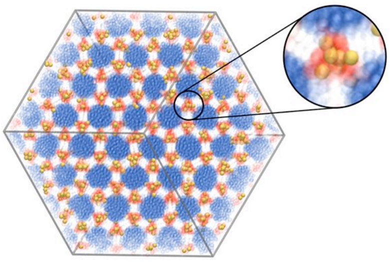
Centre Européen de Calcul Atomique et Moléculaire

# Coarse-Grained Methods and Self Assembly



*July, 27 2011 - July 29, 2011*
*CECAM-USI, Lugano, Switzerland*

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ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

# 1 Description

Self-assembly concerns the organization of individual molecules to create supramolecular architectures. The final superstructures are characterized by unique properties, which are different from the isolated molecules that formed them.

Motivated by the desire to build new molecular structures with striking features, scientists have, during the last decade, synthesized molecules that can self-assemble in different environments. Successful examples of these attempts can be found for example in material science where the ability of liquid crystals [1] to self assemble in ordered phase is widely used in information-display technology, or in polymer science where polymer chains with controlled distribution of hydrophobic/hydrophilic monomers can self assemble in vesicles , or in the formation of nanoparticles that can encapsulate dyes, small proteins or drugs. [2] Moreover, more recently a new field termed “soft-nanotechnology” tries to exploit the controlled self-assembling (and disassembling) of macromolecules as responsive polymers, dendrimers or biopolymers for a wide range of applications from drug delivery to nanoreactors. [3]

However, despite many efforts spent to achieve high control over the synthesis of building block molecules and the recent progresses made in devising experimental techniques to investigate the organization of the molecules within nanoaggregates, the prediction of the shape and properties of the assembled structures is far from being achieved. Indeed, the ability to identify the correct experimental conditions to obtain structures with the desired properties and to predict the morphology of the final supramolecular structures, starting only from the knowledge of the single building block, is very difficult and remains a real challenge in this field. [4]

A key problem is that even though the chemistry of the building blocks can be known in detail, the prediction of the lowest minimum energy configuration [5] is still challenging. Moreover, entropic (and sometimes enthalpic) effects arising from the influence of solvent interactions provide a further complicating factor.

Molecular simulations can help in clarifying and rationalizing many aspects of self assembly. [6] The computational challenge is that the self assembling process is a multiscale problem where different length and time scales are involved. This is particularly true for what is known as hierarchical self-assembly. Here, single molecules self assemble in superstructures that in turn assemble in larger organized objects. [7, 8] In this contest, brute force atomistic simulations have the advantage of describing realistically the non-covalent interactions (such as hydrogen bonds, hydrophobic interactions and electrostatics) responsible for the formation of the aggregates but such simulations are mainly valuable for simple problems due to the enormous number of structures that must to be sampled . The use of coarse-grained models represents a valuable way to overcome the problem of the large sampling. Reducing the degrees of freedom of the building units decreases the number of local minima to explore and hence making the simulation much faster. In addition, the employment of simplified models allows the use of standard simulation methods such as molecular dynamics where, integrating the equation of motion, the dynamics of the self-assembly process can be followed. However, key problems have still to be solved. For example, how can we efficiently include directional non-bonded interactions (such as H-bonding or electrostatics) responsible for the self assembly mechanism [8] within CG models; or how do we recognise which (of many) degrees of freedom can be coarse-grained away without loosing the chemical specificity of molecular system. Major challenges also occur in sampling configurational space efficiently. Here, modern simulation methods allowing fast exploration of phase space and detection of multiple minima are particularly useful.

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## Key references

*[1] T. Kato, N. Mizoshita, K. Kishimoto Angewandte Chemie-International Edition, 45, 38 (2006)*

*[2] M. A. Cohen Stuart et al., Nature Materials, 9, 101 (2010)*

*[3] A. Blanazs, S. P. Armes, A. J. Ryan, Macromolecular Rapid Communications, 30, 267 (2009)*

*[4] M. McCullagh, T. Prytkova, S. Tonzani, N. D. Winter and G. C. Schatz, J. Phys. Chem. B, 112, 10388 (2008)*

*[5] V. Percec et al. Nature, 391 161 (1998)*

*[6] A. J. Crane and E. A. Müller, Faraday Discussions, 144, 187 (2010)*

*[7] T. P. J. Knowles et al., Nature Nanotechnology 5, 204 - 207 (2010)*

*[8] M. L. Klein and W. Shinoda , Science 321, 798 (2008)*

*[9] H. A. Karimi-Verzaneh, P. Carbone, F. Müller-Plathe, J. Chem. Phys, 129, 129, 154904 (2008)*

# 2 Program

## Day 1 - July, 27 2011

### Self-assembly of synthetic systems

- 9:15 to 9:30 - Welcome
- 9:30 to 10:00 - **George Schatz**
  Modeling soft material self assembly: peptide amphiphiles and dna-linked materials
- 10:00 to 10:30 - **Doros Theodorou**
  Coarse-graining of polymers and liquid crystals with the iterative boltzmann inversion method

- 10:30 to 11:10 - Coffee Break
- 11:10 to 11:40 - **Dennis C. Rapaport**
  What can we learn about self-assembly from simulating simple models?
- 11:40 to 12:10 - **Luigi Delle Site**
  Adaptive resolution simulation: linking quantum, atomistic and continuum in a concurrent way

  12:10 to 14:00 - Lunch

- 14:00 to 14:30 - **Athanassios Panagiotopoulos**
  Coarse-grained models for nanoparticle organic hybrid materials
- 14:30 to 15:00 - **Denis Andrienko**
  Versatile object-oriented toolkit for coarse-graining apllications
- 15:00 to 15:30 - **Michael Allen**
  Monte Carlo studies of adsorbed molecules using the Wang-Landau method

- 15:30 to 16:10 - Coffee Break
- 16:10 to 16:40 - **Christos N. Likos**
  Self-assembly scenarios for soft colloids
- 16:40 to 17:10 - **Clare McCabe**
  Developing coarse-grained models for the molecular simulation of the self assembly of skin lipids

## Day 2 - July, 28 2011

### Self-assembly in biosystems

- 9:00 to 9:30 - **Berend Smit**
  Mesoscopic simulation of proteins embedded in membranes

- 9:30 to 10:00 - **Durba Sengupta**
  Self asssembly of lipid-peptide systems: understanding stalk/pore complexes

- 10:00 to 10:30 - **Ard A. Louis**
  Self-assembly of patchy colloids and dna nanostructures

- 10:30 to 11:10 - Coffee Break

- 11:10 to 11:40 - **Aline Miller**
  Engineering the self-assembly of peptide and peptide conjugate materials for regenerative medicine.

