

www.eu-softcomp.net

Editorial

This is the first newsletter of SoftComp as a self-supporting network, after the EU funding came to an end. Since then SoftComp has attracted eight new partners, demonstrating thereby the scientific viability of the network. This significantly strengthens the Softcomp goal to integrate the European Soft Matter Research community and promises further growth potential. The new groups are:

- Malvern Instruments Ltd, United Kingdom
- T. Univ. Eindhoven, The Netherlands
- Univ. Göttingen, Germany
- Univ. Halle, Germany
- Univ. Lund, Sweden
- Univ. Luxembourg, Luxembourg
- Univ. Vienna, Austria
- Univ. Wageningen, The Netherlands

Furthermore, with the funding negotiation for the European Soft Matter Infrastructure (ESMI) a major step has been taken towards opening the SoftComp infrastructure including some new partners in the European Soft Matter Community. Information on ESMI may be found under www.esmi-fp7.net. Access proposals for this new infrastructure are foreseen starting from 1 January 2011.

The Softcomp Annual Meeting in 2011 will take place in Crete, Greece, 16 -18 May 2011. We like to stimulate the interest of our members to join the Annual Meeting, that has changed its format compared to earlier times. The Meeting will not be like a regular conference, but it should be a project meeting for scientific discussions around the joint scientific projects within SoftComp. The SoftComp Annual Meeting should also catalyze further joint scientific activities.

Details of the SoftComp Annual Meeting programme can be found on page 5 and at: www.eu-softcomp.net/news

We also would like to take this opportunity of wishing you all a happy and successful New Year.

Friedrich Hugo Bohn & Dieter Richter

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news letter

No. 8 · Dec. 2010

A colloid physics approach to understanding cataract formation

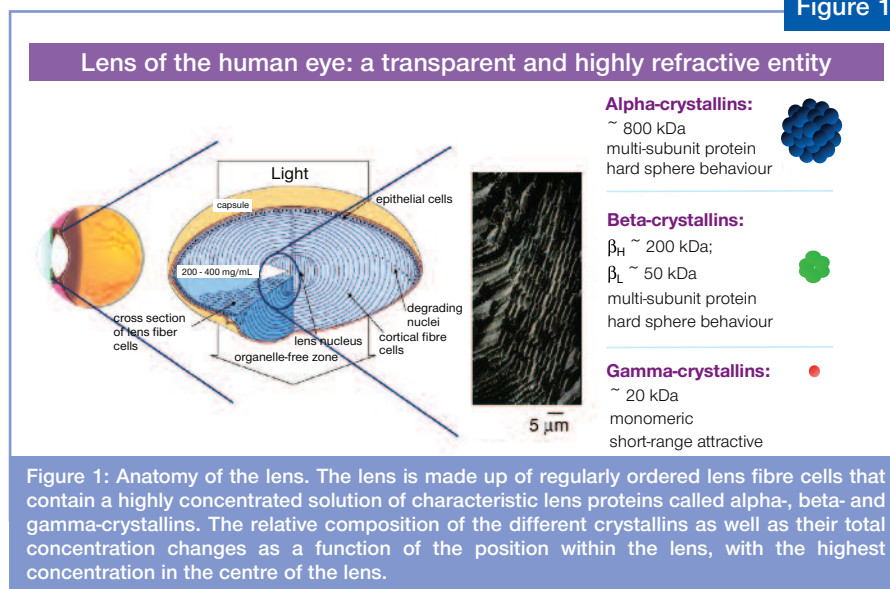
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Figure 1



Making stable concentrated colloidal dispersions is by no means an easy task, in particular if the colloids themselves represent mixtures of particles with different sizes and charges. However, nature has succeeded in this task, and we find numerous examples of cells that contain a vast number of different proteins at often exceedingly high volume fractions. However, not even nature is always perfect, and sometimes things go wrong and proteins start to aggregate or phase separate. There are actually a number of so-called protein condensation diseases such as cataract disease, sickle-cell disease, as well as Alzheimer's disease and numerous other neurodegenerative diseases,

where protein aggregation and phase separation play a central role [1]. Cataract for example – the loss of lens transparency due to increased light scattering – is a leading cause of blindness worldwide [2]. It is the consequence of various processes, the most important of which is condensation of lens proteins into aggregates. In our research we thus attempted to investigate and model the lens using analogies to colloidal suspensions in order to arrive at a sound understanding of the molecular interactions among lens proteins under conditions typical of the lens. The ultimate goal of these studies is to use our extensive know-how on phase transitions in colloidal suspensions such as liquid-liquid and liquid-

