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Computational Soft Matter: From Synthetic Polymers to Proteins

edited by
Norbert Attig
Kurt Binder
Helmut Grubmüller
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Winter School, 29 February - 6 March 2004
Gustav-Stresemann-Institut, Bonn, Germany
Poster Abstracts

organized by
John von Neumann Institute for Computing
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Max Planck Institute for Biophysical Chemistry, Göttingen
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Preface

The John von Neumann-Institut für Computing (NIC) - a joint institute of Deutsches Elektronen-Synchrotron (DESY) and Forschungszentrum Jülich - supports a large number of research projects in computational science, mainly through the Zentralinstitut für Angewandte Mathematik (ZAM) in Jülich and its supercomputing facilities. Furthermore, NIC also plays an active role in the education of young researchers in the various areas of computational science. It may already be called a tradition that every second year in February/March NIC offers a Winter School about a topic of outstanding methodological importance to the NIC user community.

This year the focus of the Winter School is on Computational Soft Matter which has become a very active field of research. Characteristic features of soft matter simulations are the nontrivial geometric structures that occur from the atomistic to the mesoscopic scales, the importance of entropic effects, and the cooperative complex dynamics. Different application fields profit from the recent progress of simulation methods.

The Winter School covers the following research topics:

- Introduction to Simulation Methods
- Polymer Solutions and Melts
- Liquid Crystals, Surfactants and Membranes
- Biopolymers

The target group of the School are again young scientists, especially graduate students and postdocs, in the areas of theoretical/computational physics, chemistry, and biophysics who have a basic knowledge of classical, statistical, and quantum mechanics. They benefit from this School by learning about recent methodological advances within and outside their field of specialization.

The Winter School is organized by the John von Neumann-Institut für Computing (Forschungszentrum Jülich), Institut für Physik (Johannes Gutenberg-Universität Mainz), Max-Planck-Institut für Polymerforschung (Mainz), and Max-Planck-Institut für biophysikalische Chemie (Göttingen).

Financial support mainly came from the Forschungszentrum Jülich. Due to the lack of additional funding either from the EU or the German Ministry of Education and Research (BMBF), the number of participants is restricted to about 80 participants compared to about 150 in previous times. This allows for a much closer contact between the lecturers and the students and fosters direct discussions between all participants throughout the School. Applicants for the School were selected on the basis of scientific background and excellence. In spite of this barrier, we received a wide-spread national and international resonance of applications, in many cases together with the submission of a poster abstract. This reflects the attractiveness of the programme and demonstrates the expectation of the participants to play an active role in this high-level scientific School. We are sure that the School is stimulating for both sides, the students as well as the lecturers.

This preface also offers an opportunity to thank all the individuals and institutions that significantly contributed to the success of the School. First of all we wish to thank those participants for their contribution, who are presenting a poster during the School. We also wish to thank the Forschungszentrum Jülich, which this year was the main sponsor of the School. For their most valuable help with the local arrangements we are greatly indebted to several staff members of the Forschungszentrum Jülich, namely Rüdiger Esser (finance), Rene Gail (conference service), and last but not least the School's secretaries Anke Reinartz and Yasmin Abdel-Fattah. Special thanks go to Anke Visser for her commitment concerning the composition and realization of this Book of Poster Abstracts.

This Book of Abstracts of the poster presentations is also published in the internet at http://www.fz-juelich.de/nic-series/volume22/.

Jülich, Mainz, and Göttingen
February 2004

Norbert Attig
Kurt Binder
Helmut Grubmüller
Kurt Kremer

Programme

Computational Soft Matter:
From Synthetic Polymers to Proteins

NIC Winter School

29 February - 6 March 2004
Gustav-Stresemann-Institut, Bonn, Germany

Monday, 1 March

09:00-10:30	*Daan Frenkel* **Introduction to Monte Carlo Methods**
10:30-11:00	**Coffee Break**
11:00-12:30	*Jörg Baschnagel* **Monte Carlo Simulation of Polymers: Coarse-Grained Models**
12:30-13:30	**Lunch Break**
13:30-15:00	*Mike P. Allen* **Introduction to Molecular Dynamics Simulations**
15:00-15:30	**Coffee Break**
15:30-17:00	*Christian Holm* **Dealing with Long Range Interactions: Polyelectrolytes**

Tuesday, 2 March

09:00-10:30	*Wolfgang Paul* **Chemically Realistic Simulations of Polymer Melts: Equilibration Issues and the Study of Relaxation Processes**
10:30-11:00	**Coffee Break**
11:00-12:30	*Burkhard Dünweg* **Advanced Simulations for Hydrodynamic Problems: Lattice Boltzmann and Dissipative Particle Dynamics**
12:30-13:30	**Lunch Break**

13:30-21:30	**Excursion to the Research Centre Jülich** *Gerhard Gompper* **Soft Matter Research in Jülich** *Thomas Lippert* **The John von Neumann Institute for Computing** *Bernd Mohr* **Parallel Programming Models and Tools** **Reception and Dinner at the See-Casino**

Wednesday, 3 March

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10:30-11:00	**Coffee Break**
11:00-12:30	*Alan E. Mark* **Simulating Self-Organization in Peptide and Lipid Systems**
12:30-13:30	**Lunch Break**
13:30-15:00	**Poster Session A**
15:00-15:30	**Coffee Break**
15:30-17:00	*Friederike Schmid* **Surfactants at Interfaces: Simulation of Structure and Phase Behavior**

Thursday, 4 March

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12:30-13:30	**Lunch Break**
13:30-15:00	**Poster Session B**
15:00-15:30	**Coffee Break**
15:30-17:00	*Helmut G. Grubmüller* **Molecular Machines**

Friday, 5 March

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10:30-11:00	**Coffee Break**
11:00-12:30	*Cameron F. Abrams* **Inhomogeneous Coarse-Graining of Polymers and Polymer/Metal Interfaces**
12:30-13:30	**Lunch Break**
13:30-15:00	*Ole G. Mouritsen* **A Lattice Model Approach to Biomembranes**
15:00-15:30	**Coffee Break**
15:30-17:00	*Marcus Müller* **Phase Behavior and Chain Conformations in Polymer Blends and Copolymer Mesophases**

Final Programme of NIC Winter School

	Monday, 1 March	Tuesday, 2 March	Wednesday, 3 March	Thursday, 4 March	Friday, 5 March
09:00 - 10:30	Daan Frenkel ***Introduction to Monte Carlo Methods***	Wolfgang Paul ***Chemically Realistic Simulations of Polymer Melts: Equilibration Issues and the Study of Relaxation Processes***	Klaus Schulten ***Protein Mechanics***	Alexander Grosberg ***Statistical Mechanics Approach to Protein Folding***	Mike P. Allen ***Liquid Crystal Systems***
10:30 - 11:00	Coffee Break				
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12:30 - 13:30	Lunch Break				
13:30 - 15:00	Mike P. Allen ***Introduction to Molecular Dynamics Simulations***	Excursion to the Research Centre Jülich Gerhard Gompper ***Soft Matter Research in Jülich*** Thomas Lippert ***The John von Neumann Institute for Computing*** Bernd Mohr ***Parallel Programming Models and Tools***	Poster Session A	Poster Session B	Ole G. Mouritsen ***A Lattice Model Approach to Biomembranes***
15:00 - 15:30	Coffee Break		Coffee Break		
15:30 - 17:00	Christian Holm ***Dealing with Long Range Interactions: Polyelectrolytes***		Friederike Schmid ***Surfactants at Interfaces: Simulation of Structure and Phase Behavior***	Helmut G. Grubmüller ***Molecular Maschines***	Marcus Müller ***Phase Behavior and Chain Conformations in Polymer Blends and Copolymer Mesophases***
Evening		Reception and Dinner			Farewell Dinner

Contents

Improving the Poisson-Boltzmann Theory by Including Counterion Correlations on a Density Functional Level

Dmytro Antypov[1], **Christian Holm**[1], **Markus Deserno**[1], **and Marcia Barbosa**[2]

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We consider a density functional extension to the Poisson-Boltzmann (PB) theory[1,2], which allows taking into account the inter-ionic correlations neglected in the mean-field approach. These include both electrostatic correlations treated within the recently developed Debye-Hückel-Hole-Cavity (DHHC) theory[2,3] and excluded volume effects treated in the way proposed by Tarazaona[4] for hard spheres. While the latter is a *local* density functional approach, the steric correlations, due to their short range nature, are incorporated using the *weighted* density method. The results of the free energy functional minimisations are compared to those obtained from our cell model MC simulations of a single charged colloid surrounded by its counterions. We find a marked improvement on the predictions of the PB theory, which neglects the correlations between counterions and treats them as an ideal gas.