- 11:40 to 12:10 - **Christian Holm**
  Simulational study of polyelectrolyte multilayers- recent advances

12:10 to 14:00 – Lunch

- 14:00 to 14:30 - **Gregory Voth**
  Coarse-grained simulation of multi-protein assemblies

- 14:30 to 15:00 - **Stefan Auer**
  Thermodynamics and kinetics of alpha-helical and beta-sheet forming peptides

- 15:00 to 15:40 - Coffee Break

- 15:40 to 16:10 - **Juan J. de Pablo**
  Coarse graining of dna. structure, properties, dynamics and assembly.

- 16:10 to 16:40 - **Siewert-Jan Marrink**
  Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites

- 16:40 to 18:30 - Poster Session

- 19:00 to 20:30 - Dinner

## Day 3 - July, 29 2011

### Self assembly in soft matter

- 9:00 to 9:30 - **Kurt Kremer**
  Adaptive resolution simulations: towards open systems molecular dynamics simulations

- 9:30 to 10:00 - **Roland Faller**
  Systematic coarse-graining in mixtures – state dependence and applications

- 10:00 to 10:30 - **Gordon Tiddy**
  Self-assembly in soft matter: lyotropic liquid crystals & experimental limitations.

- 10:30 to 11:10 - Coffee Break

- 11:10 to 11:40 - **Anna Balazs**
  Designing communicating colonies of biomimetic microcapsules

- 11:40 to 12:10 - **Marcus Müller**
  Modeling self-assembly of copolymer melts with soft coarse-grained models

- 12:10 to 12:30 - Closing words

# 3 Abstracts

## *Modeling soft material self assembly: peptide amphiphiles and dna-linked materials*

**George Schatz**

In this talk I describe research in my group concerning two self-assembly projects: the formation of cylindrical micelle structures from peptide amphiphiles (a collaboration with Sam Stupp) and the formation of gel-like materials composed of DNA-linked gold nanoparticles (a collaboration with Chad Mirkin). In both of these studies, a combination of atomistic and coarse-grained molecular dynamics methods has been used, as well as simple models, to understand both the mechanism of self-assembly process and the structural and thermodynamic properties of the self-assembled material that is produced. In the case of the peptide amphiphile assembly, I show how different levels of coarse-graining lead to different levels of understanding of the formation process and of the micelle structures that result. Of particular interest are recent results where my group has obtained an atomic level description of the micelle structures, enabling a detailed understanding of the quality of several levels of coarse-graining. For the DNA-linked gold particles, my group has developed a coarse-grained model of DNA (based on de Pablo's earlier work) that provides understanding of cooperative melting effects. Also, atomistic simulations show the role of osmotic pressure effects that dictate DNA density, and they provide insight about the correlation of base-pair composition and structural properties of the aggregate and crystalline materials.

## *Coarse-graining of polymers and liquid crystals with the iterative boltzmann inversion method*

**Doros Theodorou**

The derivation, from detailed atomistic force fields, of coarse-grained models, in which multiatom moieties are represented by single “superatoms,” is a promising strategy for addressing the long time and large length scale properties of soft matter systems. A straightforward approximate coarse-graining method is Iterative Boltzmann Inversion (IBI) [1,2]. Here, the potential of mean force with respect to the degrees of freedom retained at the coarse-grained level is assumed to be expressible as a sum of additive contributions from effective bond lengths, bond angles, torsion angles, and pairwise nonbonded interactions between superatoms. Initial estimates for these contributions are obtained by Boltzmann inversion of intramolecular distribution functions and intermolecular pair correlation functions defined by the superatoms in an atomistically simulated oligomeric analogue of the system of interest. Effective intra- and intermolecular potentials are then refined through an iterative process, which eventually causes the distribution and correlation functions from coarse-grained simulation to converge to their atomistically computed counterparts. IBI has been applied to long-chain polystyrene [3] and poly(ethylene terephthalate) [4] melts. Here, combination of coarse-graining with powerful connectivity-altering Monte Carlo methods that ensure equilibration of long-chain melts at all length scales led to excellent estimates of conformational characteristics, chain dimensions, and entanglement properties. Furthermore, reverse-mapping well-equilibrated coarse-grained configurations back to the atomistic level and subsequent atomistic molecular dynamics simulation yielded diffraction patterns and volumetric properties that are in good agreement with experiment. IBI has also been applied to 4-cyano- 4'- pentyl biphenyl (5CB), a common thermotropic liquid crystal [5]. The isotropic phase at 315 K and 1 atm was used for development of the coarse-grained effective potentials. The coarse-grained model was found to undergo a first-order ordering transition at 288 K with small hysteresis and negligible system size effects. A detailed investigation, in terms of various structural and dynamical measures, indicated that the ordered phase is of smectic type, rather than nematic as observed experimentally. The ordering temperature can be brought close to the experimental value of 308.5 K through simple rescaling of the intermolecular effective interaction potentials. A nematic ordered phase, however, can only be obtained from the coarse-grained model if IBI head-head and tail-tail effective interaction potentials are scaled down. These observations underline the difficulty of using IBI-based coarse-grained models across phase boundaries.

