Patchy Colloids, Proteins and Network Forming Liquids: Analogies and new insights from computer simulations

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February 7, 2007

1 Workshop Details

1.1 Details

Timing
Number of days : 3
Start : 2006-06-26
end : 2006-06-28

Location of the activity
CECAM
46 allée d'Italie
69007 Lyon
France

1.2 Description

No description provided

2 Requested Support

Simbioma

CECAM

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4 Presentation List

SIMPLE MODELS WITH PATCHY SITES: From intuitive speculations to rigor

Ivo Nezbeda
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Gelation and modulated phases in attractive colloidal systems

Emanuela Del Gado
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Abstract

In colloidal suspensions, the competition between attractive and repulsive interactions gives rise to a rich and complex phenomenology. I will discuss the results based on a model system with competing attraction and repulsion, which has been studied by means of molecular dynamics simulations and a thermodynamical approach. At low temperature, the competition between attractive and repulsive interactions induces a typical modulation length clearly detected at very low volume fraction in the cluster phase. As the volume fraction is increased, clusters are prone to aggregate in spite of the long-range repulsion. This results in the growing of elongated structures which keep track of the modulation length. Eventually, a perfect modulated phase forms, with a hexagonal geometry, or a lamellar one at higher volume fraction. At low temperatures, increasing the volume fraction, the system undergoes a transition from the disordered cluster phase to an ordered hexagonal phase and, at higher volume fraction, to an ordered lamellar phase. Due to the presence of defects such as local inhomogeneities and branching points in the precursors of the modulated structures, when the volume fraction is high enough, an interconnected spanning structure can be formed and a gel-like behavior is observed as it is frequently the case in the experiments. As a consequence, the system may enter in a "supercooled" metastable liquid state until structural arrest (gel) occurs. This finding strongly suggests that the transition to the gel phase observed in some experiments and in numerical simulations occurs in a metastable state. In real colloidal suspensions, the observation of such ordered phases may be hindered by the long relaxation times or by the presence of defects (polydispersity, anisotropy of the particles...).

Energy landscape of a simple model for strong network-forming liquids

Angel Moreno
DONOSTIA INTERNATIONAL PHYSICS CENTER, SAN SEBASTIAN, Spain

Abstract

We present a numerical study of the potential energy landscape of a simple model for strong network-forming liquids. The model is a system of spherical particles interacting through a square well potential, with an additional constraint that limits the maximum number of bonds, N_max, per particle. Extensive simulations have been carried out as a function of temperature, density, and N_max. The dynamics of this model are characterized by Arrhenius temperature dependence of the transport coefficients and by nearly exponential relaxation of dynamic correlators, i.e. features defining strong glass-forming liquids. This model has two important features: (i) landscape basins can be associated with bonding patterns; (ii) the configurational

volume of the basin can be evaluated in a formally exact way, and numerically with arbitrary precision. These features allow us to evaluate the number of different topologies the bonding pattern can adopt. We find that the number of fully bonded configurations, i.e. configurations in which all particles are bonded to N_max neighbors, is extensive, suggesting that the configurational entropy of the low temperature fluid is finite. We also evaluate the energy dependence of the configurational entropy close to the ground state, and show that it follows a logarithmic functional form, differently from the quadratic dependence characterizing fragile liquids. We suggest that the presence of a discrete energy scale, provided by the particle bonds, and the intrinsic degeneracy of fully bonded disordered networks differentiate strong from fragile behavior.

References

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A.J. Moreno, I. Saika-Voivod, E. Zaccarelli, E. La Nave, S.V. Buldyrev, P. Tartaglia, F. Sciortino, J. Chem. Phys. (to be published); cond-mat/0601053

Structure and Dynamics of a Gel-Forming System

Walter Kob
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Abstract

We will present the results of molecular dynamics computer simulations done to investigate the structure and dynamics of a simple model for a colloidal gel. In this model the particles interact via a radial potential, a contribution that stems from a ”decoration” of the particles, and a three-body potential. Due to this interaction the system does not show any sign of phase separation, even at low volume fraction (at least in the temperature range investigated). We will discuss to what extend the concentration of the particles and the temperature affects the structure and relaxation dynamics of the system and show that these results are indeed very similar to the one found in real colloidal gels.