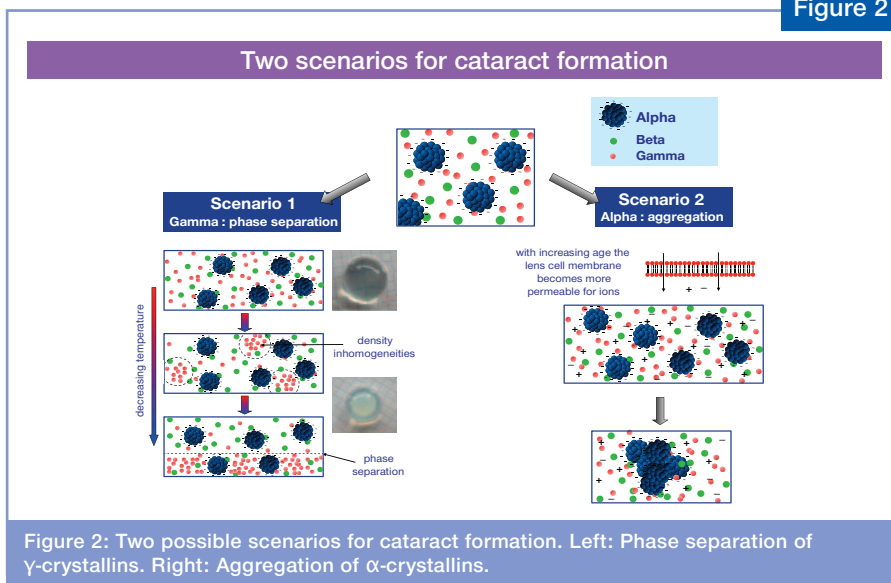
Figure 2


Figure 2: Two possible scenarios for cataract formation. Left: Phase separation of γ -crystallins. Right: Aggregation of α -crystallins.

implanted artificial lens cannot dynamically adapt its refractive power despite the fact that the neural mechanism for accommodation is still functioning. Thus great advantages, both socio-economic and in terms of quality of life, should result from understanding the mechanism of protein condensation in the lens, the prerequisite for developing an approach to prevent cataract formation.

There are many possible scenarios for cataract formation, two of which are illustrated in Figure 2. The first possible mechanism focuses on the properties of γ -crystallins, which are thought to interact via a temperature-dependent short-range attraction. Due to these short-range attractions, mixtures of lens crystallins as present in the lens, phase separate as the temperature decreases below the critical temperature for liquid-liquid phase separation (**see left side of Figure 2**). This leads to an increased scattering of visible light because of critical fluctuations already when approaching the critical temperature. The result is an opacification of the lens and blurred vision (“cold cataract”) [2]. In the healthy eye, this critical temperature lies well below body temperature. However, as a result of modifications of the protein or variations in the salt concentration the critical temperature can increase and already lead to a turbid lens already at body temperature. A second possible scenario is based on aggregation of α -crystallins, which are known to carry a small residual charge at physiological conditions. This could be one reason for the apparent hard sphere behaviour of the α -crystallins, which would then however be on ionic strength dependent. As it is also known that with increasing age the lens cell membranes become more permeable to (cat)ions and the ionic strength within the lens protein solution increases, one might speculate that this could finally lead to an aggregation of the

solid transitions in order to understand the development of cataracts, and combine this with the traditional viewpoints of molecular biology, i.e. the investigation of specific interactions and their action.