*[1] Schommers, A. Phys. Rev. A 1983, 28, 3599.*
*[2] Reith, D.; Pütz, M.; Müller-Plathe, F. J. Comp. Chem. 2003, 24, 1624.*
*[3] Spyriouni, T.; Tzoumanekas, C.; Theodorou, D.; Milano, G.; Müller-Plathe, F. Macromolecules 2007, 40, 3876.*
*[4] Kamio, K.; Moorthi, K.; Theodorou, D.N. Macromolecules 2007, 40, 710.*
*[5] Megariotis, G.; Vyrkou, A.; Leygue, A.; Theodorou, D.N. Ind. Eng. Chem. 2010, in press.*

## *What can we learn about self-assembly from simulating simple models?*

**Dennis C. Rapaport**

Despite its importance, the phenomenon of supramolecular self-assembly remains an enigma. The formation of exquisitely designed virus capsids is a well-known example. Capsid assembly can be modelled using molecular dynamics simulation of simple rigid particles designed to form polyhedral shells. Simulations incorporating an explicit solvent have provided new insight into the mechanism of self-assembly. The original work focused on the formation of icosahedral shells from triangular particles, where, contrary to expectation, assembly was observed to proceed via a cascade of strongly reversible steps; this feature helps avoid growth-impeding kinetic traps because partial shells tend to lose rather than gain members. Current work, requiring more extensive computation, deals with the formation of T=1 shells, each containing 60 trapezoidal particles, and again reversibility is seen to play an important role. The growth processes are robust, and are capable of a high yield of complete shells under suitable conditions, with no mutant structures. A further observation is that despite the large variety of possible intermediate structures, assembly pathways tend to involve only a very small fraction of highly bonded forms.

## *Adaptive resolution simulation: linking quantum, atomistic and continuum in a concurrent way*

**Luigi Delle Site**

I will introduce the Adaptive ResolutionSimulation method (AdResS). This method allows to change molecularresolution on-the-fly during a simulation by changing the number ofdegrees of freedom in the specfic regions of space where the desiredresolution must be higher than the rest of the system. I will discuss the principles on which the algorithm is based and show the results of the most recent applications.

## *Coarse-grained models for nanoparticle organic hybrid materials*

**Athanassios Panagiotopoulos**, Bingbing Hong, Alexandros Chremos

We develop coarse-grained models to study the structure and dynamics of nanoparticle organic hybrid materials and nanoparticle-based ionic liquids. The systems of interest consist of nanometer-size inorganic core particles with with tethered organic chains, and their charged analogs with ionic surface groups and linear or three-arm counterions. We use Boltzmann inversion methods to obtain the potentials for the bead-bead and bead-core interactions from "half-atomistic" simulations of polyethylene glycol chains with particles interacting via an integrated potential. Of particular interest are questions related to the scaling of diffusivities and viscosities between the atomistic and coarse-grained systems. For the ionic systems, even though electrostatic interactions between oppositely charged ions at contact are much greater than the thermal energy, we find that chain dynamics at intermediate time scales are dominated by chain hopping between core particles, resulting in superionic conductivity.

## *Versatile object-oriented toolkit for coarse-graining apllications*

**Denis Andrienko**

Coarse-graining is a systematic way of reducing the number of degrees of freedom representing a system of interest. Several coarse-graining techniques have so far been developed, such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. However, there is no uni&#64257;ed framework that implements these methods and that allows their direct comparison. We present a versatile object-oriented toolkit for coarse-graining applications (VOTCA, J. Chem. Theory Comput. 2009, 5, 3211–3223) that provides a flexible modular platform for their implementation and development. All methods are illustrated and compared by coarse-graining the SPC/E water model, liquid methanol, liquid propane, and a single molecule of hexane.

## *Monte carlo studies of adsorbed molecules using the wang-landau method*

**Michael Allen**

We have carried out Monte Carlo simulations, using the Wang-Landau method, of very coarse-grained lattice models of small molecules, polymers and peptides, adsorbed on planar surfaces. The method enables us to investigate a wide range of state points, locate phase transitions, and identify ground states. This talk will describe the steps that we have taken to improve the convergence of the method, and present some results for self-assembled structures.

## *Self-assembly scenarios for soft colloids*

**Christos N. Likos**

In soft, polymer-based colloids, the effective pair interaction can be externally tuned by means of modifications in the polymer architecture, of the solvent quality and also by external additives, such as homopolymer chains. In this talk, we will discuss the possibilities to induce attractions to star polymers, either by changing the solvent quality or by adding homopolymers. The resulting phase- and rheological behavior will be discussed and the possibilities to control the glass transition of the concentrated mixture will be analyzed. Finally, the behavior of soft colloidal systems under external shear and the scenarios of self-organization under external drive will be presented.

## *Developing coarse-grained models for the molecular simulation of the self assembly of skin lipids*

**Clare McCabe**

The outermost layer of the skin (the stratum corneum) consists of skin cells embedded in a rich lipid matrix, whose primary role is to provide a barrier to foreign agents entering the body and to water leaving the body. This lipid system is unique in biological membranes in that it is composed of ceramides, cholesterol, and free fatty acids, with phospholipids, which are the major components of most biological membranes, being completely absent. This unique composition enables the organization of the stratum corneum lipids into lamella, which in turn is believed to control barrier function. While much is known about the nature of the skin lipids from extensive experimental studies, a clear understanding of how and why these molecules assemble into the structures observed through microscopy and biophysical measurements does not yet exist. In order to probe the molecular level arrangement, we have developed coarse-grained models for the key stratum corneum lipids and water to enable us to simulate complex mixed lipid systems and study their structural characteristics on timescales accessible to molecular dynamics simulations. The development and validation of the coarse-grained models will be presented alongside the results of self-assembly studies in simple mixed lipid systems that enable us to validate the models developed and work towards the study of a realistic stratum corneum system.