References

Structure and Relaxation Dynamics of a Colloidal Gel
E. Del Gado and W. Kob
Europhys. Lett. 72, 1032 (2005).

Length scale dependent relaxation in colloidal gels
E. Del Gado and W. Kob
cond-mat/0510690

Jamming and clustering in colloidal suspensions of rods and spheres

Hartmut Lö wen
Heinrich-Heine-Universitä t Duesseldorf, Germany

Abstract

Clustering and jamming effects are discussed for colloidal suspensions of rods and spheres

obtained by Brownian dynamics computer simulations. Examples include: i) partial equilibrium clustering a in a two-dimensional binary suspensions of spheres [1], ii) rhythmic clustering generated a colloidal sphere dragged through a suspension of rods which are in a nematic phase [2], iii) jamming in a suspension of rotating rods [3,4].

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[3] R. Kirchhoff, H. L´owen, T-structured fluid and jamming in driven Brownian rotators, Europhysics Letters **69**, 291-297 (2005).
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Positive Design in Self Assembly

Ard Louis
University of Cambridge, Department of Chemistry, United Kingdom

Abstract

abstract: to come later

Experiment and computer simulation studies of heterogeneous nucleation of protein crystals on porous media

Richard Sear
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Abstract

One of the most important problems in the study of protein solutions is their crystallisation. Protein crystals are needed for protein structure determination via X-ray crystallography but many proteins are hard or impossible to crystallise into the large crystals needed. Crystallisation is a first-order phase transition and so proceeds via nucleation, an activated process, and growth. I will focus on nucleation. Nucleation occurs in contact with a surface, thus its rate depends on the properties of the surface. This has led to the idea of adding substances to a protein solution that provide a surface upon which the barrier to nucleation is especially low. These substances are called nucleants. I will describe recent experimental work on using porous media nucleants, and computer simulation work on nucleation at pores aimed at understanding these experiments. The simulations show that nucleation occurs orders of magnitude faster at pores than on flat surfaces and that there is a pore size at which the nucleation rate is maximal. These findings suggest that pores can be designed to maximise the nucleation rate.

Stability and two-phase coexistence for polydisperse fluids of adhesive colloidal particles

Achille Giacometti
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References

R. Fantoni, D.Gazzillo and A. Giacometti, J. Chem. Phys. 122, 034901 (2005)
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Non-equilibrium dynamics and structure of interfacial ice

Oliviero Andreussi
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Abstract

Stimulated by recent experiments [1], we have performed molecular dynamics and ab initio structural studies of the laser-induced heating and restructuring processes of nanometer-scale ice on a substrate of chlorine terminated Si(111). Starting from proton disordered cubic ice configurations the thin film behavior has been characterized at several temperatures up to the melting point. The surface induces order with crystallization in the Ic lattice, but with void amorphous regions. The structure changes on the ultrashort time scale and restructures by heat dissipation depending on the relaxation time and final temperature. Our results show the general behavior observed experimentally, thus providing the nature of forces in the atomic-scale description of interfacial ice.

References

[1] C.-Y. Ruan, V.A. Lobastov, F. Vigliotti, S. Chen and A.H.Zewail, Science 304, 80-84 (2004)

Structure, dynamics and gelation in a transient network fluid

Ludovic Berthier
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Abstract

Transient-network fluids consist of a dispersion of junction points connected by transient elastic bridges. They have a wide range of practical applications, from synthetic polymers to surfactant solutions, soft biological systems, gels, glues, rubbers... Their dynamical behaviour, in particular in rheology, is extremely rich and strongly non-linear: they exhibit both shear-thinning and thickening, and in some cases, ”rheochaos”.

A simple experimental model system was devised in our lab in Montpellier. It is a ternary mixture of oil-in-water microemulsion droplets and telechelic polymers connecting the droplets. The phase behaviour has been well characterized experimentally: it comprises a liquid-gas phase separation and a percolation transition towards a gel phase.