The human eye lens and its characteristic proteins, the lens crystallins

The lens of the human eye lens is a major element of the eye’s optical system that must enable perfect image transmission onto the retina (**see Figure 1**) [3]. To achieve this goal the lens has to be transparent and must dynamically adapt its refractive power. In order to provide these properties the lens is completely devoid of blood vessels and consists of regularly ordered elongated eye lens fibre cells containing highly concentrated aqueous mixtures of characteristic lens proteins, the so-called crystallins. There are three major classes of lens crystallins, called α , β , and γ in order of decreasing size. This highly concentrated and normally stable protein mixture then produces a high refractive index that aids the eye in adaptive focusing of light. It is in fact remarkable that, although the lens is composed of very high concentrations of protein (200-500 mg/ml), it remains

relatively transparent throughout most of an individual’s life [3]. To understand the origin of normal lens transparency, it is essential to recognize that of the proteins in the lens scatters light independently of its neighbours. Instead, the scattering in the lens strongly depends on the correlations in the position of pairs of proteins, i.e. on the interactions between different proteins. A homogeneous packing of lens proteins has indeed long been recognized to be fundamental for lens transparency, and has been characterized on molecular length scales using small-angle X-ray and neutron scattering [4,5].

Cataract and some possible scenarios for its formation

However, we are currently still far from understanding all the properties of the quite complex mixtures of proteins which exhibit the pathological processes involved in cataract formation that has inspired their study. Currently a cataractous lens has to be surgically replaced with an artificial lens. Cataract extraction is the most frequently performed operation worldwide, and is extremely successful in restoring a clear image on the retina from a given distance. However, the

A colloid physics approach to understanding cataract formation (continued)

alpha-crystallins and corresponding increased light scattering and decreased transparency (see right side of Figure 2). This clearly indicates that we need information about the interactions between the different protein components of the lens and the resulting solution structure. In particular, we have to reinvestigate the question whether γ -crystallins can indeed be modelled as colloids with short-range attractions and the applicability of the hard sphere analogy for α -crystallins at high ionic strength and high volume fractions.

Measuring and modelling interactions between proteins

Information about the interactions between the individual proteins can be obtained using scattering methods. Here we rely on a so-called coarse-graining approach, where we model the proteins as colloidal particles that interact with each other through an effective (isotropic) interaction potential. Direct analogies between colloids and globular proteins have been used in the past quite successfully to understand the phase behaviour of globular proteins and to rationalize some of the phenomenological observations made

during protein crystallization. We have thus used a combination of different scattering techniques, rheological measurements and determination of the phase diagram through visual inspection in order to test the two hypotheses described in Figure 2. Our investigations with the individual crystallins up to high concentrations and high ionic strength can be summarized as follows [6-9]:

Both the α - and β -crystallins can be described by hard sphere theory up to very high volume fractions and ionic strengths. We can thus exclude the second scenario in Figure 2. The γ -crystallins can indeed be modelled quantitatively as sticky spheres, and we do find liquid-liquid phase separation at temperatures below the corresponding coexistence curve. It is worth pointing out that this coexistence curve is in fact metastable with respect to the liquid-solid phase boundary, which is one of the hallmarks of colloids interacting via a short-range attraction. This quantitative agreement between colloid theory and scattering experiments that we used to extract detailed information on the interactions between individual lens crystallins is illustrated in (Figure 3). Our experiments with pure γ - and α -solutions

thus strongly support scenario 1 in Figure 2, where an age-related increase of the critical temperature could lead to dramatically increased light scattering and a corresponding opacification of the lens.

Complex protein mixtures and their investigation

The next question to ask is of course how relevant these experiments with individual protein components are for the much more complex multi-component protein solutions in the lens. The fact that protein phase separation could be important is illustrated in Figure 2 (left side), where we see that an intact lens indeed opacifies when the temperature is lowered due to a temperature-induced phase separation and the concomitant critical fluctuations. This phenomenon is called “cold cataract”. However, while the individual α -, β - and γ -crystallins have been investigated systematically, our current knowledge of the phase behaviour and the structural and dynamic properties of concentrated mixtures of lens proteins that resemble the lens cell under physiological conditions remains limited. We thus started a systematic investigation of lens protein mixtures with increasing complexity. In the first step, we looked at mixtures of α - and γ -crystallins up to concentrations corresponding to those found in the lens. We used small-angle neutron scattering experiments in order to extract information about the relevant interactions between the different proteins and the resulting structural properties. However, extracting interaction potentials from scattering data in multi-component mixtures is by no means straightforward, and we thus combined these experiments with molecular dynamics computer simulations that allow us to isolate mutual interactions between different components and investigate their effect on the overall structure and the scattering data

