced small changes in the synthetic route impose a rather high variation in the electronic conductivity of the resulting material, presumably owing to defects in the PPy microstructure. In this work, we present solid state NMR results, revealing the nature of defects that are possibly present in the respective samples. Indeed, □□ coupling as well as oxidation or reduction products affect the conductivity and these limit its application. The presence of defects varied depending on the oxidation reagent.[5] The peak assignment of the NMR spectra is supported by ab initio chemical shift calculations. However, conducting NMR samples posses inherent difficulties (e.g. currents create a magnetic field that interact with the NMR rf pulses). Therefore, samples were preferably reduced to alleviate the conductivity; if this was not possible the use of lower magnetic fields or dilution by SiO2 facilitated the measurements.

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Talk

Numerical simulation of a free surface evolution of a binary mixture on the solid substrate

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The problem of coupled demixing and dewetting of binary mixture films is frequently occuring in nano-technological applications, where the thickness of the internal interfaces between two phases may be comparable to the droplet size or layer thickness. Theoretical approaches to the demixing problem are commonly based on the Cahn--Hilliard theory [1] using the Landau--Cahn free energy functional approximation to model phase separation while neglecting the effects of the moving surfaces [2].

In this contribution, we present the static limit of the model, given in [3], specialized for a 2D film lying on a solid substrate.
Based on his model, we derived the Finite Element (FE) numerical procedure and computed droplet solutions for selected parameters of the model, using a continuation procedure with surface tension of the free surface, as the continuation parameter. Resulting solution branch is compared with the related circular-symmetric droplet solution and its effective sharp interface approximation.

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Poster

MD Simulations of Sheared Polymer Brushes with Explicit Solvent

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Polymer brushes play an important role as lubricants in many technical applications, e.g. in hard disk drives or artificial joints[1]. They are furthermore believed to be crucial for minimizing friction between synovial joints[2], such as human knees or hips. Polymer chains in brushes are forced to stretch away from the grafting surface by steric repulsion, such that two compressed brushes can carry extremely large normal loads. On the other hand, when subject to lateral shear, the chains can incline along the shear direction and minimize fricitional dissipation. Hence, the resulting friction coefficients can be extremely small (of the order 10−4 [2]). Using Molecular Dynamics simulations of a standard coarse grained model we study the lubrication properties of short chain polymer brushes. We extend further approaches (see, e.g. Refs. [3–5]), which have been performed without explicit solvent, to new simulations, where we now account for hydrodynamic interactions via including solvent molecules. We investigate the static properties of isolated and compressed brushes, and study the response of these systems to stationary and non-stationary external shear. This is done under variation of the molecular parameters, i.e. grafting density and chain length. By comparing to previous simulation results of the same model without explicit solvent, we aim at understanding the role of hydrodynamic interactions in polymer brush lubrication.

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Poster

Hybrid complexes from biological and synthetic materials for light-harvesting and charge separation applications

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Light harvesting chlorophyll a/b complex (LHCIIb) is a major component of the photosynthetic apparatus in higher plants. It non-covalently binds 8 chlorophyll a, 6 chlorophyll b and 4 carotinoids. These pigments serve to harvest light energy and to transfer it to the photosynthetic reaction centers. LHCIIb exhibits an astonishing ability to assemble in vitro from the denatured, bacterially expressed apoprotein and plant pigments.

We want to utilize the light-harvesting function of LHCIIb in organic/inorganic/biological hybrid complexes. Therefore we bind it to organic rylene dyes and inorganic semiconductor nanocrystals (quantum dots, QD). Our aim is to analyse and optimise both the chemical and optical coupling between these components. To this end we studied the binding capabilities of LHCIIb to QD type I, seeing the N-terminus and the His-tag of the protein responsible for the binding. Both binding possibilities lead to energy transfer from the QD to the LHCIIb. We also investigated the interaction of LHCIIb with two rylene dyes, one being an energy acceptor the other an energy donor for the LHCIIb. For both dyes we could show efficient binding and energy transfer.