In this talk, I will present the results of large scale molecular dynamics simulations of this system. I will focus in particular on the structure and the equilibrium dynamics of both the sol and the gel phases at various volume fractions, discussing the possible link and analogies with the physics of colloidal gelation and jamming transitions in dense systems.

Aggregation of sticky hard spheres:

Sujin Babu

Université du Maine, France

Abstract

We will present results from simulation of reversible aggregation of sticky hard spheres (i.e. with zero interaction range or surface adhesion). In that case as no ternary collisions are possible the average number of neighbors per particles cannot exceed 2. As a consequence of this no phase separation is observed. The aggregation is kinetically driven and the properties of the system at equilibrium are governed by the life time of an encounter between 2 particles. The difference between an encounter and a collision will be addressed. In these systems we observe a cross over from flocculation to percolation characterized by the change in the cluster fractal dimension from 2 to 2.7 and in the polydispersity exponent from 1.5 to 2.1. As soon as we introduce an interaction range (square well model) we observe a phase separation. In these square well systems the properties of the homogenous phase will also be addressed close to the percolation line where same phenomena as in zero interaction range are observed. A detailed comparison between zero interaction and square well systems will be shown.

References

S.Babu, M. Rottereau, T. Nicolai, J. C. Gimel,D. Durand ”Flocculation and percolation in reversible cluster cluster aggregation” Eur. Phys. J .E 19, 203(2006)

Controlling crystallization and its absence: Proteins and patchy colloids

Jonathan Doye

Department of Chemistry, University of Cambridge, United Kingdom

Abstract

Controlling crystallization and its absence: Proteins and patchy colloids
We will introduce an evolutionary perspective on the general difficulty of crystallizing proteins [1]. Namely, that there is a selective pressure against protein crystallization, and more generally native state aggregation, because they are normally deleterious to the cell. We will then review some ‘exceptions that prove the rule’, examples of proteins that do crystallize in the cell, because this achieves some functional purpose [2]. Finally, we will examine the results of simulations trying to crystallize patchy colloids, showing how the geometry of the interactions can be used to aid or frustrate crystallization.

References

[1] Physical Biology 1, P9-P13 (2004)
[2] Curr. Opin. Colloid In., 11, 40-46 (2006)

Analytical Results for charged fluids including polyelectrolytes

Lesser Blum

Department of Physics, University of Puerto Rico, Puerto Rico

Computer simulation studies of the phase diagram of water

Carlos Vega

Universidad Complutense, Madrid, Spain

Patchy Baxter spheres

Mark Miller
Department of Chemistry, University of Cambridge, United Kingdom

Abstract

Anisotropic interactions are an intrinsic feature of globular proteins in solution, since the surface of a protein is heterogeneous: charged residues interact through screened electrostatic forces, hydrophobic groups seek to minimise contact with water, and specific hydrogen-bonding patterns may be present. Despite this complexity, the generic features of many protein phase diagrams are similar to those of isotropic colloids. However, attempting to ”collapse” all proteins into one uniform description is clearly an over-simplification.

I will present a patchy version of Baxter's adhesive hard sphere model in which the spheres reversibly adhere only when the point of contact between the spheres lies inside a sticky patch on both particles. The free parameters are the stickiness (or temperature), the fraction of the sphere surface covered in patches (or the second virial coefficient, B2) and the geometry of the patches. The simplicity of the model's definition allows the effects of directionality to be isolated and controlled.

The arrangement of patches has a strong effect on the position and shape of the fluid-fluid coexistence curve. In particular, the value of B2 at the critical point can be significantly raised or lowered relative to isotropic adhesive spheres. It is known that density fluctuations near the critical point can assist protein crystal nucleation if the critical point lies in the ”crystallisation slot” of slightly negative values of B2. The present work suggests that this condition is unlikely to be satisfied given the anistropy of protein-protein interactions, and this effect may therefore contribute to the difficulty of obtaining protein crystals.