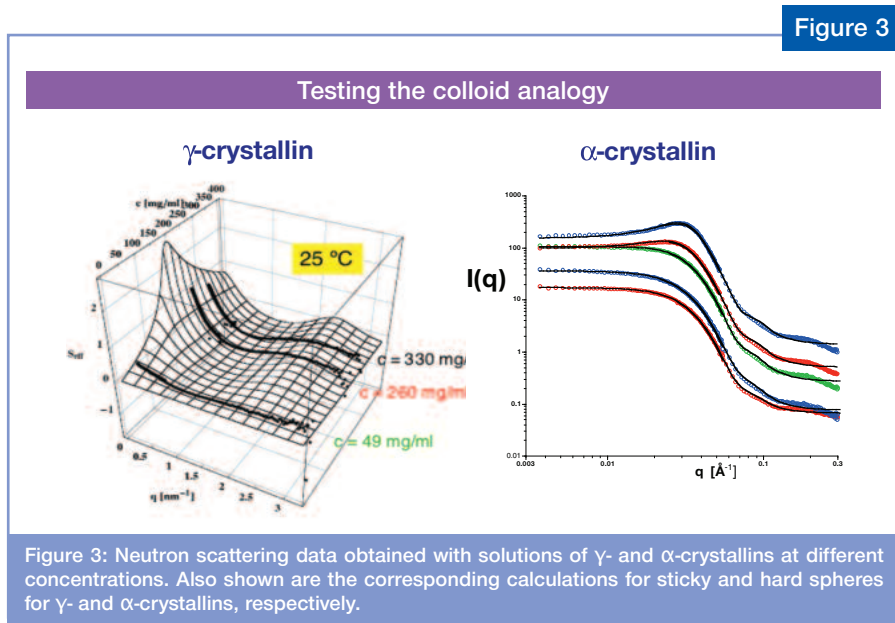
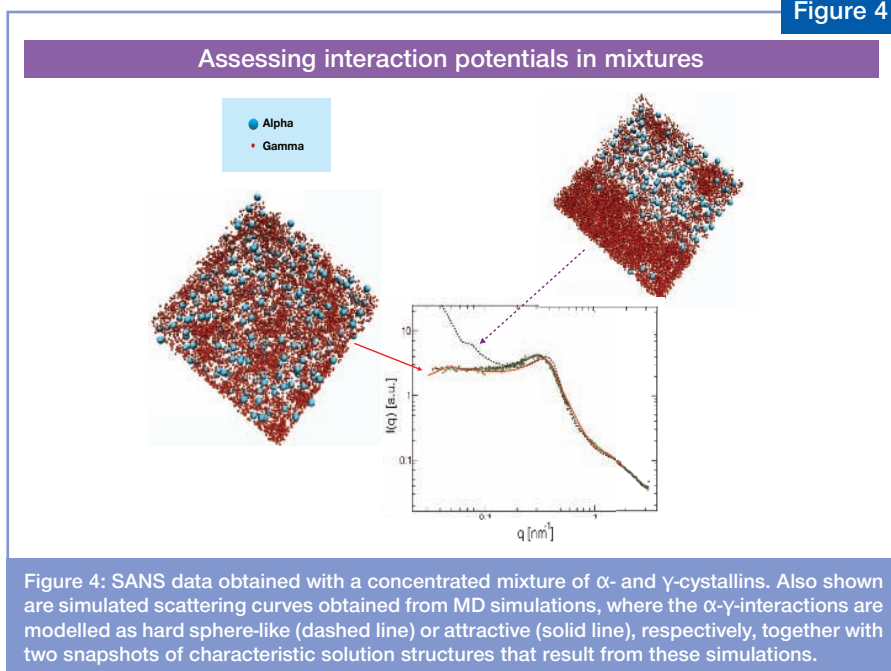


Figure 4


aggregation and cataract formation to not only understand cataract, but to extend this work to the broad class of protein condensation diseases.

Acknowledgements

We gratefully acknowledge the important contributions made by Nicolas Dorsaz, Giuseppe Foffi, Gabriela Savin, George Thurston and Lia Verhoeff. Financial support from the Swiss National Science Foundation, the State Secretariat for Education and Research in Switzerland, the Marie Curie Network on Dynamical Arrest of Soft Matter and Colloids, SoftComp and the Adolphe Merkle Foundation is gratefully acknowledged. SANS experiments were performed at the SANS I facility at the Swiss spallation neutron source SINQ, Paul Scherrer Institute, Villigen, Switzerland and at D22 at the Institut Laue Langevin, Grenoble, France. We thank the PSI and the ILL for neutron beam time.