## *Mesoscopic simulation of proteins embedded in membranes*

**Berend Smit**, Jocelyn Rodgers

The interactions between proteins embedded in a membrane are to a significant extent influenced by the membrane. For example, the hydrophobic mismatch between proteins and membranes causes a perturbation of the local structure of the membrane close to the proteins. These perturbations can result in long-range attraction between the proteins, causing the proteins to cluster. In this presentation a mesoscopic model of the membrane-protein system is presented, which allow us to study the effect of changes in the hydrophobic thickness on the interactions between proteins. Despite that this model is orders of magnitudes more efficient compared to all-atom simulations, it does not allow us to study the collective behavior of a large number of proteins embedded in a membrane. To study the collective behavior we map our mesoscopic model on a two-dimensional model of disks. The effective interactions are obtained from the potentials of mean force from the mesoscopic model. We use this model to explain the differences in clusters sizes observed in systems with positive and negative hydrophobic mismatch.

## *Self asssembly of lipid-peptide systems: understanding stalk/pore complexes*

**Durba Sengupta**

The action of membrane-active peptides is an essential process in biology and encompasses fusion, poration and translation. These self-assembled processes involve the interplay of peptides and lipids via specific protein-protein and protein-lipid interactions as well as generic physio-chemical forces. We have performed atomistic/coarse-grain molecular dynamics simulations and biophysical characterisation to probe the interaction of membrane-active peptides with model membranes. Using BPC194, a cyclic antimicrobial peptide as an example, we show that these peptides may often perform dual action such as poration and fusion. For isolated membranes, the peptide acts only via the poration pathway causing leakage through membrane pores. For membranes in close proximity, the lipid-peptide system may self-assemble to form complex phases such as the stalk/pore complex. In this state, a membrane pore is opened in the vicinity of a fusion stalk. It appears that the peptides can stabilise the saddle-splay (Gaussian) curvature leading to the stalk/pore complex and thereby lowering the energy barrier towards membrane fusion. Thus, a framework of computer simulations and biophysical experiments may be used to rationalise the differences in self-assembled states based on differences in the initial conditions.

## *Self-assembly of patchy colloids and dna nanostructures*

**Ard A. Louis**

I will briefly review some generic properties of self-assembling systems, using a simple model of patchy particles [1]. Otimal self-assembly emerges from a compromise between structural specificity and kinetic accessibility. I will then introduce a coarse-grained rigid nucleotide model of DNA that reproduces the basic thermodynamics of short strands: duplex hybridization, single-stranded stacking and hairpin formation, and also captures the essential structural properties of DNA: the helical pitch, persistence length and torsional stiffness of double-stranded molecules, as well as the comparative flexibility of unstacked single strands [2]. We apply the model to calculate the detailed free-energy landscape of one full cycle of DNA `tweezers', a simple machine driven by hybridization and strand displacement. We also study other nanomachines as well as processes such as force-induced melting, cruciform formation, and the dynamics of Holliday junctions.

*[1]Reversible self-assembly of patchy particles into monodisperse clusters Alex W. Wilber et al., J. Chem. Phys. 127, 085106 (2007);Self-assembly of monodisperse clusters: Dependence on target geometr, Alex Wilber et al, J. Chem. Phys. 131, 175101 (2009); Monodisperse self-assembly in a model with protein-like interactions, Alex W. Wilber et al., J. Chem. Phys. 131, 175102 (2009)*

*[2] DNA nanotweezers studied with a coarse-grained model of DNA Thomas E. Ouldridge, Ard A. Louis, Jonathan P.K. Doye Phys. Rev. Lett. 104 178101 (2010); Structural, mechanical and thermodynamic properties of a coarse-grained model J. Chem. Phys. 134, 085101 (2011)*

## *Engineering the self-assembly of peptide and peptide conjugate materials for regenerative medicine.*

**Aline Miller**

Self-assembly represents a simple and efficient route to the construction of large, complex structures. Peptide self-assembly in particular offers the possibility to design new functional bio-materials that find application in drug delivery and tissue engineering. The beta-sheet motif is of particular interest as short peptides can be designed to form beta-sheet rich fibres that entangle and consequently form hydrogels. These hydrogels can be functionalised using specific biological signals and can also be made responsive through the use of enzymatic catalysis and/or conjugation with responsive polymers. Here I will outline the influence of molecular design on the self-assembly and gelation behaviour of short oligopeptides with the aim of controlling and tailoring material properties for target applications. In particular, some basic questions regarding experimental phase behaviour, structure, and dynamics will be tackled in addition to the effect of conjugation with responsive polymers.

## *Simulational study of polyelectrolyte multilayers- recent advances*

**Christian Holm**, Q. Baofu, J.J. Cerda, M. Sega

Polyelectrolyte multilayers (PEMs) are composed of alternating layers of oppositely charged polyelectrolytes (PEs), which are generally built up based on the Layer-by-Layer technique. PEMs have stimulated great interests from both academic researchers and industries due to their potential applications, such as membrane, encapsulation, and matrix materials for enzymes and proteins in sensor applications. Nevertheless, despite the large amount of experimental works, theoretical and computational studies are relatively scarce . Our goal is to understand the interphase and interface structures and interactions via simulation methods. We try to combine coarse- grained (CG) and all-atom (AA) molecular dynamics (MD) simulations to construct a viable model for PEMs. The CG-MD method is very efficient in dealing with the systems in larger time and length scale, and AA-MD approach is necessary to understand the details, e.g., the conformation of adsorbed PE chains, the influence of the aqueous solvent at a higher resolution. We find that the first layers, and in particular the second layer, is very important in PEM buildup. Our AA-MD simulations reproduce the experimental dielectric constant and diffusion of waters in the central (interphase) region of PSS/PDADMA PEMs. On the other hand, the PSS adsorption has been investigated in AA-MD to understand the interfacial behavior close to the adsorbing substrate. We find that both, the surface charges and surface hydrophilic groups, enhance the adsorption of PSSs.