Gel formation in naturally occurring triglycerides and synthetic beta-peptides. Results from atomistic and coarse grain models

Juan J. de Pablo
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Self-assembly of patchy particles: The shapes of things to come

Sharon C. Glotzer
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Abstract

Recent breakthroughs in particle synthesis leading to nanoscopic and colloidal particles of unusual shape and patterning have paved the way for a revolution in materials formed from the self-assembly of these building blocks. The unprecedented anisotropy of today's new nanoparticle and colloidal building blocks starkly contrasts with the isotropic, spherical colloids that have been the focus of particle assembly for more than a generation. As the materials community gains further control over the design and fabrication of these new particles, they are poised to become the “atoms” and “molecules” of tomorrow's materials and devices, provided we can learn to assemble them into predictable and useful structures [1].

Fundamentally, no comprehensive theory exists to predict the range of structures possible for

these new building blocks as a function of thermodynamic conditions, and the complementary problem of inverse design of a particular building block that can self-assemble into a desired target structure is difficult with as yet no standard design algorithm. In this talk, we discuss the need for a conceptual framework and common language with which to describe these new building blocks and their assemblies [2]. We present results of computer simulations of patchy particle [3] and polymer-tethered nanoparticle [4] "shape amphiphiles" undergoing self-assembly, and, where possible, make connections between these particulate building blocks and their molecular analogs. We show how various measures of anisotropy, including particle shape, patterning, functionalization and interaction selectivity, can be combined and exploited to achieve complex mesoscale one-, two- and three-dimensional structures such as wires, sheets, shells, helices, gyroid, diamond, virus-like and other complex structures through self-assembly [5-13].

References

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12. C. R. Iacovella, A.S. Keys, M.A. Horsch and S.C. Glotzer, "Icosahedral packing of polymer-tethered nanoparticles and stabilization of the gyroid phase," preprint.

Monte-Carlo simulations of a coarse-grained model for DNA-coated colloids

Benhaz Bozorgui
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Abstract

Colloidal particles coated with DNA with a hybridizable end group can selectively bind to colloids coated with a complementary DNA sequence. This can lead to the formation of clusters of different size. Recent experimental data on systems with two types of colloids shows strong attraction between such coated colloids, yet the size of the clusters remains finite. By means of Monte-Carlo simulations we studied the clustering of complementary coated colloids in which the DNA chains are modeled as soft colloids. When such a DNA chain bridges two colloids, it can act as an entropic spring. As a single colloid can carry many DNA chains, the model allows for the formation of large clusters but also for the formation of multiply bounded dimers. We discuss the effect of number density of polymers on cluster size and the center to center distribution functions. The results are in a good agreement with experimental observations. The distribution function of colloids always has a peak at contact distances. We find that the growth of the clusters saturates at a finite size where the steric stabilization due to the DNA inhibits further colloid addition.

Limited-valency models for attractive colloids

Emanuela Zaccarelli
SOFT-INFM-CNR Istituto dei Sistemi Complessi, Via dei Taurini 19 Roma, Italy

Aggregation and Gelation of the protein ocr - a DNA mimick

Wilson Poon
University of Edinburgh, United Kingdom

Abstract

Restriction enzymes represent one of the main mechanisms E. coli uses to defend itself against infection by lambda bacteriophage. These enzymes have the ability to recognise, bind to, and destroy phage DNA. Phage, however, has a counter defence mechanism. The first protein that the lambda phage DNA manufactures when it enters its bacterial host is ocr ('overcome classical restriction'). This protein geometrically (it has a bent-rod, or banana, shape) and electrostatically mimicks DNA, and competes for binding with the restriction enzymes. For the purpose of this meeting, then, ocr is banana-shaped nanoparticle with patches of negative charges arranged in a spiral pattern. Very strange behaviour was noticed by my collaborators in Edinburgh when they tried to purify this protein - it did not precipitate even under 80% saturated ammonium sulphate. Instead, at this sort of salt concentration, a transparent gel forms. In this talk, I will review our investigation of this phenomenon, and suggest that it may be due to the formation of novel salt bridges between negatively charged patches on adjacent proteins.