[10-12]. The simulations are once again based on a coarse-graining procedure, where all the molecular details of the protein structure are omitted, and the proteins are treated as simple spheres interacting via effective pair potentials. The particles generated in the simulations have the same overall dimensions as the different crystallins, and the pair potentials that describe the interactions between two γ -crystallins ($U_{\gamma\gamma}$) and between two α -crystallins ($U_{\alpha\alpha}$), respectively, are chosen such as to correctly reproduce the phase diagrams and the scattering data obtained with the individual proteins. The only unknown thus remaining is the interaction between the alpha and the gamma crystallins, $U_{\alpha\gamma}$. As a first guess, we assumed a purely hard sphere interaction between gammas and alphas. However, the simulations quickly revealed that such a particle system would not be stable, but would immediately phase separate as shown in **(Figure 4)**. A direct comparison between the experimentally obtained SANS data and the scattering curves obtained from the simulated structures also demonstrates that the

two protein species must experience a mutual interaction potential that is clearly not hard-sphere-like. It turned out that we had to assume a weak mutual attraction between alphas and gammas in order to reproduce the neutron scattering results **(Figure 4)** [10-12].

Our experiments clearly demonstrated that variations in intermolecular interactions can have strongly non-monotonic effects on the resulting solution structure and the stability of mixtures. Given the extremely delicate balance of weak intermolecular interactions that decides about stability or instability in lens protein mixtures, we thus have to strive for a sound understanding of the actual consequences of the interactions between the different protein components. We believe that the lens provides an excellent testing ground for elucidating key statistical physics principles that not only bear directly on cataract, but which will also be of far-reaching applicability in other more complicated and dynamic cellular contexts. In a long-term perspective we thus hope to be able to generalize the link between phase separation,

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SoftComp Annual Meeting 2011

The SoftComp Annual Meeting 2011 will take place at the Knossos Beach resort, Crete. Greece, May 16-18, 2011. The SoftComp Consortium aims to stimulate the interest of its members towards the SoftComp Annual Meeting, that should not be just like a regular conference, but has to be seen as an important informal meeting where free scientific discussions on joint scientific projects and/or new projects may take place. The SoftComp Annual Meeting is seen as the catalyst of the SoftComp scientific activities. Therefore, the SoftComp NCC members reformulated the SoftComp Annual Meeting programme in the following way: The number of plenary talks on the first two days is reduced to two. This gives rooms for network area meetings where the different joint research activities could be discussed in some depth. Following the activity plan that we have agreed upon in Sicily the network area coordinators are asked to organize debates around the different

plan activities. This would be a top down element that allows to better structure the discussions. At the same time the SoftComp Annual Meeting will also live from a bottom up organization where the different partners are asked to present their wishes for presentations to the respective coordinators. Thus our meeting should assume in some way the character of a project meeting. In this sense we also plan for a longer discussion time after lunch, where different project partners could join forces for the discussion of results and the planning of new endeavours. On the third day we'll conclude the discussion on our joint activities with hopefully some decision in which direction we shall go in the different areas. Thereafter we'll have an ESMI – day. In this context we are going to have two prominent external plenary speakers. Then the different ESMI partners that offer access to their facilities and laboratories will present opportunities and research highlights

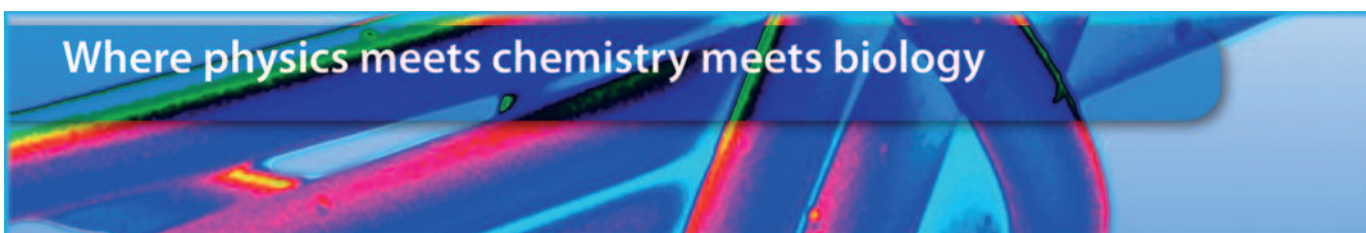
in their fields. I think this will become a highly interesting day with a plethora of new opportunities and scientific results interesting for all of us.