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Statistical Properties of Off-Lattice Heteropolymers

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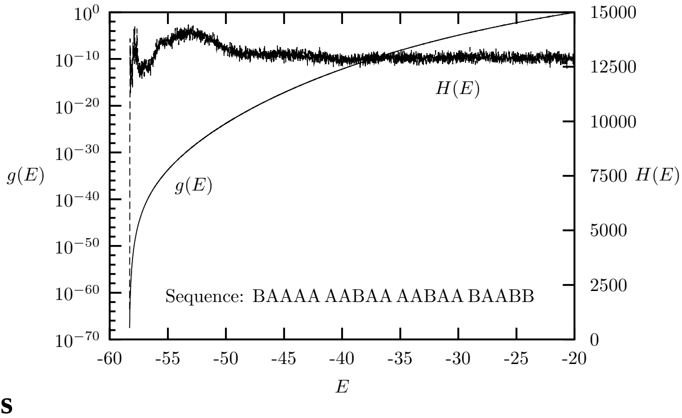
We apply a multicanonical algorithm to variants of the AB model[1,2] being an off-lattice model for heteropolymers. Heteropolymers are considered as chains of hydrophobic (A) and hydrophilic (B) monomers only. Into the energy function enter the bending energy and a Lennard-Jones-like potential between nonbonded monomers, where short-range repulsion and long-range attraction compete. Contacts between hydrophobic monomers are favoured, thereby assuming that the global energy minimum state of proteins is characterized by a compact hydrophobic core screened from the solvent by a shell of hydrophilic residues. We calculate thermodynamic quantities for known sequences by means of a modified AB model[2] and identify the temperatures, where conformational pseudo transitions are expected. Since the multicanonical algorithm allows for an accurate sampling of the low-temperature region, we also obtain good estimates for the global energy minimum. Therefore we apply our algorithm to sequences where minimum energies were recently quoted[3] and compare with lowest-energy states found by minimizing procedures. The figure shows the flat histogram $H(E)$ from the multicanonical sampling of a 20mer and the density of states $g(E)$ that has accurately been determined over 70 orders of magnitude.



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Folding and Unfolding of an Elastin-Like Oligopeptide

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and Dominik Marx**

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Elastin, a principle protein component in vertebrate's connective tissues, features unusual viscoelastic properties[1–3]. Remarkably, upon increasing the temperature beyond 40°C this protein folds, while regular proteins would undergo denaturation. The term "inverse temperature transition" (ITT) was coined for this apparently paradoxical change from a "disordered" (extended) to an "ordered" (folded) conformation upon heating. The origin of elastin's properties is controversially discussed, calling concepts such as rubber elasticity[4], librational entropy[1–3], hydrophobic collapse[5], and multi–phase models[3, 5, 6]. Beyond doubt is the decisive role of water as a plasticizer (dry elastin is *brittle*[3]), but the aspect of the protein's hydration water *dynamics* remains unexplored.

A significant experimental finding was the recent finding[7] that oligopeptides of the kind GVG(VPGVG)$_n$ display the ITT even in the limit of only one pentameric repeat unit. Using the limiting value n = 1 opens up the possibility to perform molecular dynamics (MD) simulations that allow for fairly long simulation times with sufficiently many solvating water molecules.

We present classical MD-simulation results[8, 9] which demonstrate that the peptide GVG(VPGVG) undergoes an ITT leading to a folding at about 40-50°C. In addition, an unfolding transition is identified at unusually high temperatures approaching the boiling point of water. A detailed molecular view involving a thermodynamic order parameter, or reaction coordinate, for this process is presented along with a time-correlation function analysis of the hydrogen bond dynamics within the peptide as well as between the peptide and solvating water molecules. This picture is emphasizing the role of the hydrogen bond dynamics at the protein-water interface and peptide backbone librational entropy.

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δ-Amino Acids as Building Blocks for the Structural Design of Peptides and Foldamers

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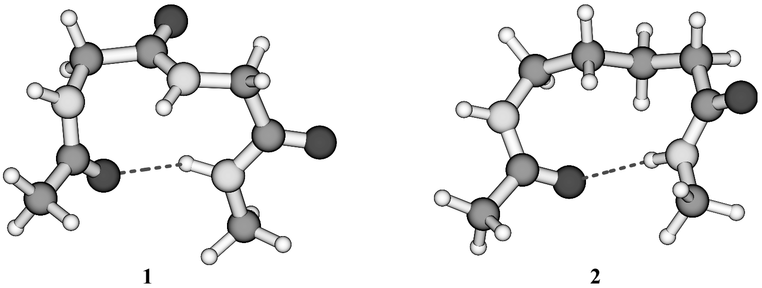
In the last years, numerous studies demonstrated that oligomers of α-, β- and γ-amino acids are able to form stable secondary structures with interesting properties. The consistent extension of the homology principle leads to δ-peptides, which are solely composed of δ-amino acids. Elements of secondary structures could be expected in this class of compounds, too. In comparison to β- and γ-amino acids, δ-amino acids show a special aspect. The size of a δ-amino acid constituent corresponds approximately to a dimer unit in the native α-peptides. Thus, a single δ-amino acid could replace a dimer unit in α-peptides and secondary structures in δ-peptides should be rather similar to the typical secondary structures in native peptides.

In this study, we performed a systematic conformational analysis on hexamers of δ-amino acids at the HF/6-31G* and B3LYP/6-31G* level of ab initio MO theory to find the possibilities of helix formation in δ-peptides. Solvation effects were estimated by the polarizable continuum approach (PCM//HF/6-31G*). A wide variety of helical structures with H-bonds pointing forward and backwards along the sequence was found. The most stable ones form 10-membered hydrogen bonded pseudocycles like the 3_{10}-helix of α-peptides.

Beside the possibility of helix formation in oligomers of δ-amino acids, δ-amino acids can also serve as β-turn mimetics. Our studies show that the two central β-amino acids in a β-turn can be replaced by a δ-amino acid without changes of the structure (see Fig. 1). However, some alternatives for β-turn formation with δ-amino acids appear which are even more stable than these β-turn analogues.



1 **2**

Figure 1. Comparison of a βII-type turn (**1**) in native peptides with a blocked δ-amino acid (**2**).

Vanadate Embedded in Hydrogen Bonding Network: DFT Study of Active Site of Vanadium Haloperoxidase

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Vanadium containing haloperoxidases (VHPO) catalyse[1,2] the two electron oxidation of a halide by hydrogen peroxide. The reactive species 'hypohalous acid' thus formed, either haloginates the organic compounds, or in absence of organic substrates consumes another hydrogen peroxide to produce singlet oxygen. Crystal structure of chloroperoxidase[3] from *Curvularia Inaequalis* revealed enzyme's active site and a vanadate anion was found with vanadium within covalent bonding distance to His496 residue while anionic oxygens of vanadate engaged themselves in hydrogen bonding with other residues Lys353, Arg360, Ser402, Gly403, His404 and Arg490. These residues, in one way or the other, optimize electron density at vanadate centre for peroxide attack and subsequent oxygen-transfer to halide ion.

Interestingly, amino acid sequence of active site of VHPOs was found to be conserved in three families of acid phosphatases including mammalian glucose-6-phosphatase[4]. This led to anticipation that these phosphatases might exhibit haloperoxidase activity, which actually was shown to be possible[5] but observed catalytic rates were much lower than those for haloperoxidase. At first glance this might seem surprising as active site architecture of two enzymes is astonishingly similar but some subitle differences in hydrogen bonding network in two active sites can prove to be vital for fine turning of haloperoxidase activity. In present work DFT calculations are carried out to elucidate the hydrogen bonding network in active site of vanadium chloroperoxidase[3] from *Curvularia Inaequalis* and acid phosphatase[6] from *Escherichia Blattae*. It is shown that the two enzymes, despite having structural similarities in active site, have differences in their hydrogen bonding networks. Particularly Arg183 in phosphatase is not equivalent to it's Arg490 counterpart in VHPO in this respect.

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Dynamical Properties of the Slithering Snake Algorithm: A Numerical Test of the Activated Reptation Hypothesis

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Correlations in the motion of reptating polymers in a melt are investigated by means of Monte Carlo simulations of the three dimensional slithering snake version of the bond-fluctuation model.[1] Surprisingly, the slithering snake dynamics becomes inconsistent with classical reptation predictions at high chain overlap (created either by chain length N or by the volume fraction ϕ of occupied lattice sites), where the relaxation times increase much faster than expected. This is due to the anomalous curvilinear diffusion in a finite time window whose upper bound $\tau_+(N)$ is set by the density of chain ends ϕ/N. Density fluctuations created by passing chain ends allow a reference polymer to break out of the local cage of immobile obstacles created by neighboring chains. The dynamics of dense solutions of "snakes" at $t \ll \tau_+$ is identical to that of a benchmark system where all chains but one are frozen. We demonstrate that the subdiffusive dynamical regime is caused by the slow creeping of a chain out of its correlation hole. Our results are in good qualitative agreement with the activated reptation scheme proposed recently by Semenov and Rubinstein.[2] Additionally, we briefly comment on the relevance of local relaxation pathways within a slithering snake scheme. Our preliminary results suggest that a judicious choice of the ratio of local to slithering snake moves is crucial to equilibrate a melt of long chains efficiently.