*[1] Qiao, Baofu and Cerd`a, Juan J. and Holm, Christian Poly(styrenesulfonate)-Poly(diallyldimethylammonium) Mixtures: Towardthe Understanding of Polyelectrolyte Complexes and Multilayers viaAtomistic Simulations*,
Macromolecules **43** 7828--7838 (2010)
[2] Qiao, Baofu and Cerd`a, Juan J. and Holm, Christian *Atomistic Study of Surface Effects on Polyelectrolyte Adsorption:Case Study of a Poly(styrenesulfonate) Monolayer*,
Macromolecules **44** 1707--1718 (2011)
[3] Cerd`a, J. J. and Qiao, B. and Holm, C. *Modeling strategies for polyelectrolyte multilayers*,
Eur. Phys. J. Spec. Top. **177** 129--148 (2009)

## *Coarse-grained simulation of multi-protein assemblies*

**Gregory Voth**

A multiscale theoretical and computational methodology will be presented for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is a method for deriving coarse-grained models from protein structures and their underlying molecular-scale interactions. A critical component of the modeling is also its connection to experimental structural data such as cryo-EM or x-ray, thus making it “hybrid” in its character. Recent applications the overall multiscale approach to describe the self-assembly of large multi-protein complexes such as the HIV-1 virion will be presented. The highly scalable computational implementation of the multiscale simulations will also be described.

## *Thermodynamics and kinetics of alpha-helical and beta-sheet forming peptides*

**Stefan Auer**

A characteristic feature of polypeptides chains is their ability toform structural motives such as alpha-helices and beta-sheets. Thisleads to a complex phase behaviour in which proteins can assemble into various types of aggregates including liquid-like phases of folded or unfolded proteins and amyloid fibrils. In my talk I will give anoverview of our attempt to characterise the thermodynamics andkinetics of a alpha-helical and beta-sheet forming peptide system. Inparticular we have tried to calculate the peptide phase diagram [1],calculated a nucleation barrier underlying the aggregation of peptidesinto beta-sheets [2,3], and how these peptides aggregate on a nanoparticle surface [4].

*[1] Phase diagram of alpha-helical and beta-sheet forming peptides S. Auer,and D. Kashchiev, Phys. Rev. Lett., 104 168105 (2010)*

*[2] Self-templated nucleation in peptide and protein aggregation S. Auer, C. M. Dobson, M. Vendruscolo, and A. MaritanPhys. Rev. Lett., 101 258101 (2008)*

*[3] Atomistic nucleation theory for amyloid fibril formation R. Cabriolu, D. Kashchiev, and S. AuerJ. Chem. Phys., 133 225101 (2010)*

*[4] A condensation-ordering mechanism in nanoparticle-catalyzedpeptide aggregation S. Auer, A. Trovato, and M. Vendruscolo PLoSComput Biol, PLoS Comput Biol, 4 e1000458 (2009)*

## *Coarse graining of DNA. structure, properties, dynamics and assembly.*

**Juan J. de Pablo**, Gordon Freeman, Daniel Hinckley, Vanessa Ortiz

Beyond its importance to biology, the assembly of nanoscale objects on the basis of DNA hybridization is finding an increasing range of applications in materials science and engineering. In genetics, the flow and translocation of long DNA molecules are of considerable applied and fundamental interest. In that context, design of effective genomic devices requires control of molecular shape and positioning at the level of microns and nanometers. This presentation will provide an overview of hierarchical models and computational approaches developed by our research group to investigate the effects of confinement, hydrodynamic interactions, and salt concentration, on the structure and properties of DNA, both at equilibrium and beyond equilibrium. A particular emphasis will be placed on emerging, detailed models and methods that are capable of describing melting and rehybridization at the single nucleotide level, as well as the packaging of DNA in chromatin. The validity of the models will be assessed by comparison to experimental data for dehybridization temperatures, molecular size and flexibility, rate constants for duplex formation, and nucleosome positioning.

## *Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites*

**Siewert-Jan Marrink**, Andrzej Rzepiela, Christine Peter

In this contribution I discuss a straightforward scheme to perform hybrid all-atom (AA) - coarse grained (CG) simulations, making use of virtual sites to couple the two levels of resolution [1]. With the help of these virtual sites interactions between molecules at different levels of resolution, i.e. between CG and atomistic molecules, are treated the same way as the pure CG–CG interactions. Within the &#64257;eld of biomolecules, our method appears ideally suited to study e.g. protein-ligand binding or protein-protein interactions with the site of interaction modeled in full detail and the surrounding coarse-grained. The method is still in the testing phase, but I expect to show some preliminary applications.

*[1] A.J. Rzepiela, M. Louhivuori, C. Peter, S.J. Marrink. Hybrid simulations: combining atomistic and coarse-grained force fields using virtual sites. Phys. Chem. Chem. Phys., in press, 2011. DOI:10.1039/C0CP02981E*

## *Adaptive resolution simulations: towards open systems molecular dynamics simulations*

**Kurt Kremer**

The relation between atomistic structure, architecture, molecular weight and material properties is a basic concern of modern soft matter science. This longstanding aim by now goes far beyond standard properties of bulk materials. A typical additional focus is on surface interface aspects or the relation between structure and function in nanoscopic molecular assemblies. Here computer simulations on different levels of resolution play an increasingly important role. To progress further adaptive schemes are being developed, which allow for a free exchange of particles (atoms, molecules) between the different levels of resolution. The lecture will concentrate on the coupling between microscopic and coarse grained particle based methods, however will also include first approaches to connect particle based simulations to continuum as well as to include quantum effects. For a general review on part of the methodology see: M. Praprotnik, L. Delle Site, and K. Kremer, Multiscale Simulation of Soft Matter: From Scale Bridging to Adaptive Resolution, Annu. Rev. Phys. Chem. 59, 2008

## *Systematic coarse-graining in mixtures – state dependence and applications*

**Roland Faller**, Beste Bayramoglu, David M. Huang

Systematic Coarse-Graining of Soft Matter by the Iterative Boltzmann Method has become standard in recent years. More and more of these systems involve mixtures. However, in mixed systems the number of distribution functions to be optimized increases with the square of the number of components. Here, we are discussing some fundamental observations on the fundamental applicability and efficiency of this technique. We will then discuss several examples. This includes a polymer blend, namely polyisoprene and polystyrene and especially a mixture of a polymer (polythiophene P3HT) and a fullerene (C60). This system has important applications for the understanding of the morphology in polymeric solar cells. For both systems we will discuss the phase behavior and the dependence of the models on the concentration as an example of a state variable.