Minimal Models for Modeling Protein Crystallization

Sanat Kumar
RPI, United States

Abstract

The crystallization of proteins is a topic of great interest since the availability of macroscopically large crystals represents almost the only means available to characterize native protein structures by scattering techniques. Two decades of experiments have shown an extremely sim-

ple phenomenology describes this crystallization process: proteins crystallize if their second virial coefficients fall in a very small band ["crystallization slot"]. Since such universal behavior has been observed it appears reasonable that simple models, such as spheres interacting through isotopic interactions, are sufficient to understand these situations. We have employed a series of computer simulations to study the validity of this simple model in describing protein crystallization: the results of this investigation will be discussed in this talk.
A parallel study, on "patchy" polymers has been conducted which allows us to understand the competition between gelation and phase separation. The relationship of this work to that of protein crystallization will also be considered.

Dynamics in patchy colloids and network forming liquids: gels and glasses

Francesco Sciortino
Dipartimento di Fisica, Universita' di Roma La Sapienza, Italy

Maximum Valency Lattice Gas Model

Emilia La Nave
INFM CRS-SOFT, Physics Dep. University of Rome , Italy

Phase diagram of patchy colloids: empty liquids and ideal gels

Emanuela Bianchi
università di Roma La Sapienza, Italy

Making Patchy Colloids

David Pine
New York University, United States

Abstract

A method for synthesizing a versatile new class of nearly spherical colloidal particles that interact with well-defined non-spherical symmetries is described. These particles are typically several hundreds of nanometers in diameter and have attractive interaction potentials with twofold, threefold, fourfold, or higher symmetries. For example, a colloidal suspension of particles with attractive potentials possessing twofold symmetry forms chains while a suspension of particles possessing fourfold symmetry forms aggregates with local tetrahedral symmetry. Thus, these particles have a well-defined "valence" analogous to atoms: the particles with twofold and fourfold attractive interactive potentials are analogous to sulfur and carbon, respectively, for example. Exotic higher symmetry particles are also available, particles with 7-fold or 12-fold icosahedral symmetries can be made.

Model for the Assembly and Gelation of DNA "Dendrimers"

Francis Starr

Wesleyan University, United States

Abstract

The disordered-arrested state of matter is ubiquitous in existing materials like glasses, and is prevalent in many new materials, due to the uncommon mechanical, thermal and electrical properties. The “bottom-up” construction of new materials is one of the central aims of nanotechnology. DNA is potentially an optimal choice for the construction of three-dimensional supramolecular assemblies since it can self-assemble into long and fairly rigid helices, based simply on sequence complementarity. We numerically study a model designed to mimic the behavior of recently synthesized single-stranded DNA dendrimers. Complementarity of the base sequences of different strands results in the formation of strong cooperative intermolecular links with a valency controlled by the number of strands. We simulate the bulk behavior of a system containing many 4-armed DNA dendrimers and find that in an extremely narrow temperature range the system forms a large-scale, low-density network via a thermo-reversible gel transition. The sharpness of the crossover the gel state can be controlled by the length of the DNA strands, since longer strands will form cooperative bonds over a narrower temperature range. As a result, the percolation temperature of the network formed by the dendrimers can be made arbitrarily close to the gel transition by tuning the length of DNA strands. This is in contrast with recent model systems designed to understand thermo-reversible gelation. Given that gelation and percolation coincide in irreversible chemical gels, this system provides an excellent model material to bridge the understanding between reversible and chemical gels.

To be announced

Julio Largo
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Thermodynamics and dynamics of short range-range attractive colloids down to the Baxter limit

Giuseppe Foffi
Institut Romand de Recherche Numerique en Physique des Materiaux, Ecole Polytechnique Federale de Lausanne , Switzerland