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Ab Initio Investigation of Structure and Stability of Two-Fold Rings in Silicates

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We present *ab initio* many-body calculations on the strain energy of W-silica, taken as a model system for edge-sharing tetrahedral SiO_2-systems with respect to corner-sharing ones as in α-quartz. The mean-field results were obtained using the restricted Hartree-Fock approach, while the many-body effects were taken into account by the second-order Møller-Plesset perturbation theory and the coupled-cluster approach. Correlation contributions are found to play an important role to determine the stability of edge-sharing units. The most sophisticated method used in our calculation, i.e., the coupled-cluster approach with single and double excitations, yields a strain energy of 0.0427 a.u. per Si_2O_4 unit with respect to α-quartz, which is even smaller than the value obtained by a previous DFT calculation[1]. The results indicate that edge-sharing SiO_4 tetrahedra in (partially) amorphous systems are possible at a modest energetic expense.

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Free Interfaces in Binary Hard-Platelet Mixtures

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Suspensions of platelike colloids like blood, clay sols, or liquid crystal dispersions are of increasing interest because of possible applications in biomedicine, geophysics, or liquid crystal display technology. So far, most theoretical investigations on platelets have only been devoted to bulk properties like the formation of isotropic and nematic phases. In contrast, this work is dedicated to interfaces between demixed fluid-fluid phases of binary mixtures of hard platelets.

The most adequate approach to treat inhomogeneities like interfaces is the density functional theory. In order to apply the currently most sophisticated excess free energy functional, the fundamental measure functional, platelets are described within the Zwanzig model, which allows only three mutually orthogonal orientations.

Two different binary hard-platelet mixtures have been considered: A mixture of large thin and small thick platelets as well as a mixture of large and small thin platelets. Besides non-fluid phases, the first mixture shows one isotropic and one nematic phase whereas the second mixture exhibits one isotropic and two nematic phases. Additionally, the second mixture shows an isotropic-nematic-nematic triple point.

Density and orientational order parameter profiles at interfaces between coexisting phases as well as the interfacial tension are determined. In the mixture of large thin and small thick platelets, a density inversion, oscillatory density profiles, and a Fisher-Widom line have been found. The lowest interfacial tension corresponds to the mean bulk orientation of the platelets being parallel to the interface. For the mixture of large and small thin platelets, an isotropic-nematic interface is completely wetted by a film of a second nematic phase when approaching the isotropic-nematic-nematic triple point. This has been confirmed by both the asymptotic logaritmic divergence of the film thickness and the vanishing of the dihedral angle of a lense of the wetting phase.

For further details see *M. Bier, L. Harnau, and S. Dietrich, cond-mat/0310716* and the references therein.

Molecular Simulation of the Adsorption of Molecules out of Dilute Solutions

W. Billes, R. Tscheliessnig, F. Bazant-Hegemark, M. Wendland, and J. Fischer

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The minimum in the free energy yields the preferred position of a molecule and in case of more complex molecules like proteins also its preferred configuration. The change of the free energy is obtained by integration over the mean force on a molecule. This method is physically obvious as it says that the change in free energy is the work required on a reversible path. In addition the potential of mean force can be related to the logarithm of the local density[1]. The molecule is fixed in a certain position and the mean force exerted on it from the surface and the fluid particles is calculated. Then the mean force is integrated over an appropriate path to yield the potential of mean force.

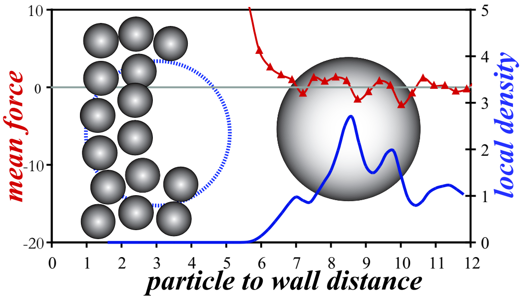

Figure 1. This graphic shows the mean force and the relative local density of a dilute component B as function of the distance from the wall as obtained by integration of the mean force. The system is a LJ mixture in contact with a 9/3 LJ wall. The A-particles form the solvent which are rather densely packed close to the wall. The blue dotted circle at the left side represents a B-particle which one would intuetively center at the minimum of the wall potential. The result of the MDS give clear evidence that the B-particle is shielded off from the wall by the A-particles. The B-particle is centered at the maximum of the local density. [2].

Based on this theory we first considered rather simple systems of various 1-center Lennard-Jones (LJ) mixtures at a 9/3-Lennard-Jones wall[1]. As a representative result see Figure 1. In a second step, we will study the adsorption of 2-center-LJ fluids at those walls. We will outline the possibilities to handel even more complex systems: like the adsorption of a bio-molecule at structured carbon surfaces.

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Monte Carlo Simulations for Instantaneous Electrodeposition Processes

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We introduce a very simple model for the instantaneous electrodeposition process that takes into account the kinetic roughening during the film growth. The main ingredients of the model are the characteristic time for the cation particles to attain their steady state velocity, and the choice of a velocity dependent probability for the particles to relax on the substrate. The model is capable of reproducing the experimental results for the density current as a function of time for a fixed value of the external potential during the electrodeposition experiment, as well as typical voltammograms. The model was investigated through a suitable continuous Monte Carlo algorithm where the number of particles to be deposited in a Monte Carlo step (MCs) changes with time. For small values of the particle velocities the deposition is essentially described by a pure random deposition model, while for high values of velocity a dominant local relaxation process is assumed. At each MCs we compute the surface width in order to determine the roughness of the surface. From the plots of the surface width versus time we found the growing β, dynamic z and roughness α exponents for this model.

Crossover from 2D to 3D Demixing in Binary Polymer Blends: A Monte Carlo Simulation

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Monte Carlo simulation of the Bond Fluctuation Model are performed in order to study the unmixing behavior of symmetrical polymer blends (chain length $N_A = N_B = N$) confined in ultrathin films. The critical temperature T_c of unmixing has been located by finite-size scaling analysis for different values of chain length (from $N = 16$ to $N = 256$) and film thickness (from D=2 to D=19 in units of lattice spacing). A crossover from two–dimensional to three–dimensional, bulk-like behavior in the scaling of the critical temperature with N is observed for D close to the screening length of the polymer melt, $\xi_s \sim 7$. This crossover is independent of the chain length. In the limit of large film thicknesses ($D >> \xi$), we show that the critical temperature asymptotically approaches the linear scaling ($T_c \sim N$) predicted by the Flory-Huggins theory. When we reduce the film thickness ($D \lesssim 2\xi_s$), we observe a weaker increase of T_c with N. Assuming the power law $T_c \sim N^{\alpha(D)}$, for ($D << \xi_s$), our results are compatible with $\alpha(D) \sim 1/2$. For $2 < D < \xi_s$, the exponent $\alpha(D)$ grows from 0.68 to 0.83 (15%), instead, for $\xi_s < D < 19$, it increases only from 0.83 to 0.9 (7%). This allows us to identify ξ_s as a crossover length between the two regimes. The anomalous scaling of the critical temperature with the chain length for ultrathin films and the crossover from the two–dimensional to the three–dimensional demixing can be rationalized in terms of geometrical arguments.

Static and Dynamic Properties of Tethered Chains at Adsorbing Surfaces: A Monte Carlo Study

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We present extensive Monte Carlo simulations of tethered chains of length N on adsorbing surfaces, considering the dilute case in good solvents, and analyze our results using scaling arguments. We focus on the mean number M of chain contacts with the adsorbing wall, on the chain's extension (the radius of gyration) perpendicular and parallel to the adsorbing surface, on the probability distribution of the free end and on the density profile for all monomers. At the critical adsorption strength ϵ_c one has $M_c \sim N^{\phi}$, and we find (using the above results) as best candidate ϕ to equal 0.59. However, slight changes in the estimation of ϵ_c lead to large deviations in the resulting ϕ; this might be a possible reason for the difference in the ϕ values reported in the literature. We also investigate the dynamical scaling behavior at ϵ_c, by focusing on the end-to-end correlation function and on the correlation function of monomers adsorbed at the wall. We find that at ϵ_c the dynamic scaling exponent a (which describes the relaxation time of the chain as a function of N) is the same as that of free chains. Furthermore, we find that for tethered chains the modes perpendicular to the surface relax quicker than those parallel to it, which may be seen as a splitting in the relaxation spectrum.