*1. Q. Sun, R. Faller: Systematic coarse-graining of a polymer blend: Polyisoprene and Polystyrene J Chem Theor Comp 2(3) 607-615 (2006)*
*2. Q. Sun, R. Faller: Phase Separation in Polyisoprene/Polystyrene Blends by a Systematically Coarse-Grained Model J Chem Phys 126(14) 144908 (2007)*
*3. J. Ghosh, R. Faller: State Point Dependence of Systematically Coarse-Grained Potentials Molecular Simulation 33(9 & 10) 759-767 (2007)*
*4.Q. Sun, J. Ghosh, R. Faller: State Point Dependence and Transferability of Potentials in Systematic Structural Coarse-Graining in Coarse-Graining of Condensed Phase and Biomolecular Systems (CRC Press, 2008, Editor G. Voth )*
*5.D. M. Huang, R. Faller, K. Do, A. J. Moule: Coarse-grained computer simulations of polymer/fullerene bulk heterojunctions for organic photovoltaic applications J Chem Theor Comp 6(2) 527-537 (2010)*
*6.D. M. Huang, A. J. Moule, Roland Faller: Characterization of Polymer-Fullerene Mixtures for Organic Photovoltaics by Systematically Coarse Grained Molecular Simulation Fluid Phase Equilibria 302 (1-2) 21-25 (2011)*

## *Self-assembly in soft matter: lyotropic liquid crystals & experimental limitations.*

**Gordon Tiddy**

Soft matter is a topic that covers a very wide range of materials, from creams, pastes and lotions to fibre assemblies and living cells. This talk will focus on lyotropic liquid crystals formed by surfactants and related systems. Surfactants are molecules containing a non-polar “tail” bound to a polar “head group”. These chemically distinct moieties give rise to the formation of a wide range of aggregates in solution (usually in water). The aggregates (termed micelles) can be spheres, rods or discs. At high concentrations the micelles become ordered, resulting in the formation of various liquid crystalline phases (cubic, hexagonal, lamellar etc.). There is a reasonably good understanding of the link between surfactant chemical structure & liquid crystal architecture for the water-continuous liquid crystals. But there remain some significant unsolved problems in linking these two for the “oil- continuous” (reversed) phases. In addition to the liquid-like phases a range of phase states occur where either the non-polar or the polar regions contain additional degrees of order. If the order occurs in the alkyl chains these are usually called “gel” phases. They are similar to the “rotator” phases of hydrocarbons and are comprised of surfactant mono- or bi-layers. Most of the alkyl chains are in the all-trans conformation, but there is a significant fraction of gauche conformations also present. The “L&#946;” and “P&#946;” phases of phospholipids fall into this category. Many properties of these systems are not properly understood. For phospholipids, in this author’s opinion, there is no experimental study of the lamellar/gel phase transition where both the phases have been demonstrated to be at thermodynamic equilibrium. Nor are there any molecular simulations that fulfil this criterion. A second class of phases with additional order comprises systems where the ionic groups are ordered to some extent, but the chains are molten. The liquid crystal structures found to date appear to include both layer and rod phases. A proper understanding of their structure & formation is at a very early stage. It requires a detailed knowledge of the arrangements of the ionic species. This would appear to be a good area for modelling. A very brief mention will be made of several additional related areas. Other lyotropic liquid crystals where self-assembly is the dominant process are the chromonic mesophases formed by many dyes and drugs. These aggregate via. &#960;-stacking, again in water. In addition, the author will point to (a few) major problems that should have been elucidated, but have not. It may well be that recent advances in molecular simulations will allow these finally to be resolved.

## *Designing communicating colonies of biomimetic microcapsules*

**Anna Balazs**, German V. Kolmakov, Victor V. Yashin, Steven P. Levitan

## *Modeling self-assembly of copolymer melts with soft coarse-grained models*

**Marcus Müller**

Representing a large number of monomeric repeat units of a macromolecule by a single particle of a coarse-grained polymer model allows us to investigate the self-assembly of copolymer materials on large time and length scales. Inspired by systematic coarse-graining procedures, the interactions between the coarse-grained segments are soft, ie they do not include the harsh repulsion (excluded volume of the beads). Advantages (e.g., realistic strength of fluctuations, fast equilibration, computation of chemical potential, connection to field-theoretic models) and difficulties (e.g., crossability of polymers, lack of resolution of narrow polymer-solid interface) that are caused by this very coarse representation will be discussed and selected application in area of pattern replication will be presented.

# 4 Posters

### *Relation between molecular shape and the morphology of self-assembling aggregates*

**Robert Vacha**, Daan Frenkel
University of Cambridge, United Kingdom

We report a wide variety of self assembled structures obtained with a simple model of a rod like particle with attractive (hydrophobic) stripe on its side. All predicted structures by our model were identified with an experimentally observed protein self assembled structures including Coiled Coils, amyloid Ribbons, barrels, and vesicles. Our Monte Carlo simulations showed that aggregate morphologies crucially depend on two parameters. The first one is the width of the attractive stripe and the second one is a presence or absence of attractive interactions at the particle ends. The results provide us a generic insight into conditions needed for a given structure formation and also suggest that other structures that were not observed require more complex model.

### *Conformation state diagram of polypeptides: a chain length induced transition*

**Piero ricchiuto**, Andrey Brukhno, Emanuele Paci, Stefan Auer
University of Leeds, United Kingdom

By using a generic coarse grained polypeptide model, we perform multicanonical molecular dynamics simulations for determining the equilibrium conformation state diagram of a single homopolypeptide chain as a function of the chain length and temperature. The state diagram highlights the thermal regimes of stability for various conformational patterns in polypeptides, including swollen, random and collapsed coils, globular structures, extended and bended &#945; helices, and compact &#946; bundles. Remarkably, at low temperatures we observe a sharp transition from extended &#945; helix to compact &#946; bundles as the chain length increases. This finding indicates that the chain length is one of the intrisic factors triggering &#945;-&#946; transformations in a broad class of polypeptides.