The industrial – academic sessions will consist of an introduction to the topic, by industrial and academic scientists followed by a discussion. The joint SoftComp – ESMI session consists of the presentation of the infrastructure made available by the ESMI partners to the whole European Soft Matter Community together with the scientific highlights achieved by using that infrastructure. The ESMI project is very important for the future research activities of the SoftComp partners.

Accommodation and subsistence costs are paid by the SoftComp Central Budget up to a number of four participants per group.

More information on the meeting venue is available under:

www.knossosbeach.com



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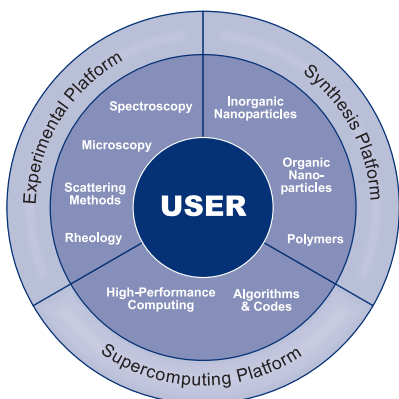
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Announcements



European Soft Matter Infrastructure ESMI

Free access to Soft Matter Infrastructure, synthesis facilities, first-class instrumentation and a fast supercomputer will be offered by the new EU project "ESMI", which stands for European Soft Matter Infrastructure and is planned to start in January 2011. The goal of ESMI is to enable all European soft matter scientists to synthesize new systems and/or to perform experiments and/or to use a supercomputer for simulations that would otherwise be difficult to implement due to the need for specialized know-how and equipment not available in house. There are a large number of groups offering external users free access to their infrastructure through ESMI. ESMI thus offers free access to a full range of synthesis facilities for several types of soft matter systems, to a comprehensive set of specialized experimental techniques and to a fast supercomputer, and, if necessary, also to theoretical support for data interpretation. The costs of travel, accommodation and use of infrastructure are fully covered by ESMI. There will be a web-based system for applications, through which proposals for free access to the ESMI infrastructure can be submitted. An independent review panel will evaluate these proposals online so that successful applications can be implemented without delay. If you would like to be informed in more detail about ESMI, please register at <http://www.esmi-fp7.net>.



Register now at
www.esmi-fp7.net
and you will be contacted
when ESMI starts!

ESMI institutions that offer access:

Catholic University Leuven (Belgium)
FORTH (Greece)
Paul Scherrer Institut (Switzerland)
Research Centre Jülich (Germany)
University of Antwerp/EMAT (Belgium)
University of Basque Country/PSMG (Spain)
University of Edinburgh/COSMIC (United Kingdom)
University of Hamburg (Germany)
University of Lund (Sweden)
University of Vigo (Spain)

Other ESMI institutions:

Adam Mickiewicz University (Poland)
Biolin Scientific (Finland)
LS Instruments GmbH (Switzerland)
Malvern Instruments Ltd (United Kingdom)
University of Twente (The Netherlands)
University of Leeds (United Kingdom)
VisiTech International (United Kingdom)

ESMI is negotiating support from the European Commission under the 7th Framework Programme. The EU Grant Agreement has not yet been signed.



ESMI Coordinator Prof. J. Dhont
ESMI Project Manager Dr. F. Carsughi
Forschungszentrum Jülich GmbH, Germany



About SoftComp



SoftComp is a Network of Excellence – a tool developed under the 6th Framework Programme of the European Commission dealing with the integration of European research, with the intention of strengthening scientific and technological excellence. In particular, SoftComp aims to establish a knowledge base for an intelligent design of functional and nanoscale soft matter composites. It will do so by overcoming the present fragmentation of this

important field for the development of new materials at the interface of non-living and living matter, where the delicate principles of self-assembly in polymeric, surfactant and colloidal matter prevail. This Network of Excellence has created an integrated team that is able to activate the European potential in soft matter composite materials and thus disseminate excellence through extensive training and knowledge transfer schemes. Since December 2009, when EU funding came to an end, Softcomp is

a self-supporting consortium consisting of 38 research groups belonging to 33 different institutions.