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Structural Dependence of the ^{15}N and ^{27}Al Chemical Shifts in Solid AlN
A Theoretical Investigation

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AlN is a III-V semiconductor with high thermal conductivity, low compressibility and a wide band gap. Thin films of AlN may be produced from molecular precursors by chemical vapor deposition.
In order to assist the characterisation of the resulting materials we calculated the ^{15}N and ^{27}Al chemical shifts in thermodynamically stable wurtzite type AlN and in metastable zinc-blende AlN. The shifts were computed from H-saturated clusters which were chosen as cutouts from the crystal structure.
Experimental ^{15}N and ^{27}Al chemical shifts in wurtzite AlN could be reproduced with good accuracy. It was found that the ^{15}N chemical shift is much more sensitive to changes in the local environment than the ^{27}Al chemical shift. The ^{15}N chemical shifts can be classified according to the number of H-Atoms in the neighbourhood.
No experimental NMR data for zinc-blende AlN is available until now. From our calculations we can predict that the ^{15}N chemical shifts in zinc-blende and wurtzite AlN are very similar.

The Sequence Design of Heteropolymers with Saturating Bonds

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Heteropolymers with saturating bonds attract scientists as a very coarse-grained model of biopolymers like DNA and RNA. In our research we investigate the formation of stable secondary structure caused by the hydrogen bonds between corresponding bases and the statistical behavior of model energy spectra. Our goal was to analyze the influence of the initial sequence and other factors on the bottom part of these spectra and to reveal the properties of the ground state of such systems. The simple matrix model we use corresponds to the case of AB-copolymer which can have only saturating bonds between the A- and B-units. The parameters of our system are: N is the number of monomer units in the chain, q is the number of different interactions and δ is the dispersion of energies. The energies are determined from the random matrix of interaction B_{ij} which depends on the set of parameters. The simplified model we use provides with good accuracy the results close to those obtained in the exact 3d-simulation, but requires much less computational resources. For small values of N we use full enumeration of the low-energy structures, while for $N > 20$ we use Monte Carlo simulation. The investigation of the obtained spectra showed that on average there is only a little difference between the ground state and the next states. It also showed that the ground states of the different realizations can vary in quite a wide range. Only an exponentially small part of the random realizations has the unique and "rough" enough ground state. The phase diagram in terms of (N, q, δ) was obtained. This diagram shows which combination of these parameters can cause the unique ground state. Nearest perspective is to estimate whether this ground state is steady or not, and if it can be achieved at finite temperatures within kinetic motion.

Phase Diagrams of Ising Mixtures

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The mean field theory for the pure Ising fluid was recently extended to binary mixtures of an Ising and a van der Waals fluid[1]. Depending on three parameters describing the relative magnetic and nonmagnetic interaction strengths, the theory predicts a rich multicritical behavior in the three dimensional x, T, p-phase diagrams, featuring tricritical consolute and plait point lines, lines of critical end points and magnetic consolute point lines. In order to ascertain if the predicted topologies are also found in the presence of fluctuations we have performed extensive Monte Carlo simulations, investigating both first order (liquid-vapor and demixing) and second order (paramagnetic-ferromagnetic) phase transitions for mixtures of a Lennard-Jones fluid and a Lennard-Jones Ising fluid as well as for the Ising fluid itself. The computational methods we have used include Gibbs Ensemble MC, Multi-histogram Reweighting, Hyper-parallel Tempering, the cumulant intersection method and the newly developed Density of States MC technique. We present the resulting ρ, T phase diagrams of pure Ising fluids with varying strengths of the magnetic interaction as well as constant pressure and temperature sections of the phase diagrams of Ising mixtures with different system parameters. The results show that in the accessible temperature range the mean field topology is obtained.

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Mixed Helices - A Novel General Folding Pattern in Homologous Peptides

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The periodic structure elements of the native α-peptides are defined by the backbone torsion angles ω, ϕ and ψ. All hydrogen bonds in the α- and 3_{10}-helix point into the backward direction along the sequence and form pseudocycles with 13 and 10 atoms, respectively. In β-peptides, which are homologues of the α-peptides, a novel unique type of a periodic secondary structure was found by Seebach and co-workers, which they named 'mixed helix'.[1] In this structure, the repeating unit is not the monomer, but a dimer unit. The peptide bonds are alternately involved in hydrogen bonds pointing backwards and forward along the sequence (see Fig. 1).

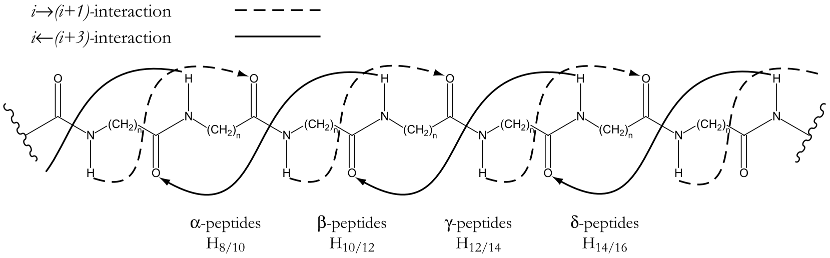

Figure 1. Hydrogen bonding pattern in mixed helices of homologous α- (n=1), β- (n=2), γ- (n=3) and δ-peptides (n=4).

The finding of mixed helices of β-peptides might be a hint for the existence of similar structures in α-peptides and their homologous γ- and δ-peptides. The conformational space of these homologues was screened by a systematic variation of the backbone torsion angles in the dimeric subunits of hexamers. The resulting structures were starting points for geometry optimizations at the HF/6-31G* and B3LYP/6-31G* level of ab initio MO theory. For each of the homologous peptides one or more mixed helices were found. Some of them were at least as stable as their classical helical counterparts. Calculations at the PCM//HF/6-31G* level reveal, that a polar solvent is unfavorable for the formation of mixed helices due to the low dipole of these structures. Only the experimentally described mixed helix of the β-peptides[1] remains very stable in water.

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Comparison of Theory and Experimental Data on the Rheology of Dense Colloidal Suspensions

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The rheological properties of soft materials like particle suspensions are a challenge in soft matter science. While dilute suspensions flow with a viscosity only slightly higher than that of the solvent, concentrated ones behave as weak amorphous solids and elastically withstand finite stresses. On increasing the external shear rate a strong decrease of the viscosity is observed. This feature of a non-Newtonian fluid is usually referred to as shear thinning. Temperature sensitive core-shell latex particles[1] provide model dispersions that show this behaviour. Depending on the concentration of suspended particles phenomena like shear thickening and jamming are also observed and can even be analyzed quantitatively[2].

In principle linear flow theories fail to describe the behaviour of dense suspensions and have to be abandoned in favour of non-linear ones. The later account for the crucial role that the imposed shear itself plays for the internal particle dynamics. We compare non-Newtonian viscosity data with model calculations suggested by a recent first-principles approach to non-linear rheology of dense colloidal suspensions[3]. It predicts a universal transition between yielding of amorphous solids and shear thinning fluid flow. The significant mechanism behind is the advection of density fluctuations. Hydrodynamic interactions, non-linear flow profiles and ordering phenomena are neglected. The data analysis indicates that the predicted transition is experimentally accessible.

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Polymers Confined Between Two Parallel Plane Walls

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Single three dimensional polymers confined to a slab, i.e. to the region between two parallel plane walls, are studied by Monte Carlo simulations. They are described by N-step walks on a simple cubic lattice confined to the region $1 \leq z \leq D$. The simulations cover both regions $D << R_F$ and $D >> R_F$ (where $R_F \sim N^\nu$ is the Flory radius, with $\nu \approx 0.587$), as well as the cross-over region in between. Chain lengths are up to $N = 80,000$, slab widths up to $D = 120$. In order to test the analysis program and to check for finite size corrections, we actually studied three different models: (a) Ordinary random walks (mimicking Θ-polymers); (b) Self-avoiding walks (SAW); and (c) Domb-Joyce walks with the self-repulsion tuned to the point where finite size corrections for free (unrestricted) chains are minimal. For the simulations we employ the pruned-enriched-Rosenbluth method (PERM)[1] with Markovian anticipation[2–5]. In addition to the partition sum (which gives us a direct estimate of the forces exerted onto the walls), we measure the density profiles of monomers and of end points transverse to the slab, and the radial extent of the chain parallel to the walls. All scaling laws and some of the universal amplitude ratios are compared to theoretical predictions[6].

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Cooperative Dynamics of Multicontact Friction: Creep and Stress Relaxation

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It has been recently shown experimentally that the cell wall extends logarithmically under the application of a constant, unidirectional force. We have described this phenomenon in analogy with the frictional dynamics of rough multicontact surfaces, by means of the Burridge and Knopoff (BK) model at finite temperature. In this model contacts move, driven by temperature, to relax the internal stresses at the interface between two surfaces. We show that, depending on the strength of interactions between contacts, different regimes for the microscopic motion can be identified, which in turn affect macroscopic friction, stress relaxation and their temperature dependence. In this way, experimental information can be used to get insight on the microscopic structure of this complex system. We have also simplified the problem of stress relaxation in the BK-model by developing an automaton-like version of the model, and have shown that the BK-model can also behave logarithmically slow when driven by a low force and temperature, much like the cell wall.