*[1] F. Chiti and C. M. Dobson, Annu. Rev. Biochem. 75,333 (2006).*
*[2] Feng Ding, Jose M. Borreguero, Sergey V. Buldyrey, H.*
*Eugene Stanley, and Nikolay V. Dokholyan. PROTEINS: Structure, Function, and Genetics, 2003, 53:220–228.*
*[3] M. J. Buehler and Y. C. Yung, Nature Materials 8, 175(2009).*
*[4] S. Auer, C.M. Dobson, M. Vendruscolo, HFSP J. 1, 137 (2007).*
*[5] A. E. Garcia and K. Y. Sanbonmatsu, PNAS 99, 2782 (2002).*
*[6] G. S. Jas and K. Kuczera, Biophysical Journal 87, 3786 (2004).*
*[7] J. M. Scholtz, S. Marqusee, R. L. Baldwin, E. J. York, J. M. Stewart, M. Santoro, and D. W. Bolen, Proc. Natl Acad. Sci. USA 88, 2854 (1991).*
*[8] W. Dzwolak, T. Muraki, M. Kato, and Y. Taniguchi, Biopolymers 73, 463 (2004).*

### *Molecular simulation of nanoparticles and proteins at liquid interfaces*

**David Cheung**
University of Warwick, United Kingdom

### *Simulation studies of crystallisation in diesel*

**Valentina Erastova**, Mark Wilson
Durham University, United Kingdom

## *Pseudo liquid-solid transition of self-assembled spherical coarse-grained dendron clusters*

**Erich A. Müller**, Andrew J. Crane
Imperial College London, United Kingdom

We present a coarse-grained molecular dynamics study into the thermotropic liquid crystalline phase behavior of tapered monodendron polyphilic molecules. At low temperatures, the dendrons self-organise, apex centrally, into spherical aggregates with a narrow cluster size essentially behaving as a fluid phase of supramolecular spheres of roughly the same size. At lower temperatures this pseudo-fluid crystallises into a body-centered cubic arrangement, in effect resembling a liquid-solid transition. The liquid crystalline nature of both aggregate phases was confirmed visually, with both intra and inter aggregate dendron diffusion monitored. Moreover self-assembly from a quench isotropic state to the crystalline aggregate state confirmed the fluid nature of the phase, as well as elucidating the formation mechanism.

## *Discrete molecular dynamics simulations of protein aggregation using a physics-based coarse-grained model*

**Agusti Emperador**, Modesto Orozco
Institute for Research in Biomedicine, Spain

We are developing a coarse-grained protein model to simulate protein dynamics, interactions and aggregation. In our model each amino acid is defined with one bead for the backbone and up to four beads for the sidechains, depending on the size and characteristics of the residue [1]. The interaction potentials between the beads that we have defined are physically derived from the Lazaridis-Karplus solvation potentials [2] devised for an atomistic representation of the proteins. We generate the trajectories with Discrete Molecular Dynamics, a simulation technique faster than standard MD. In the trajectories for isolated proteins we verify that the native structure is conserved. In the simulations of several contacting proteins, in some cases we find partial unfolding through loss of tertiary structure and aggregation. Previous studies of protein aggregation based on simulations of coarse-grained protein models usually dealt with intrinsically disordered proteins [3,4], therefore without a native conformation. Here we apply our model to stable proteins, in order to study how they can be destabilized due to its interaction with other proteins and their possible oligomerization.

*[1] L. Monticelli et al, J. Chem. Theory and Comput. 4, 819 (2008)*
*[2] T. Lazaridis and M. Karplus, Proteins 35, 133 (1999)*
*[3] A. J. Marchut and C. K. Hall, Biophys. J. 90, 4574 (2006)*
*[4] S. Yun et al, Biophys. J. 92, 4064 (2007)*

## *Multiscale modelling of soft-matter dynamics: toward a hybrid molecular-dynamics/finite-element approach*

**Florian Müller-Plathe**, Mohammad Rahimi, Hossein Ali Karimi Varzaneh, Michael Böhm, Sebastian Pfaller, Gunnar Possart, Paul Steinmann
Technical University of Darmstadt and Center of Smart Interfaces, Germany

In the development of a horizontally coupled hybrid scheme we aim to describe an "interesting" region at the molecularly detailed level and the environment by continuum mechanics. To this end, a molecular dynamics (MD) region has to be embedded in finite-element (FE) surroundings, which creates compatibility problems in the overlap region where particle simulation meets continuum simulation. The poster reviews our efforts to communicate displacements and forces between the two domains by so-called anchor points without creating too many artefacts. The method is to be applied in structure and failure mechanics of interphases and nanocomposites.

*M. Rahimi, H. A. Karimi-Varzaneh, M. C. Böhm, F. Müller-Plathe, S. Pfaller, G. Possart, P. Steinmann, J. Chem. Phys. 134, 154108 (2011). [DOI:10.1063/1.3576122]*
*S. Pfaller, G. Possart, P. Steinmann, M. Rahimi, F. Müller-Plathe, and M. C. Böhm, Comput. Mech. (submitted).*

## *Hybrid model atomistic-coarse-grained for soft material molecular dynamics simulations*

**Nicodemo Di Pasquale**, Paola Carbone
Politecnico di Torino, Italy

We present a hybrid coarse-grained-atomistic model for soft materials that enables an easy and smooth change on-the-fly of the number of degrees of freedom considered during the simulation. The model employs the coarse-grained force fields developed using the Iterative Boltzmann Inversion and classical atomistic force fields. [1] The resolution of the model can be automatically controlled by the software and there is no need of any type of interface when switching on or off the degrees of freedom. The model is used on melt of atactic polystyrene of different molecular weight showing that the soft coarse-grained potential merges extremely well with the atomistic force field. The model is able to reproduce correctly all the global and local structural properties at any level of resolution. The method has been implemented in our simulation code IBISCO and can be readily used to simulate any kind of material interface allowing a proper multiscale approach to material science. [2]