Poster

Synthesis of polymer nanoparticles with new topologies in non aqueous emulsions

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Nanofunctional materials, e.g. polymer latex particles, find wide-spread applications ranging from electronics, pharmaceutics and photonics to cosmetics, coatings and catalysis. This can be attributed to their ell-defined morphology and their unique physical and chemical properties such as the size, their optical roperties and the defined nature of the surface. trategies to form polymer nanoparticles usually include a direct synthesis in emulsion, miniemulsion, or dispersion. Due to the presence of water in these traditional methods, latex preparation using moisture sensitive reactions or monomers cannot be applied. To overcome this drawback, non-aqueous emulsions consisting of organic aprotic solvents have been developed.[1-4] This technique dramatically increases the number of applicable monomers in emulsion processes. Stable non-aqueous emulsions are obtained by the emulsification of two immiscible organic aprotic solvents. Suitable solvent combinations are DMF dispersed in n-hexane or acetonitrile dispersed in cyclohexane. A poly(isoprene)- block-poly(methyl methacrylate) copolymer (PI-b-PMMA) serves as the emulsifier to suppress the separation of the solvents yielding stable droplets. The general synthesis of the particles is achieved by mixing a monomer with the dispersed phase, formation of a stable emulsion via ultrasonification and afterwards dropwise addition of the second monomer or initiator / catalyst, respectively, which diffuse into the droplets and start the intended polymerization. Since the first monomer is insoluble in the continuous phase, the reaction takes placeexclusively inside the droplets. In this way it is possible to obtain polymer particles (e.g. polyurethane (PU), polyester or polyacetylene) from water sensitive monomers or reactions. A combination of these resulting polymers can be used to prepare novel polymeric nanosized core-shell particles. For example structures containing a polyurethane core and a polymethacrylate shell or shells obtained from Ring Opening Metathesis Polymerization (ROMP) can be synthesized[5]. This approach reveals the advantage of non-aqueous emulsions to form core-shell particles applying water sensitive reactions, because no prepolymer formation is necessary to obtain high molecular weight polymers, as in classical emulsions, and also no multi-step synthesis are needed since the formation of the core and the shell are carried without intermediate work-up. This enables a simple and efficient formation of particles with special material properties, e.g. optimized film forming abilities or adhesion behavior on surfaces necessary for coatings or paints.

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Talk

Parameter Optimization and Data Mining in Molecular Simulations

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Simulation of complex systems is receiving increasing research attention over the past years. We consider the description of systems of the condensed matter by force fields on an atomistic level. We thereby focus on Molecular Dynamics based on the (12,6)-Lennard-Jones (LJ) potential, which describes interactions between uncharged, non-bonded atoms. The two goals of my PhD thesis, which will be presented in the talk, are the application of Parameter Optimization and Data Mining techniques on Molecular Simulations.

1. The LJ parameters ☼ and ← have to be optimized, in order to reproduce known experimental data such as the density and the heat of vaporization. To solve this task, Faller u. a. (1999) used the Nelder Mead simplex method, but it requires a lot of expensive function evaluations and is a quite heuristic approach. The focus now lies on finding more efficient optimization algorithms, e.g. gradient based methods from the field of Numerical Optimization, in order to improve the convergency. Bourasseau u. a. (2003) have developed a gradient based algorithm resulting in the solvation of an LES. The talk will give an overview of the embedding of such algorithms in a simulation workflow and how gradient based methods can be applied.
2. In many projects, only a small number of system properties are calculated and evaluated, and the system behaviour is studied only in a limited and manual way. Thereby, a quite big quantity of information in the simulation data remains hidden and is not taken into account. Hence, there is need for an automated detection of patterns in the trajectories, which can be used for example to find the reasons of undesired and

erroneous simulations. Therefore, a concept for an automated information extraction process has to be developed. Unsupervised Data Mining algorithms make it possible to test the data for regularities and to detect correlations to other simulations. In the talk, the recent ideas of applying this kind of techniques in Molecular Simulations will be summarized.

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Poster

Understanding the properties of lipid bilayers

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Understanding the properties of lipid bilayers under physiological salt conditions is a first step to comprehend the complex biomolecular assembly of a cell membrane essential for all life on earth. Remarkably, recent results from molecular dynamics and in vitro experiments suggest that the major lipid component of cellular membranes, phosphatidylcholine (PC), although zwitterionic, can adsorb sodium ions with significant effect on the structural and dynamic properties of the bilayer. We have used molecular dynamics simulations to study the effect of cation size on the interaction with PC lipids. Potassium ions, rather, were found to be depleted from PC lipids, whereas lithium ions bound more strongly to PC. These findings may have important biological and medical implications, as sodium or potassium ions are the respective major cations in extra- or intracellular environments of animals and humans, whereas intake of lithium can have both curative and toxic effects.

Poster

Theoretical study of Morphology and Charge Transport in Amorphous tris(8-hydroxyquinoline) aluminium (Alq3)

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A force-field for tris(8-hydroxyquinoline) aluminium (Alq3) - a compound widely used in organic light emitting diodes -has been developed and verified comparing classical and ab-initio molecular dynamics simulations. This force-fied was then used to obtain a large scale morphology of amorphous Alq3. Giving the realistic morphology, charge transport in thin films of amorphous Alq3 can be analyzed withing the framework of high temperature non-adiabatic Marcus theory.