Bilayer Material Properties from Dissipative Particle Dynamics Simulations

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Dissipative Particle Dynamics simulations are used to extract the material parameters (bending modulus and area stretch modulus) of a bilayer membrane patch. The area stretch modulus is an important property of biological membranes, and some experiments indicate that it varies little as the chain length of the lipids composing the bilayer increases. Here we show that the interactions between the hydrophilic headgroups of the model lipids must be proportional to the hydrophobic tail length if the above result on the area stretch modulus is to be observed. We also show the effects of changing the amphiphile architecture on the membrane material properties.

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Molecular Dynamics Simulations of Polymer Friction Coefficients and Collision Dynamics in Sieving Media

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We utilize large scale non-equilibrium Molecular Dynamics simulations with an explicit solvent to systematically explore the friction coefficient $\xi(N)$ of polymers in conformations commonly occurring in sieving media. In particular we examine i) random coil polymers ii) rigid polymers moving either parallel or perpendicular to their major axis and iii) hydrodynamically coupled molecules. We compare these friction coefficients with predictions from macroscopic hydrodynamics. We also examine the collision of single polymer chains with obstacles in three regimes: i) a polymer (in the presence of an external force) colliding with a fixed obstacle ii) a polymer (in the presence of a fluid flow) colliding with a fixed obstacle and iii) a polymer (in the presence of an external force) colliding with a free polymer in solution. We present analytical models for these three regimes and compare them to results from Molecular Dynamics simulations with explicit hydrodynamic interactions.

The Unusual Behavior of the DMSO/Water Mixture

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DMSO–water mixtures exhibit a marked freezing point depression (60 K at n_{DMSO}=0.33)[1]. Additionally, the phase diagram[2] is very complex at n_{DMSO}=0.25–0.33, in which lies the possible origin for its cryopreserving ability.
As explanation stable 1DMSO-2H_2O (1–2), 2DMSO-3H_2O (2–3) and especially 1DMSO-3H_2O (1–3) cluster were suggested. Whereas the 1–2 and the 2–3 clusters were seen in traditional (based on pair potential) molecular dynamics (MD) simulation studies, the presence of a 1–3 cluster was not established.
Static quantum chemical calculation identified the structural patterns of small clusters[3]. These are spatially very different from those formed in MD simulation. In accordance with the discussion of the weak C-H$\cdots$O hydrogen bond by Steiner et al.[4] interaction energies of the methyl groups with water up to 8 kJ/mol are found. To identify characteristic structural features of the DMSO–water mixtures temperature-dependent high-resolution FT-Raman spectra[5] are compared to DFT calculations, which also consider anharmonicity effects.
Finally, the mixture is studied with Car–Parrinello MD simulation[6]. A 3-fold coordination at the DMSO oxygen, C-H$\cdots$O contacts, and 1–3 clusters are observed. The angular distribution for different distant water molecules around the methyl group shows a complex behavior: Close water molecules orient with the oxygens to the methyl hydrogen, far water molecules vice versa.

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Polymers in DPD

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DPD[1] is a novel method to describe systems on mesoscopic length and time scales with the correct thermo and hydrodynamics. After applying a few modifications to the original DPD scheme we can accurately model long polymer chains. DPD consists of two parts, a set of interaction forces and a thermostat. Normal DPD uses a random and dissipative force as a thermostat. The problem with this type of thermostat is that it does not even guarantee a correct temperature. To solve this we use a different thermostat which acts like an Andersen thermostat from molecular dynamics but then for particle pairs[2].

Polymers are included in this model by attaching fluid elements to each other with harmonic springs. If we choose the resulting Kuhn length four times larger than the hydrodynamic radius of a single element, we can show that relatively short chains (N=16) already behave similar to very long chains.

Another modification is the lack of the conservative force in polymer simulations. This still gives the correct thermo and hydrodynamics but makes for a very simple algorithm. We do this because it is the only way to model something which corresponds to a real system (a polymer in a theta-solvent). If we include the conservative forces also we still model polymers in some solvent, but it is not possible to relate such a system to reality.

Note that even though we lose all the original ingredients of DPD, we end up with a model which is similar to it, but actually simulates a real system.

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Atomistic Simulations of *tert*-Butanol and Water Mixtures

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Studies on the liquid structure of alcohol-water mixtures provide important insights in the role of hydrophobic interactions that are believed to control aggregation of amphiphilic molecules in biological systems. Especially *tert*-butanol is of great interest as it is the largest monohydric alcohol that remains fully miscible with water at room temperature. Hydrophobic interactions between *tert*-butyl moieties cause highly non-ideal solution behaviour, which depends strongly on the solution composition and temperature.

Our goal is to parameterise an atomistic *tert*-butanol (*tba*) model capable of reproducing the non-ideal solution behaviour over the full composition range. For water the single-point-charge (SPC) model is used. We make use of the Kirkwood-Buff theory of solution,[1,2] which provides relations between thermodynamic quantities (known from experiment) and molecular distribution functions. The molecular distribution functions obtained from our simulation relate to thermodynamic quantities through Kirkwood-Buff (KB) integrals, which reveal whether a solution component is preferentially solvated by molecules of the same species or by the other component. Our optimised model quantitatively reproduces the excess *tba*-*tba* association observed experimentally[3] at low *tba* concentrations while stronger excess water association at slightly higher *tba* concentrations is underestimated.

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A New Polarizable and Dissociable Potential for Water: Clusters and Transferability to Bulk Water

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A new polarizable and dissociable potential for water is presented and validated through the study of microclusters. It is shown that several properties compares well to the available experimental data and the results of ab initio studies. In particular, the geometries and the vibrational properties of the ground states and of several local minima and the molecular dipole moments are satisfatorily reproduced.
With regard to transferability to the description of bulk water, we remark that the employed potential keeps a relatively simple and physically transparent form; the small number of parameters it contains makes it more likely that they are close to the real ones. Besides, the range of predicted physical properties is rather wide, quantitatively and qualitatively, compared to other studies of this kind. Finally, the trends of some important quantities, like the average oxygen-oxygen distances and the average molecular dipole moment- with increasing number n of molecules in the clusters- are in agreement with ab initio calculations and clearly show that the absolute errors decrease with n.

Flory-Huggins Parameter from Atomistic Molecular Dynamics Simulations

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The miscibility of two polymers is determined by the free energy of mixing which includes both entropic and enthalpic terms, modelled in the Flory-Huggins approximation as:

$$\frac{\Delta G_{mix}}{RT} = \left(\frac{\Phi_A}{N_A}\right) \ln \Phi_A + \left(\frac{\Phi_B}{N_B}\right) \ln \Phi_B + \chi_{FH} \Phi_A \Phi_B$$

where R is the gas constant, Φ_A the volume fraction of polymer A and χ_{FH} the Flory-Huggins parameter. The first two terms of the right hand side of the equation above reported represent the combinatorial contribution to the entropy of mixing the last term is the enthalpic contribution.

In principle, once the Flory-Huggins parameter is known the entire phase diagram of the system can be calculated.

Different approaches can be implemented to extract Flory-Huggins parameter from molecular simulations. Different applications to systems of increasing complexity, going from mixtures of low molecular weight organic molecules to polymer/solvent systems will be presented.

On the Curvature of Oceanic Arcs: New Insights from a 3-D BEM-FEM Method for Subduction

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A well known feature of subduction zones is the curvature of oceanic arcs. Arc curvature is often held to be due to the Earths sphericity. This would imply that the radius of curvature is everywhere similar to the order of the radius of the Earth. However, the observation shows that there is a significant departure of smaller arcs towards higher curvature. We investigate this problem using our newly developed coupled analytical-solid-mechanical FEM model for the dynamics of slab-mantle feedback during subduction.

The method consists of embedding a solid lithosphere, modeled with a Lagrangian finite-element code, into a creeping flow mantle, where the drag is solved analytically by the Stokeslet method. Such a method consists of calculating analytically the stress profile on the subducted plate, using a second order approximation of mantle drag flow. The solution is obtained by a so-called lubrication theory where the stress profile is given by the volumetric flow constraints of the subduction process. The solution is discretized and applied as different singular solutions (Stokeslet) for each node of the boundary of the FEM model. The new tool permits to perform three-dimensional subduction simulations at reasonable computation cost, because solutions for the largest domain in the calculation, the mantle, is obtained analytically.

We analyze separately, two effects being lateral density inhomogeneities of the slab and side flow of the mantle on the ends of the arc and consider their competition. It is shown that the oceanic arcs can be obtained as the effect of the lateral mantle flow on the side of the slab, without the necessity to consider the Earth curvature. It is also shown, that the lateral density inhomogeneities in the slab play an essential role in controlling the trench dynamics, the trench shape and the plate motion and it is identified as the dominant effect for open subduction systems.