SoftComp partners details

www.eu-softcomp.net/about/part

Registration

If you would like to register under the SoftComp portal, please contact:

f.h.bohn@fz-juelich.de

Second International Soft Matter Conference ISMC-2010: A Review

*Juan de Vicente and R. Hidalgo-Álvarez,
Applied Physics Department, University of Granada, Granada, Spain*



The International Soft Matter Conference 2010 was held in Granada, Spain at the Granada Exhibition Conference Centre on 5 to 8 July 2010. The Biocolloid and Fluid Physics Group led by Prof. R. Hidalgo-Álvarez planned and organized an international conference focusing on multicomponent composites and mixtures, wide length and time scales, hierarchical metastable structures

and many interacting degrees of freedom, leading to complex structures, phase behaviour and dynamics.

The conference brought together students and scientists interested in soft matter systems such as polymers, colloids, surfactants, membranes, biomaterials and their composites. Soft matter implies high sensitivity to external fields and ubiquitous and significant

non-equilibrium phenomena, and requires an interdisciplinary approach connecting theoretical, computational and experimental physics, physical chemistry, materials science and biology. A special focus of discussion in this context was the application of soft matter concepts to biological and biomimetic systems. In this field, basic science and a broad range of modern technological applications also encompassing many aspects of nanoscience are closely related. These links were emphasized during the conference, thereby fostering an exchange between academia and industry.

The conference was therefore organized along themes associated with biophysics, colloids, polymers, surfaces and interfaces, membranes, dynamics soft nanotechnology and self-assembly. There were four types of presentations: plenary, invited, contributed talks, and posters. These were chosen by the Programme Committee in cooperation with the Advisory Board. In numbers, the conference registered a total of 570 participants presenting 8 plenary lectures, 38 invited talks, 88 oral communications and 561 poster communications

The ISMC 2010 conference benefited from technical and financial support from the Spanish Ministry of Innovation and Science, the Andalusia Government, the University of Granada, the Donostia International Physics Center, Forschungszentrum Jülich, the Science Park and the SoftComp European Excellence Network.

Plenary speakers were:

- L. M. Liz-Marzán, Colloids
- P. Schurtenberger, Dynamics of complex fluids
- S.A. Safran, Hybrid lipids
- M. Olvera, Ionic membranes and gels
- D. Langevin, Foams stabilized by particles
- C. Bustamante, Homeostasis and rheology of the cellular membrane
- K. Landfester, Soft nanotechnology
- H. Watanabe, Entanglement dynamics in homopolymer liquids

Vacancies

PhD position in the area of computer modelling Martin Luther University Halle

The Theoretical Polymer Physics group at Martin Luther University Halle has an open PhD position in the area of computer modelling of the structure and dynamics of polymer nanocomposites.

Contact: Wolfgang.Paul@physik.uni-halle.de

A post-doc position

... available in the field of large-scale polymer dynamics under confinement investigated by neutron scattering, dielectric spectroscopy and simulation. The work will be done partly in Jülich, Germany, and partly in San Sebastian, Spain.

Contact: neutronsattering@fz-juelich.de
http://www.fz-juelich.de/iff/d_ins_stellen/

PhD student position

As a part of the recently launched Marie Curie Initial Training Network COMPLOIDS, a 3-year PhD student position is available immediately at Jožef Stefan Institute in Ljubljana, Slovenia (www.ijs.si).

Contact: primoz.zihel@ijs.si

Post-doctoral position

A position for a post-doctoral research associate is available at ETH Zürich, in the Department of Civil and Environmental Engineering, in the new group of Microstructure and Rheology headed by Emanuela Del Gado of the Institute for Building materials (<http://www.ifb.ethz.ch/micro>).

More information can be obtained at the site above and in particular at the link:

<http://www.ifb.ethz.ch/micro/jobs/index>

Contact: delgadoe@ethz.ch

Post-doctoral position

The group for "Theory of Soft Condensed Matter" at the university of Luxembourg offers a PhD position: Simulation of Crystallization in Polymermelts under Shear-Flow.