Poster

Homogeneous and Heterogeneous Nucleation in Colloidal Systems

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We are presenting a computer simulation study of nucleation in two simple model systems: hard spheres and a Lennard Jones fluid.
As nucleation is a rare event, it cannot be accessed by standard MC or MD methods. Therefore we use Flux Forward Sampling, a transition path sampling kind of method.

Poster

Mechanical properties of pore spanning membranes probed by AFM

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The mechanics of membranes play a pivotal role in cell function, i.e. blood transport through narrow veins. To characterize the mechanical parameters of native and artificial membranes a model system of pore spanning membranes is employed solving the problems of close membrane surface contact and concomitant lateral mobility. Porous silicon with pore diameters ranging from 450 nm to 1,2 µm, covered with a 60 nm thick layer of gold are used as substrates. This model system is suitable for scanning probe techniques like atomic force microscopy (AFM) and for optical methods like fluorescence microscopy.

Nano black lipid membranes (Nano-BLMs)[1] consisting of DPhPC prepared on octanethiol (OT), octadecanethiol (ODT) or cholesterylpolyethylenoxythiol (CPEO3) functionalized substrates are used as model systems for free standing artificial membranes. Due to the special geometry of the porous substrates we are able to study the same position with atomic force and fluorescence microscopy. DPhPC bilayers are stained with 1 mol% of Bodipy-PC.

Indenting these "nano drums" centrally with an AFM tip yields force indentation curves exhibiting the apparent spring constant of the free standing membrane. Force indentation curves for artificial lipid bilayers are quantitatively analyzed by solving the corresponding shape equations of continuum curvature elasticity. Since the measured response depends in a predictable way on the system geometry (pore size, tip radius) and on material parameters (bending modulus, lateral tension), this opens the possibility to monitor local elastic properties of membranes in a well-controlled setting by addressing each pore separately[2][3].

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Poster

Charge Transfer Organic Molecules

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One of the first true organic synthetic metals, called TTF-TCNQ, was made by many different groups in 19721. This conducts electricity but does not superconduct. Then in 1979, Denis Jerome2 of the University of Paris at Orsay and Klaus Bechgaard of the University of Copenhagen discovered the first organic superconductor3, a related compound based on tetramethyltetraselenafulvalene (TMTSF), with a formula (TMTSF)2PF6, and a transition temperature of 0.9 K . These compounds are crystalline solids called electron charge-transfer salts. Such salts consist of regular arrays of cations and anions, just as sodium chloride (rock salt) does. The difference is that the ions are charged molecules, not atoms and the crystal structures are much more complicated. The salts are made from organic electron-donor or electron-acceptor molecules. That is, molecules that are easily oxidized (by losing electrons) or reduced (by gaining electrons) in chemical or electrochemical reactions with suitable ions, known as counter ions. Our purpose is theoretical investigations of these charge transfer salts. We are working on some other macromolecules for finding suitable Acceptors and Donors for these charge transfer salts.

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Poster

Phase-Shaping of Spin-Wave Pulses by Non-Resonant Parallel Pumping

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Parallel pumping is a versatile technique to amplify spin waves.

From a quantum mechanical point of view it can be described as a three-particle-process where the pumping photon is split up into two magnons.

Momentum and energy conservation have to be fulfilled. Moreover, the dispersion law for spin waves places another condition on the frequency and wave vectors of spin waves which can be excited. Overall, effective pumping is mainly possible, if the frequency of the excited spin waves is exactly half the pumping frequency $\omega_{SW} = \frac{\omega_{Pump}}{2}$.

As has been shown in [1], by introducing a suitable phase shift between the travelling spin wave under investigation and the pumping signal, parametric amplification can be used not only to increase the spin wave amplitude but also to shape it.

This effect has been explained by the scattering and phase accumulation of the propagating spin wave inside of a magnetic spin-wave barrier created around a pumping transducer due to effective parametric generation of other spin-wave groups.

Using non-resonant travelling spin waves with $\omega_{SW} \neq \frac{\omega_{Pump}}{2}$, the direct influence of the spin-wave barrier on the phase profile (instead of the amplitude) is investigated in the presented work. This has two advantages: firstly, the non-resonant nature ensures that no direct amplification of the travelling spin wave is possible which simplifies the interpretation of the results. Secondly, the spin-wave phase is much more sensitive to the value of the barrier than the amplitude.