Hydrogen Bonding Properties of Sphingomyelin Bilayers - A Molecular Dynamics Simulation Study

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Sphingomyelin molecules are, among phosphatidylcholines and cholesterol, most important components of cellular plasma membranes. Sphingomyelin shares many common features with other lipids, although significant differences arise from a few specific details in molecular structure[1]. Especially, the higher hydrogen bonding capacity together with the higher degree of saturation in fatty acyl chains, as compared with phosphatidylcholines, makes them most likely to interact with cholesterol. This interaction has been postulated to be the driving force in formation of lateral domains (rafts) in biomembranes[2].

Only a few molecular simulation studies have been carried out on sphingomyelins[3–5] and yet no studies have concentrated on the interaction of sphingomyelins with other lipid components in biological membranes. Our aim is to first create and validate a molecular dynamics model for sphingomyelins and then create a combined bilayer model of sphingomyelins together with phosphatidylcholines and cholesterol molecules. Later on, coarse graining techniques will be applied to finally achieve biologically relevant time scales and system sizes.

The presentation at the NIC Winter School 2004 in Bonn will discuss some aspects and structural properties of sphingomyelin molecules and bilayers[6].

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Fusion and Fission of Bilayer Membranes: Brownian Dynamics

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We have studied the dynamics of vesicles, closed bilayer membranes, by three-dimensional Brownian dynamics simulations: (1) self-assembly into vesicles[1], (2) spontaneous fusion[2], (3) the adhesion of a nanoparticle[3], (4) fission[4] or fusion[5] induced by mechanical force, and (5) the formation of polyhedral vesicles[6].
We have clarified the two pathways of spontaneous fusion[2]. The contacted vesicles form neck-like structure connecting only outer monolayers. This intermediate agrees with stalk intermediate predicted by the stalk hypothesis. At high temperature, a pore on a vesicle by the side of stalk opens, and the elliptic stalk bends around it. Then a fusion pore connecting insides of vesicles is formed. On the other hand, at low temperature, the fusion pore opens through the trans monolayer contact from the stalk state. A nanoparticle, which interacts attractively with the hydrophilic segments, induces fusion-pore opening through stalk-bending process from stalk intermediates.

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Effect of Surface Topology on Hydrophobicity by Atomistic Molecular Dynamics Simulation

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My work is to understand the superhydrophobic 'lotus effect' at the nanometer level. The strongly reduced wettability of leaves is an obvious and long known phenomenon. The theory of wettability was to a large extent worked out in the last century, but in detail it is still subject to intensive research today. As a rule the following can be stated: The wettability of a material with air and water as the surrounding media depends on the ratio of the interfacial tension between water/air, material/water and material/air. The ratio of the tensions determines the contact angle of a water droplet to the surface. A contact angle of 0 indicates complete wetting, the water droplet spreading out into a mononuclear film. A contact angle of 180 means complete unwettability, the droplet making contact with the surface in only one point. Materials with a high interfacial tension are more wettable than those with a low interfacial tension, such as Teflon. The behavior of water on a surface is to a large extent dependent on the roughness of the surface. The wettability of a smooth, easily wettable surface is even improved through roughening. On a smooth, hydrophobic surface, roughening results in a superhydrophobic (i.e. extremely unwettable) surface. In the latter case air is enclosed between the droplet and the microstructures. A single water droplet applied to a waxy leave rolls off the leave like on a hotplate. The roughness of the surface minimizes the contact area between leave and droplet, making a seemingly frictionless rolling possible.

We investigate the static properties of water at the water-hydrophobic surface interface with respect to the surface topology of the hydrophobic surface by molecular dynamics simulation. The model of the hydrophobic surface, in our system, is a crystal made up of the n-eicosane molecule. The properties we are interested in are the density, chemical potential, hydrogen bonds and the orientation of water at the interface.

Condensation Phenomena in Nano-Pores

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The non-equilibrium dynamics of condensation phenomena in nano-pores is studied via Monte Carlo simulation of a lattice gas model. Domains perform a random walk in the pores with a diffusion constant that turns out to grow with the domain size l as $\mathcal{D}(l) \sim l^{0.76}$. The evaporation of particles from a pore is described by a stretched exponential decay of the particle density $\rho(t) \sim exp\left[-(t/\tau)^{\beta}\right]$ with $\beta \approx 0.74$. Moreover, it is found that the domain growth is significantly slowed down in the presence of a rough wall. Finally results for the hysteretic behavior of the particle density as a function of the density of a reservoir are presented for various pore geometries in two and three dimensions.

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Orientational and Positional Phase Transitions in Geometric Confined Systems of Alkanes - A Numerical Study

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A classical phenomenological atom-atom potential is used to study alkane chains in a single 2D hexagonal pore via the Monte Carlo method. We find different phases characterized by orientational and positional order and discuss the influence of (1) the surface structure of the pore wall and (2) the pore diameter on the correlation functions. Our calculations for the confinement are compared to the bulk scenario and to recent experiments on n-alkanes in nano-pores by Huber and Knorr.

Simulation of Micelle Formation

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Above the Critical Micelle Concentration (CMC), amphiphiles (*e.g.* surfactants) in solution are no longer present only as isolated monomers, but also in aggregated form: micelles. A micellar cluster can be described as a hydrophobic core, shielded from the aqueous environment by a hydrophilic corona. The CMC is an important quantity for surfactants and it is difficult to determine theoretically. As far as we know, the CMC for a molecular model has not yet been determined.

Using molecular simulations of solvent/surfactant mixtures we aim to obtain the CMC for various surfactants and acquire information on free energy barriers involved in micelle formation.

The truncated and shifted Lennard-Jones (LJ, 12-6) potential is used to describe the molecular interactions. Solvent (s) molecules are represented as single LJ particles and surfactants consist of head (h) and tail (t) LJ particles, connected by a harmonic potential. tt and hs interactions are treated the same as ss interactions, while for the ts and th interactions only the repulsive part of the potential is used[1]. We have also performed simulations where the st interaction in the above parameter set has a small attraction well.

A hybrid Monte Carlo program which samples the semi-grand canonical ensemble was developed. By imposing a chemical potential difference $\Delta\mu$ between surfactant and solvent, the identity of a randomly picked molecule can be swapped (*i.e.* solvent → surfactant or vice versa). During one MC cycle, particle displacements are performed using molecular dynamics and volume changes are attempted in addition to identity swaps. The free energy as a function of cluster size is obtained from cluster size distributions, calculated from simulation data. The CMC can be calculated from this free energy profile[2].

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Hydrogen Bonding Between Histidine and Lignin Model Compounds or Redox Mediators as Calculated with the DFT Method

Effects on the Ease of Oxidation

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Using the Density Functional Theory, the effect of hydrogen bonding between imidazole (IM) and ten benzyl alcohol derivatives (BA) on the ionization potentials of the latter is calculated. IM is used as a model for histidine, which is found in the reaction sites of laccases and lignin peroxidases[1] and the BA-derivatives serve as lignin model compounds. A marked decrease ($\sim$15 kcal mol^{-1}) is found for the IPs of the BA-derivatives when paired with IM. This should facilitate the one-electron oxidation of BA in the reaction site of the enzyme. The same effect was found for the known redox mediators violuric acid, 1-hydroxybenzotriazole and N-hydroxyacetanilide assuming that they enter the reaction site of the enzymes. Furthermore, upon one-electron oxidation the strength of the H-bond from BA to IM is considerably increased and in the case of the mediators this effect is so pronounced that the relevant proton shifts from them to IM. If this occurs in the active site of the enzyme then the oxidized redox mediators are released into the aqueous phase in their neutral form rather than as radical cations (deprotonation of the radical cations). The oxidation power of the neutral radical mediators, however, is too low to initialize oxidation of lignin. A more likely reaction pathway is oxidation of the substrates via hydrogen abstraction[2]. The pertinent bond dissociation energies are similar for the BA-derivatives and the redox mediators, which in principle allows the reaction to occur.

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Experimental Analysis of Catalitic Processes of the Glutathione S- Transferase Enzyme Through Mass Spectrometry

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Enzymes are biological macromolecules consisting of proteins which act as catalysts in most chemical reactions occurring in living systems, and thus they play a vital role in many life processes. Enzymes increase the rate of a chemical reaction also by one million times with respect to the corresponding uncatalysed reaction because they lower the activation energy, by introducing an energetically more favoured reaction path from reagents to products; moreover these macromolecules intervene in all chemical processes in a highly stereospecific way, based on structural complementary between the reagent molecules (or substrates), and the active site of the enzyme. In this study we have examined some reactions catalysed by the enzyme Glutathione S- transferase (GST), which belongs to a large family of enzymes involved in the translocation of cellular material and in detoxification processes of many vegetable and animal systems, including the humans. In particular, the studied reactions are the dehalogenation of haloaromatic benzene and naphthalene compounds by conjugation with the natural tripeptide glutahione, i.e. the same reaction at the basis of the detoxification of human liver. Alternatively to the traditional UV spectroscopy, for the analysis of these catalytic processes we have adopted the experimental technique of mass spectrometry (MS), which is not much applied to the study of enzymatic reactions, but particularly useful in the cases where reagents or products of reaction are not easily detectable with UV-VIS detectors, or where they exhibit overlapping UV absorption peaks like it happens in the reactions with naphthalene substrates here examined. The mass spectrometer was coupled to electrospray ionisation source (ESI), which uses a soft method for the ionisation of compounds, and this is particularly indicated for organic and biological molecules and macromolecules, such as proteins, peptides and nucleic acids. We will illustrate some details of the experimental procedure developed for an accurate quantitative analysis with ESI-MS technique, and subsequently we will show the results obtained in this way, as well as the hypothesis advanced in order to explain the experimental data. The most interesting of our results regard: (a) the relative mobility order of halogen atoms substituted on the aromatic ring, for catalysed and uncatalysed reactions, which gives useful information about the effect of enzyme presence on the number of steps of the reaction; (b) the values of kinetic parameters appearing in the Michaelis-Menten rate equation, in particular the Michaelis-Menten constants which are a qualitative measure of the stability of intermediate enzyme-substrate complex formed during the catalytic process; and (c) the influence of a variation of temperature on the catalytic power of GST.