The topic of the PhD thesis will be a study of crystallization of a polymer melt under shear by a combination of classical MD and a novel non-equilibrium rare-event sampling method. The thesis will be carried out in close collaboration with the experimental physics group at the "Laboratory for soft matter and advanced materials" at the university of Luxembourg. It is funded within the CORE-programme of the FNR (Luxembourgish research association). (There is an opening for an experimental PhD in the context of this programme, too. If you are interested, please contact Prof. R. Sanctuary) We are looking for a candidate with a Master/Diploma degree in Physics, Materials Science or a related subject. The candidate should have experience in programming and computer simulation techniques and preferably a background in statistical mechanics.

Good knowledge of English is required.

Knowledge of French and German would be useful.

Contact: Tanja.Schilling@uni.lu

Coming Up...

SoftComp Conferences & Workshops	Date
International Workshop on Rheology and Structural Design of Complex Fluids Leuven, Belgium Prof. J. Vermant jan.vermant@cit.kuleuven.be	7-8 Feb 11
IFF Spring School on Macromolecular Systems in Soft and Living Matter Jülich, Germany Prof. J. Dhont j.k.g.dhont@fz-juelich.de	14-25 Feb 11
7 Course on Epigenetics Paris, France Dr. G. Almouzni Genevieve.Almouzni@curie.fr	9-16 Mar 11
International Workshop on Dynamics in Viscous Liquid Rome, Italy Prof. F. Sciortino francesco.sciortino@phys.uniroma1.it	30 Mar - 25 Feb 11
Mesoscale hydrodynamic simulation of non-equilibrium and driven soft-matter systems Jülich, Germany Prof. Gerhard Gompper g.gompper@fz-juelich.de	9-11 May 11
School on Nanomaterials and Their application to Biology and Medicine Poznan, Poland Prof. S. Jurga stjurga@amu.edu.pl	12-18 Apr 11
SoftComp Annual Meeting 2011 Heraklion, Crete, Greece Flavio Carsughi f.carsughi@fz-juelich.de	16-18 May 11
Laboratory Course on Dielectric Spectroscopy San Sebastian, Spain Prof. A. Alegria angel.alegria@ehu.es	30 May - 4 Jun 11
3rd Montpellier Workshop on Reinforcement and Nanocomposites Montpellier, France Dr. Julian Oberdisse oberdisse@lcvn.univ-montp2.fr	2-3 Jun 11
International Workshop on Nanoplasmonics for Energy and the Environment Sanxenxo, Spain Prof. L. Liz-Marza lmarzan@uvigo.es	8-10 Jun 11

Coming Up (continued) ...

SoftComp Conferences & Workshops	Date
ECIS European Student Conference Falkenberg, Sweden Dr. A. Howe AHowe2@slb.com	14-17 Jun 11
NMR Ampere School Zakopane, Poland Prof. S. Jurga stjurga@amu.edu.pl	19-25 Jun 11
13th European School on Rheology Leuven, Belgium Prof. C. Clasen christian.clasen@cit.kuleuven.be	5-9 Sept 11
15th JCNS Laboratory Course on Neutron Scattering Jülich and Garching, Germany Dr. R. Zorn r.zorn@fz-juelich.de	5-16 Sept 11
Juelich Soft Matter Days Bonn, Germany Prof. J. Dhont j.k.g.dhont@fz-juelich.de	15-18 Nov 11
Mainz Materials Simulation Days Mainz, Germany Prof. M. Öttel ettelm@uni-mainz.de	25-27 Nov 11
Laboratory Course on Dielectric Spectroscopy San Sebastian, Spain Prof. A. Alegria angel.alegria@ehu.es	28 May - 2 Jun 12

Personalia

On 1 June 2010, Christos Likos,

formerly Professor of Physics at the University of Düsseldorf, took up a new position as Professor of Multiscale Computational Physics at the Faculty of Physics of the University of Vienna, Austria.

On 1 October 2010, Peter Schurtenberger,

formerly Professor of Physics and Nanoscience at the University of Fribourg, Switzerland, started as a Professor at the Division of Physical Chemistry, Department of Chemistry, University of Lund, Sweden.

On 1 April 2011, David Head,

formerly post-doc at Theoretical Soft Matter and Biophysics, Institut of Solid State Research Forschungszentrum Jülich, has accepted a tenure-track fellowship for a Lecturer position in Theoretical and Translational Biofilm Research in the School of Computing at Leeds University, UK.

For more frequently updated information, please see also the SoftComp web pages...

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SoftComp Events: www.eu-softcomp.net/news/cal

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