Abstract

It is well established that the range of the attraction is a key parameter for both the thermodynamical and dynamical properties in short ranged attractive colloidal systems. I will discuss the effect of going to an extremely short range, a limit that is the basis of the celebrated Baxter (or adhesive) model. I will begin by discussing the dependence of the dynamics on the range of attraction and I will show how a trivial dynamical scaling holds once the range becomes extremely short. The main consequence, for systems with an interaction ranging from a few percent down to the Baxter limit, is that the relative location of the attractive glass line and the liquid-gas line does not depend on the range. This proves that in this class of potentials, disordered arrested states (i.e. gels) can be generated only as a result of a kinetically arrested phase separation. Moreover, the present work gives a new interpretation to the Baxter model. According to our results, the apparent long bond lifetime characteristic of the Baxter model is only induced by the extremely small thermal velocity associated to the vanishing of T implicit

in the limit of vanishing range. In the second part of my talk I will present recent results for the thermodynamics of short range systems. I will discuss the reason of the success of the Baxter model, showing that the equivalence of all the short range potential systems (the Noro and Frenkel ”generalized law of correspondent states”), can be explained in the rigorous PEL thermodynamic formalism as arising from the multiplicative contribution that each bond add to the vibrational entropy and from the possibility of separating vibrational and floppy contributions (a condition which requires a small bond width). Incidentally, I will show how our approach allows to count the fraction of floppy modes in a system of bonded particles.

References

[1] **WARNING : unknown g. foffi et al. phys. rev. lett. 94, 078301 (2005)g. foffi et al. j. chem. phys. 122, 224903 (2005)m. noro and d. frenkel j. chem. phys. 113, 2941 (2000**

5 Program

Day 1: June 26 2006

Session : 1 Patchy Particles
08:50 to 09:00 : Welcome

09:00 to 09:30 : Presentation
SIMPLE MODELS WITH PATCHY SITES: From intuitive speculations to rigor
Ivo Nezbeda

09:30 to 10:00 : Presentation
Self-assembly of patchy particles: The shapes of things to come
Sharon C. Glotzer

10:00 to 10:30 : Presentation
Making Patchy Colloids
David Pine

10:30 to 11:00 : Coffee Break

Session : 1 Cluster, Gel and Network Formation
11:00 to 11:30 : Presentation
Jamming and clustering in colloidal suspensions of rods and spheres
Hartmut Lö wen

11:30 to 12:00 : Presentation
Gelation and modulated phases in attractive colloidal systems
Emanuela Del Gado

12:00 to 12:30 : Presentation
Limited-valency models for attractive colloids
Emanuela Zaccarelli

12:30 to 15:00 : Lunch Break

Session : 2 Protein Crystallization
15:00 to 15:30 : Presentation
Positive Design in Self Assembly
Ard Louis

15:30 to 16:00 : Presentation
Minimal Models for Modeling Protein Crystallization
Sanat Kumar

16:00 to 16:30 : Presentation
Controlling crystallization and its absence: Proteins and patchy colloids
Jonathan Doye

16:30 to 17:00 : Coffee Break

Session : 2 More on patchy particles
17:00 to 17:30 : Presentation
Dynamics in patchy colloids and network forming liquids: gels and glasses
Francesco Sciortino

17:30 to 17:50 : Presentation
Phase diagram of patchy colloids: empty liquids and ideal gels
Emanuela Bianchi

17:50 to : Discussion

Day 2: June 27 2006

Session : 3 DNA (I)
09:00 to 09:30 : Presentation
Aggregation and Gelation of the protein ocr - a DNA mimick
Wilson Poon

09:30 to 10:00 : Presentation
Model for the Assembly and Gelation of DNA ”Dendrimers”
Francis Starr

10:00 to 10:30 : Presentation
Monte-Carlo simulations of a coarse-grained model for DNA-coated colloids
Benhaz Bozorgui

10:30 to 11:00 : Coffee Break

Session : 3 DNA (II) ; Integral Equations
11:00 to 11:30 : Presentation
To be announced
Julio Largo

11:30 to 12:00 : Presentation
Analytical Results for charged fluids including polyelectrolytes
Lesser Blum

12:00 to 12:30 : Presentation
Stability and two-phase coexistence for polydisperse fluids of adhesive colloidal particles

Achille Giacometti

12:30 to 15:00 : Lunch Break

Session : 4 Gels
15:00 to 15:30 : Presentation
Structure and Dynamics of a Gel-Forming System
Walter Kob

15:30 to 16:00 : Presentation
Gel formation in naturally occurring triglycerides and synthetic beta-peptides. Results from atomistic and coarse grain models
Juan J. de Pablo