Off-Lattice Monte Carlo Simulations of Diffusion Limited Cluster Aggregation of Hardspheres

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Many systems such as silica gels, globular proteins gels undergo an aggregation process and lead to a gel formation. Monte Carlo algorithm allows to mimic such a behavior[1,2].
Simulations of hard spheres aggregation was performed using an off-lattice diffusion-limited cluster-cluster-aggregation ($DLCA$) model inside a cubic box. After the initial stage consisting of randomly distributing No spheres in the simulation box of size L leading to a concentration $c = N_0/L^3$, the $DLCA$ process is applied and a Brownian motion is assumed for each cluster. Nearest neighbors clusters link up irreversibly and continue to diffuse inversely proportional to their size.
The simulation is stopped either when the number of cluster is unity or when a three dimensional network arises. We have simulated aggregation and gelation over a range of volume fraction ϕ between 0.1% to 50%. Our simulations clearly show different regimes during the aggregation process and the crossover between floculation and percolation is well defined. We analysed the kinetic evolution in term of aggregates size and distribution and the structure through the pair correlation function $g(r)$ leading to a fractal dimension[3] d_f and a correlation length ξ.

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Development of a Genetic Algorithm for Studying the Folding of Model Proteins

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The Genetic Algorithm (GA)[1,2] is a search technique, based on the principles of natural evolution, which uses operators that are analogues of the evolutionary processes of genetic crossover, mutation and natural selection to explore multi-dimensional parameter spaces. A GA can be applied to any problem where the variables to be optimised (genes) can be encoded to form a string (chromosome). Each string represents a trial solution of the problem. The GA operators exchange information between the strings to evolve new and better solutions. A crucial feature of the GA approach is that it operates effectively in a parallel manner, such that many different regions of parameter space are investigated simultaneously. Furthermore, information concerning different regions of parameter space is passed actively between the individual strings by the crossover operator, thereby disseminating genetic information throughout the population. The GA is an intelligent search mechanism that is able to learn which regions of the search space represent good solutions.

Determination of the native state of a protein from its amino acid sequence is the goal of protein folding simulations, with potential applications in gene therapy and drug design. Location of the global minimum structure for a given structure, however, is a difficult optimisation problem. Minimal models, such as the 2D HP lattice bead protein model[3] can be used to develop search techniques to determine the native state and gain insights into folding pathways. A local coordinate system is used to reduce a protein's structure into a set of directions for use within the GA, which then searches this direction space to find the lowest energy structure corresponding to the protein's native state. Investigations[4,5] have shown that a GA is an effective technique for predicting the lowest energy states with this simple model. A 3D HP lattice bead protein model based on a diamond lattice represents a more realistic model and is currently under investigation.

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Thermodynamical and Molecular Mechanisms for the Solvation of Benzene in Water

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Benzene, in contrast to small aliphatic hydrocarbons, has a negative Gibbs energy of hydration when transferred from the gas phase to water. It has been proposed that the main force contributing to this stabilisation is the formation of hydrogen bonds between water and the aromatic ring[1].
The theoretical background of the solvation of benzene in water has previously been studied via several approaches, such as thermodynamical models[2] and by looking at the structural information found via Molecular Dynamics[3].
In the current study, the solvation process is looked at by comparing the equilibrated solvation of a hypothetical benzene without any charges but the same structural properties as benzene, with the equilibrated solvation of the common model of benzene as a partially charged molecule.
The thermodynamic integration as well as the radial distribution and angular correlation analysis performed here show even more convincingly the orientation dependence as found by Linse et al.[3], but present a different view on the contributions of enthalpy and entropy in hydrogen bond formation than the one proposed in the model proposed by Graziano et al.[2]

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Glycine on a Wet Pyrite Surface at Extreme Conditions

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The recently proposed "iron-sulfur world" (ISW) scenario[1] is an intriguing contribution to the controversial field of "Origin of Life" research. At the very heart of the ISW is the idea that prebiotic chemistry might have taken place near deep sea volcanoes (hydrothermal vents) at extremely high pressures and temperatures. In particular, the interface between hot pressurized water and Fe/S minerals, such as pyrite, $\mathrm{Fe^{II}S_2}$, is crucial to this scenario. A key step for building *proteins* is the formation of the peptide bond. It has been demonstrated that this reaction, which is usually unfavorable in water, can be carried out in the presence of FeS, H_2S, and CO in aqueous solution at elevated temperature and pressure[2]. While this is a major success for the ISW, the mechanism of this unusual reaction is not yet understood. Furthermore, pressure and temperature of this experiment were much lower than the ISW requires.

In an effort to contribute to this discussion we present ab initio molecular dynamics (MD) simulations[3,4] of the simplest amino acid, glycine (GLY: CH_2NH_2COOH) at the pyrite / water interface under ISW conditions. Our aim is to understand the very first step of pyrite-assisted peptide bond formation, which is the adsorption of GLY on the pyrite surface and its possible activation. The results are not only interesting in the context of the ISW, but also explore unusual chemistry.

The simulations show that GLY bound by one carboxylate oxygen and the NH_3^+ group easily desorbs from a pyrite / water interface, while the retention time of GLY bound by both carboxylate oxygens is much longer. The desorption process is water-assisted, and the surface bonding is best understood as an electrostatic interaction. We have also found indications of a GLY activation due to the interaction with the surface. This might open an avenue into the experimentally observed peptidization and is the subject of ongoing research.

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Migration of DNA in Structured Microchannels

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Electrophoresis is still one of the main techniques when handling DNA molecules. However, many important aspects are still only poorly understood[1]. Therefore much effort has been spent on the investigation of electrophoresis in microfluidic channel devices[2–5].
In this work, DNA migration in structured microchannels was investigated with computer simulations and in experiment. The results are in good agreement with experimental data. Both computational and experimental data show that for certain geometries, DNA molecules of certain chain length exhibit two different mobilities, which are very stable[6].

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Parallelization of YASP Molecular Dynamic Package Using OpenMP Technique

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Sequential version of package for molecular modeling YASP has been parallelized to increase computed time scales are still within reasonable real time ranges that is spent for calculations. Previous results of molecular modeling using this package showed that most of wasted CPU time (70 % of all time) is spent for calculating non-bonded forces. Then calculation of constraints, dihedral angle forces, bond angle forces follow. OpenMP technique was used to parallelize this parts of the software package, namely, cycles that do these tasks were parallelized using OpenMP philosophy and tools. It was also found that parallelizing of simple cycles such as integration of motion equation is not feasible. Executed tests showed that total spent CPU time slightly increased comparing to sequential version of package. They also revealed that with increasing number of processors used for calculations real times drops with behavior that is slightly worse that linear one.

Modeling Dielectrophoresis of Colloidal Particles

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Dielectrophoresis is a phenomenon that has been known for several decades. It has been applied to biological and medical research to separate entities based on their polarizability. In particular, it can be used in micromanipulation and separation of viruses, latex spheres and polyelectrolytes such as segments of DNA. Further applications include such diverse fields as nanotechnology.

Polarizable particles experience a dielectrophoretic (DEP) force in a non-uniform electric field. The force is either attractive or repulsive, causing particle motion towards or against the electric field gradient, depending on the polarizability of the particle with respect to the medium. In the case of an external AC electric field, the DEP force changes sign at the crossover frequency f_{CF}[1]. In electrokinetic experimental measurements, the velocity of propagation of the colloids in solution can be determined and hence the mobility of the particles extracted. A further advantage is that DEP, as well as some other electrokinetic measurements can be miniatyrized and performed on microfluidic devices.

We have investigated analytically[1,2] and computationally[3] the electrokinetic effects of colloidal particles in stationary liquid in the dilute limit under non-uniform electric fields. In particular, we have analyzed the dielectric properties of colloidal particles in terms of the crossover frequency[1] and multipolar interactions between the colloids[2]. The results compare favourably to experiments. We also suggest new experiments to test our findings. The phenomena discussed there are closely related to electrorotation[4] and stability of charge inversion in electrophoresis[3].