*[1] Reith, D and Putz, M and Muller-Plathe, F Deriving effective mesoscale potentials from atomistic simulations*, JOURNAL OF COMPUTATIONAL CHEMISTRY **24** 1624-1636 (2003)

[2] Karimi-Varzaneh, Hossein Ali and Qian, Hu-Jun and Chen, Xiaoyu andCarbone, Paola and Mueller-Plathe, Florian *IBIsCO: A Molecular Dynamics Simulation Package for Coarse-GrainedSimulation*, JOURNAL OF COMPUTATIONAL CHEMISTRY **32** 1475-1487 (2011)

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## *Molecular dynamics simulations of the phase behaviour of bent-core molecules*

**Robert Sargant**, Adam Rigby, Mark Wilson, Andrew Masters
The University of Manchester, United Kingdom

There has been great interest in the bent-core or “v-shaped” mesogen due to its biaxial nature. It is both a good candidate for a biaxial nematic liquid crystal phase with three distinct optical axes [1] and for novel ferroelectric devices [2]. We have used molecular dynamics to examine the phase behaviour of simple bent-core molecules [3] from isotropic initial conditions. Our model consists on a number of fused, repulsive spherical potentials arranged in a v-shape with a fixed angle between the two arms. These systems have been run under a range of bend angles, pressures and number of potentials. For systems comprised of 11-potential molecules, two different forms of phase behaviour are observed. In systems where the bend angle is &#8804;145°, we see a transition from isotropic to a uniaxial nematic phase. This subsequently transitions to an antiferroelectric smectic phase with interlocked clusters with no distinct separable layers. At narrower bend angles, no globally aligned mesophase is observed and the system forms isotropically orientated polar clusters. We have examined other molecule sizes and found the threshold between these two behaviours tends towards larger angles as the molecule size reduces. We have also briefly examined the behaviour of binary mixtures of two different sizes molecules with the same bend angle in the hope of destabilizing some of these observed smectic phases. To date these systems have been observed as experiencing uniaxial nematic mixing, but then preferentially demixing as one component undergoes a transition to the antiferroelectric smectic phase. It has not yet been shown that the introduction of the second species affects this transition.

*[1] P.I.C Teixeira, A.J. Masters and B M Mulder. Mol. Cryst. Liq. Cryst., 323, 167 (1998)*
*[2] O. Francescangeli et. al., Adv. Funct. Mater. 19, 2592 (2009)*
*[3] A. Dewar and P.J. Camp, Phys. Rev. E 011704, 70 (2004)*

## *Coarse-grained simulations of poly(ethylene oxide) in aqueous solution and at a water-air interface*

**Khongvit Prasitnok**, Mark R. Wilson
Durham University, United Kingdom

## *Self-assembling of dppc membrane in implicit water solvent by coarse-graining simulations*

**Hossein Ali Karimi Varzaneh**, Elena Algaer, and Florian Müller-Plathe

In this work a coarse-graining model of the DPPC lipid membrane has been presented. The iterative Boltzmann inversion has been used to develop a coarse-graining force-field between the superatoms to reproduce the structural properties of the atomistic simulation. It has been found that the coarse-graining model predicts successfully chemical features of the membrane. The coarse-graining force-field developed shows also the self-assembling of the membrane from a random distribution of the lipids in the simulation box. The self-assembling of the membrane has been investigated in a range of pressures and temperatures. Phase diagram based on the simulations at different pressures reproduces different phases of membrane.

## *Wetting and spreading by molecular dynamics simulations*

**Fereshte Taherian-Tabasi**, Valentina Marcon, and Nico van der Vegt

Azobenzene undergoes a reversible photoisomerization upon changes in illumination conditions. The more thermodynamically stable state is the trans form, which has a flat planar structure Illumination with ultraviolet light converts the azobenzene into a bent cis state, which reverts back to the trans form either under illumination with visible light or by removal from light for an extended period of time. The cis- and trans-isomers have a different spatial arrangement of the aromatic moieties, and consequently show significantly different physical and chemical properties.The trans to cis photoisomerization of functionalized azobenzenes induces a change of the dipole moment in these molecules, which in turn determines the hydrophobic and hydrophilic nature of the trans and cis isomers.By means of molecular dynamics simulation we are going to understand the effect of azobenzene on wetting parameters.

## *Stability of amphiphilic tri-block copolymers in biological membranes: effect of the polymer molecular weight and structure*

**Paola Carbone**, Selina Nawaz

Amphiphilic copolymers are widely employed in nanomedicine as surface coating. Among the different amphiphilic copolymers available for these purposes the triblock copolymers (known also as Pluronics) formed by ethyl oxide (EO) as hydrophilic monomer and propylene-oxide (PO) used as hydrophobic monomer, are the most commonly employed. The study of their cytotoxicity is then a key issue but attempts in rationalizing their behaviour when interacting with the living matter have resulted in contradictory results [1] [2]. Here we present the results of atomistic molecular dynamics simulations used to investigate the stability of a model biological membrane dipalmitoylphosphatidylcholine (DPPC) upon the insertion of tri-block copolymer poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEOPPOPEO). We investigate the relation between the polymer molecular structure such as PEO/PPO ratio and polymer molecular weight on the membrane structure. We find that the stability of the membrane is affected concurrently by the two. The hydrophobic unit (PPO) holds the two leaflets of the bilayer together even when the membrane has lost its integrity. The membrane is stabilized when large quantities of the copolymer chain interact with the hydrophilic head group.

*[1] Wu, G., et al., Lipid Corralling and Poloxamer Squeeze-Out in Membranes. Physical Review Letters, 2004. 93(2): p. 028101.*

*[2] Wu, G., et al., Interaction between Lipid Monolayers and Poloxamer 188: An X-Ray Reflectivity and Diffraction Study. Biophysical Journal, 2005. 89(5): p. 3159-3173.*

# 5 Participant List

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