Here, we propose to understand the travelling spin-wave pulse as a probe to measure the spin-wave barrier. Note, that the latter is mainly formed by spin waves at the bottom of the magnon spectrum. This spin-wave group is of huge interest since the discovery of spin-wave Bose-Einstein-Condensation[2]. Up to this time this group was not accessible by conventional microwave techniques. The proposed approach now provides – besides Brillouin light scattering spectroscopy – a second experimental access to the dynamics of these spin waves.

Financial support by the MATCOR Graduate Class of Excellence is gratefully acknowledged.

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Poster

A criterion to estimate the quality of the Mapping Scheme in CG

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We propose a simple method to evaluate the approximation of separation of variables (ASV) in Molecular Dynamics (MD) and related fields. It is based on a point-by-point evaluation of the difference between the true potential and the corresponding potential where the separation of variables is applied. The major advantage of such an approach is the fact that it requires only the analytical form of the potential as provided in most of the MD codes. We provide an application of this criterion for the alkane (aliphatic) chain and compare the efficiency for two differents Mapping Schemes (MS).

Talk

Local Density of States for Individual Energy Levels in Finite Quantum Wires

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The local density of states (LDOS) in finite quantum wires is calculated as a function of discrete energies and position along the wire. By using a combination of numerical density matrix renormalization group (DMRG) calculations and analytical bosonization techniques it is possible to obtain a complete understanding of the local spectral weights along the wire in terms of the underlying many particle excitations.

Talk

MD simulations of sheared brush-like systems

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Friction forces between two solid surfaces bearing polymer brushes play a key role in many applications. However, systems with soft colloids between polymer brushes have not been investigated yet. Star polymers can be taken as a model of hairy micelles or soft colloids. We perform Molecular Dynamics simulations of such systems under shear. Statical and dynamical properties are investigated. In particular, we focus on the response to non-stationary external stimuli.

Poster

Monte Carlo Simulations of Lattice Peptides Near Surfaces

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It has recently become possible to design peptides that bind to inorganic (metal, metal oxide and semiconductor) surfaces with high specificity and stability. These peptides may be used in future sensory devices or to modify the crystalline growth of inorganic materials. The mechanism for the important property of specificity is unknown but it is thought that the conformations which the peptide forms are significant to the binding. It is currently impossible to simulate a chemically realistic model of a peptide on the time scales of conformation changes making it necessary to use coarse-grained models to study the effect the conformations formed may have on substrate binding. The HP lattice model used in this work is the simplest model that has been shown to encapsulate the basic folding problems. The rough energy landscape of peptides makes Monte Carlo simulation difficult, conventional Boltzmann distribution simulations become trapped within local energy minima and do not sample effectively. In this work the Wang-Landau algorithm, a multicanonical Monte Carlo method in which the density of states of a system is determined with increasing accuracy as the simulation progresses is used. A recently proposed move set, pull moves, has proved effective in combination with the

Wang-Landau algorithm in sampling the compact conformations of HP lattice models. When considering peptides in the presence of a surface the density of states can be calculated as a function of both the number of monomer-monomer and monomer-surface contacts. This can be used to calculate the specific heat capacity as a function of both temperature and solvent quality. As specific heat peaks indicate pseudo-phase transitions this can be used plot phase diagrams for lattice peptides near surfaces. By investigating the interaction of peptides with patterned surfaces the phenomenon of surface specificity might be better understood.

Poster

Interactions of antimicrobial peptides with lipid monolayers

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Antimicrobial peptides are an evolutionary conserved component of the innate immune response and are found among all classes of life. These peptides associate with prokaryotic but not eukaryotic cell membranes, presumably because of charge complementarity. In general, their mode of action consists of membrane permeabilization leading to cell lysis and death. Nklysin is a protein expressed in porcine NK (natural killer)cells. The highest antimicrobial activity is observed for the amino acid sequence from residue 39 to residue 65 denoted as NK2. NK2 is highly cationic with an □helical amphipathic structure when embedded in the parent protein. Mimicking previous in vitro experiments, we investigate the conformations of NK2 peptide at phospholipid monolayers using molecular dynamics (MD) simulations. Simulations of up to four NK2 molecules placed close to an anionic dipalmitoylphosphatidylglycerol (DPPG) layer were carried out. The peptides spontaneously adsorbed to the head group region of the monolayer and oriented themselves parallel to the interface. The interaction between DPPG and NK2 as a function of the surface peptide concentration is studied and compared with experimental data where available.