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Control of Electroosmotic Flow in a Nanofluidic Channel Using Grafted Polymer Chains

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Electroosmotic flow (EOF) refers to fluid flow past a surface induced by an external electric field. It initially arises near a solid-fluid boundary due to the net charge density in the Debye layer, but the bulk of the fluid is eventually dragged into a uniform flow by viscosity. The phenomenon plays a critical role in capillary electrophoresis experiments for the analysis of DNA molecules, but ways in which it may be controlled or quenched rest mostly on empirical evidence. The most common approach consists in coating the inner capillary surface with adsorbed or grafted polymer chains, but the definite mechanism by which this affects EOF remains elusive. We report on large-scale Molecular Dynamics computer simulations of EOF in a nanoscale cylindrical capillary, and discuss the impact of grafted polymers chains on the properties of EOF. The specific question we address is: are simple steric interactions between solvent molecules and grafted polymer chains sufficient to prevent the generation of EOF?

Molecular Dynamics of Biological Molecules at the Water−Membrane Interface

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Molecular dynamics of different molecules including peptides and molecular oxygen was studied. Model membranes were bilayers of two types – hydrocarbon (n−tetradecane) and lipid (1−palmitoyl−2−oleyl−phosphatidylcholine). Calculation of membrane dynamics was carried out in NVT and N PT ensembles (at isotropic normal pressure and at anisotropic, taking into account surface tension). Thermostat used was on the base of collisional dynamics (frequency of collisions 10 ps $^{-1}$, mass of collisional particles 1 amu) and forcefield employed most ly was that of Amber (Amber99). The following adjectives of the membranes were considered: specific surficial area and density of the media, diffusion parameters and parameters of lipid conformation. Also dynamics of molecules at water−membrane interface a nd inside the last one was examined. Application of external linear field enabled consideration of membrane penetration. Structural (micro− and macroscopic) characteristics are found to be in a good agreement with experimental data. Dynamics of molecules a t interface are determined by polarity, size and charge ratio. Free energy of transfer of charged molecules from water to membrane correlates with Born energy. Behavior of the molecules at interface indicates their surface−active properties. Studies at different temperatures revealed that hydrophobic effect decreases with increase of temperature.

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Dense Nematically Ordered States of a Single Semiflexible Macromolecule: Extended Ensemble Monte Carlo Simulation

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Using a coarse-grained model of a semiflexible macromolecule, equilibrium shapes of the chain have been studied varying the temperature and the stiffness. A novel enhanced sampling Monte Carlo technique for the bond fluctuation model was applied: an expanded ensemble which allows the molecules to occupy positions in 4 dimensions in junction with the Landau-Wang algorithm to generate the weights between different subensembles which are characterized by different values of the chemical potential of monomers in the 4th dimension. Chain consisting of 256, 512, 1024 monomer units has been studied. Two different types of interactions were taken into account: a potential depending on the angle between successive bonds along the chain to control the chain stiffness, and an attractive interaction between non-bonded effective monomers to model variable solvent quality. The enhanced sampling technique allows the fast equilibration of dense spatial conformations of long enough chains and the location of transition lines between different structures.

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Annealed Polyelectrolytes in Poor Solvent

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Polyelectrolytes (PELs) in poor solvent are known to exhibit rather complex phase behaviour due to the competition between the effectively attractive short-range interaction and the repulsive Coulomb interaction.

For annealed PELs, as polyacids and polybases, an additional degree of freedom becomes into play. In contrast to quenched or strong PELs, the total charge on the polymer is not fixed, but can be tuned by changing the pH of the solution. The positions of the charges along the polymer chain are not fixed. The charges can move by recombination and redissociation [1].

The pronounced plateau in titration curves of annealed PELs, where the pH remains almost constant, is related to a discontinuous transition between collapsed and stretched conformations[2–4].

We present Monte Carlo simulations on annealed PELs in poor solvent. Increasing the chemical potential of the charges, which is equal to the pH of the solution, we obtain the transition between a weakly charged globule and a highly charged extended chain. For the first time, we show that this transition is indeed a first-order phase transition as predicted by theory[5]. In addition to that we demonstrate the existence of pearl-necklace conformations[6,7] in annealed PELs. However, compared to the quenched case their existence is restricted to a rather small parameter range[8].

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Influence of Angular Potentials on the Crystallization of Model Polymer Chains

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The simplified polymer model[1,2] appeared to be extremely efficient for the study of polymer crystallization in molecular dynamics simulations. On this poster, we show the influence of different simulation parameters, and in particular of the angular potential. Our model goes one step further than usual united-atom models and resumes all atoms of a monomer into one sphere. A mapping was made for poly(vinyl alcohol) which appears to be very similar to polyethylene at this level of approximation (after a rescaling of energy or temperature scale). One sphere contains thus two backbone-carbon atoms, these spheres are connected by harmonic springs and an angular potential. This angular potential is the result of two successive dihedral angles on the atomistic scale. It has three minima corresponding to trans-trans (tt), trans-gauche (tg) and gauche-gauche (gg) torsions of the backbone.

To get a better understanding of the stability of the used model and of the essential parameters for crystallization, we vary the depths of these minima as well as the barrier heights between them. The completely stretched tt state is always energetically preferred, however, since there are less states accessible, the folded states tg and gg prevail in the melt. We characterized the melt at a reference temperature and looked for correlations with the crystallization temperature determined during continuous cooling. For most quantities as persistence length, radius of gyration or relaxation times, no trivial correlation can be found, except for the fraction of tt conformations in the melt: the higher this fraction, the easier is the crystallization and thus the higher the temperature where ordering starts. Note that there is no trivial correlation between persistence length and this tt fraction.

The morphology of crystals where chain-folding is involved ($N = 100$) seems to be controlled by the depth of the gg-minimum rather than by the persistence length or the radius of gyration in the melt. The more pronounced this gg-minimum, the easier it is to retain folds in the crystal and consequently there are more hairpins and shorter stems.

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HP Proteins on Generalized Lattices

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We present investigations of HP proteins[1] in three dimensions on simple cubic and fcc lattices as well as on the triangular lattice in two dimensions. Employing the nPERM algorithm[2] to selected sequences, we searched for ground states on these three lattices and compared the density of states and the heat capacity of sequences which are designed on the simple cubic lattice.

PERM is a chain growth algorithm which combines the Rosenbluth method with the "Go with the Winners" strategy, proposed by Grassberger some years ago.[3] Population control is implemented by cloning and pruning growing conformations depending on variable thresholds which are computed adaptively during the simulation.

The figure illustrates two of our results[4]. The left hand side shows a conformation of a HP protein with 124 monomers on the triangular lattice in two dimensions, which is not yet the ground state for this lattice type. There are still three well-separated hydrophobic domains, which upon merging lower the energy. On the right hand side, a state of a HP protein with 136 monomers on the three-dimensional fcc lattice with energy $E = -168$ a.u. is shown, which is the lowest energy we found for this protein up to now.

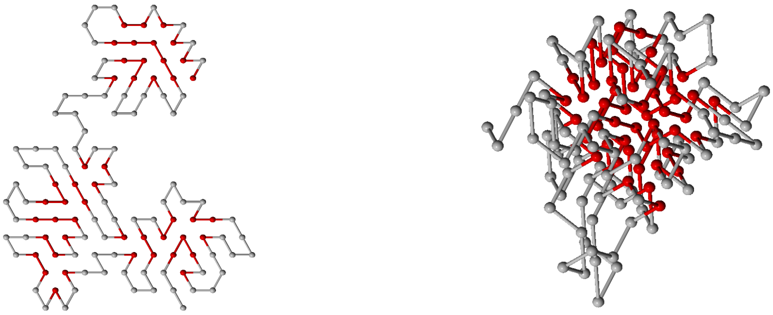

Figure 1. HP proteins on the triangular (left) and fcc (right) lattice. Hydrophobic (H) residues are depicted by dark (red) spheres and polar (P) ones by light (gray) spheres.

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A Computational Study of Chiral Discrimination: The Lindner Stationary Phase in Chiral Chromatography

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The discrimination of a series of enantiomeric 3, 5-dinitrobenzoyl (DNB) derivatives of leucine and alanine by a derivatized quinine chiral stationary phase (Lindner CSP) were simulated by computational studies. The conformations of the diastereomeic complexes formed between the CSP and the analytes were modified from known X-ray structures and from NMR data. 1 ns of molecular dynamics of the diastereomeric complexes in a continuum model of water solvent was carried out using MacroModel 7. The computed retention order and enantiodiscrimiating energy differences agree with the chromatographic data. The total energies and the intermolecular energies responsible for complex formation and for chiral discrimination are evaluated. Molecular dynamics trajectories and distributions of the stabilizing and destabilizing intermolecular forces are presented. The role of each fragment of the CSP molecule in complexation and chiral recognition is analyzed and described.

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