16:00 to 16:30 :

16:30 to 17:00 : Coffee Break

Session : 4 Water and more on patchy particles
17:00 to 17:30 : Presentation
Computer simulation studies of the phase diagram of water
Carlos Vega

17:30 to 17:50 : Presentation
Non-equilibrium dynamics and structure of interfacial ice
Oliviero Andreussi

17:50 to 18:10 : Presentation
Maximum Valency Lattice Gas Model
Emilia La Nave

18:10 to : Discussion

Day 3: June 28 2006

Session : 5 Sticky spheres and energy landscape
09:00 to 09:30 : Presentation
Patchy Baxter spheres
Mark Miller

09:30 to 10:00 :

10:00 to 10:30 :

10:30 to 11:00 : Coffee Break

Session : 5 Energy Landscape (II); Protein Crystallization (II) and Conclusions
11:00 to 11:30 : Presentation
Energy landscape of a simple model for strong network-forming liquids
Angel Moreno

11:30 to 12:00 :

12:00 to : Discussion

6 Organizer's report

6.1 Conclusions.

The CECAM workshop on Patchy Colloids, Proteins and Network-Forming Liquids was held in Lyon June 26-28 2006. It has offered to a small focused group of researchers a rather unique opportunity to interact and share ideas. Scientists working in the field of colloidal science, protein aggregation and glass-forming network liquids (both experimentalists and theoreticians) have met for three full days, finding a common language between them.

During the workshop it has become clear that the underlying physics, in particular the topology of the phase diagram and the dynamical behaviour, for these different systems is often very similar. It can be interpreted in an unifying approach. In particular, a clear emergence of close similarity between colloidal gels, as those formed by some 'patchy-like' interactions, and network-forming liquids, such as the most-common studied water and silica, arised during the talks at the workshop.

In the workshop, it was discussed in details the relation between gelation, phase separation and glassification, as well as crystallization. The importance of understanding gelation at low densities remains a challenge. Hopefully light can be shed on these questions through the use of simple primitive-like models for patchy colloids and experiments in the foreseeable future (thanks to the advancement in particle synthesis).

The design of specific colloidal particles for self assembly is enormously advancing and calls for an effort from theory and numerical simulation to provide a framework for understanding the assembly process and to guide the synthesis. In the same spirit, positive and negative design techniques are being exploited in relation to protein crystallization. Several contributions have called attention on the need for protein models which incorporate non-spherical patchy interactions.

Finally, numerous experimental/numerical works in DNA-coated colloids have been reported at the workshop, signaling the importance of DNA to become (beside a genetic carries) also a building block molecule in the design of new materials.

We are pleased to note that several young researchers have asked to participated and many of them have been given the opportunity to present their work.

6.2 Recommendations.

CECAM has provided us with the unique opportunity to organize a small, focused workshop, putting together in the same room experts of different topics. We think it is very important to have such opportunities, and we strongly hope that CECAM will continue to provide these opportunities.

The workshop was very successful in terms of participation, discussion and comments from the attendants. Due to the fast pace at which the field is growing, perhaps it will be the case to organize another workshop on the same topic in 2/3 years.

We really appreciated the easyness in organizing the workshop, through a proposal, a very careful and intelligent referral (who suggested us to invite two famous experimentalists) and a few emails. All was done very simply through the website, from the uploading of abstracts and program to the accomodation arrangements and so on. All this constitutes a major advantage while organizing a CECAM workshop.

We would really like to thank all the CECAM staff, Mmes Emmanuelle Crespeau and Emilie Bernard, Mr. Frederic Barmes, the system administrator and Prof. Berend Smit, the director of CECAM. They really gave a crucial contribution to the organization and helped us promptly in every detail.

Finally, we want to mention the sponsors of this workshop, CECAM itself and SimBioMa for additional financial support, which allowed us to reimburse local expenses to almost all participants.

We believe it would be useful to start the workshop with a welcome talk by a CECAM member, explaining what CECAM is and how it works, since the young participants are not aware of this important organism.

7 Key references

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