

Network of Excelline

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Editorial

The European Networks of Excellence aim at creating durable and sustainable structures bringing together eminent scientists in their respective fields in order to strengthen the European research area. SoftComp has succeeded in this essential task by completing a new consortium agreement (CA) which goes far bevond the funding period of the EU. In this agreement, the partners agree to support the sustainable network structure by contributing substantial funds. With the exception of a very small number of partners, most members of the SoftComp consortium have agreed to this new CA. We believe this is a great success for SoftComp showing its quality and demonstrating the benefits it offers to all its members. This new CA has also been signed by a number of new members who have not benefited from the EU funding so far – again, a demonstration of the attractiveness of SoftComp.

Finally we would like to take this opportunity to wish you all a happy and successful New Year.

Hugo Bohn & Dieter Richter 🧲

In This Issue

Vitrification and Melting Scenarios for Soft Colloidal Mixtures

About SoliComp	4
International Soft Matter Conference 2007	5
First Anniversary of the SoftComp Cluster	6
SoftComp Workshop in San Sebastian, Spain	
The SoftComp Research Road Map	7
Vacancies · Coming Up · Credits/Disclaimer · Editorial Details	8



Vitrification and Melting Scenarios for Soft Colloidal Mixtures: The Star Polymer Paradigm



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Glass transitions have captured the interest of a broad community of scientists, experimentalists and theorists alike for a long time. Both from the fundamental point of view and with regard to applications, the fact that when approaching vitrification materials under suitable conditions (typically high concentrations and/or low temperatures) display an increase of their viscosity that encompasses many orders of magnitude, has attracted great interest in the hope of gaining a deep understanding of the associated physics. A model system whose vitrification has been intensively studied, is that of colloidal hard spheres.^[1,2] When the volume fraction of the latter slightly exceeds 50%, the (metastable) hard sphere fluid undergoes a dynamical arrest towards a system that has the translational invariance of a fluid but the macroscopic rigidity of a crystal. This is a glass, i.e., a thermodynamically metastable state of matter (compared to the stable crystal), which inherits the structural spatial correlations present in the fluid phase but which does not flow; or, to put it more precisely, it flows at time scales vastly exceeding those of experimental observation, so that one can make the approximation that the dynamical correlations in the system are frozen. Translated into mathematical terms, this means that if a disturbance of the homogeneous density of the system is made, with a wavenumber k at time t = 0, this persists at all times, theoretically to t = infinity. This need not be true of all possible values of k; it suffices that some modulations don't die out in order to be able to call the system a glass. In the ergodic liquid, on the other hand, a fluctuation of the density at any wavenumber k will die out to zero as time increases.



The Star Polymer Paradigm (continued)

What is the origin of the glass transition for hard spheres? A large number of experimental and theoretical studies on the problem have led to the interpretation that the crowding of hard spheres at sufficiently high concentrations is responsible for the arrest, leading to the famous caging effect.[3,4] Particles mutually trap each other in cages that are collectively formed. As they cannot leave these restricted cages, diffusion ceases.^[5] Flow thus becomes arrested and the system shows rigidity against shear, which is a characteristic of solids for, as we know, fluids cannot be sheared. This paradigm of caging can also be carried over to soft colloids, such as star polymers of a sufficiently high number) functionalization (arm $f(\text{see Fig. 1})^{[6-8]}$.



Indeed, both experiment ^[9,10] and theory ^[11] have long established that star polymers with f exceeding, roughly, 50 arrest into a glassy state above their overlap concentration because of crowding and caging effects. The most convincing evidence of this came from experiments ^[9,10] demonstrating that an increase in temperature, which swells the stars and thus enhances crowding, leads to a *reversible glass formation*, i.e., to ergodic-to-nonergodic transitions that can be crossed by changing the temperature. This is consistent with the mode-coupling theory analysis carried out in ^[11] and the associated mapping of high-functionality stars into hard spheres.



Perhaps a naive, but descriptive representation of the caging of hard and soft colloids can be captured in Fig. 2, where the distinct differences (namely the star interpenetration) are clearly identified. This has profound consequences as will become evident below.

So, are star polymers then just an effective realization of hard sphere systems? Nothing could be farther from the truth, for star polymers are very versatile, flexible, and extremely rich in phenomenology and vitrification scenarios, as recently demonstrated by an ongoing collaboration between the SoftComp partners FORTH and the University of Düsseldorf, involving also E. Zaccarelli, F. Sciortino and P. Tartaglia from the University of Rome La Sapienza. To begin with, the star glass can be melted by the addition of smaller polymer chains, as was demonstrated by a FORTH/Düsseldorf collaboration in 2002 [12]. In fact, this might sound not so different from the well-known melting of the hard sphere glass upon addition of non-adsorbing polymer ^[13,14], but there are some crucial differences. Whereas in the melting of the hard sphere glass the added polymer induces depletion attractions between the hard spheres, which lead to cage deformation and opening up. in the case of star/linear mixtures there is no net attraction induced the stars by the chains: instead, the depletion effect of the chains has the net result of reducing the star-star repulsion, leading to a softening (but not a deformation!) of the star cages. Eventually, at linear chain concentrations higher than those needed to melt the star glass, depletion attraction takes place.^[15] Therefore, upon adding depletant to the hard sphere/polymer mixture the cage opens up whereas in the star/linear mixture the cage softens. It oscillates and *breathes* more violently as chains are added. In addition, whereas in hard sphere/polymer mixtures the melting of the glass ceases when the polymer-to-colloid ratio exceeds 10 % [16], in star/chain mixtures it persists up to size ratios of 50 %, thus showing the considerably greater possibility of tailoring the rheology of soft glasses than that of hard ones. In fact, a detailed investigation of the statics and rheology of star/linear mixtures is the subject of an ongoing FORTH/ Düsseldorf collaboration^[17].

But now what happens if we add in a glass of star polymers not linear chains but rather small star polymers that are chemically identical to the glassforming species but physically distinct? In particular, we wish to know what happens if the additives are smaller in two senses: both of a smaller functionality f_2 and of a smaller size, thereby defining the size ratio q between the two species. The question has been studied intensively by a combination of rheology (FORTH) and simulation and mode coupling theory (Düsseldorf and Rome) in the last few years and it is indeed one of the core regions of SoftComp: the rheology of soft matter composites. Through a fruitful exchange of ideas, suggestions and last but not least - puzzles between





experiment and theory, a consistent picture of the effect of soft additives on soft glasses has started to emerge. In what follows, a brief description of the phenomenology and physics involved will be given.

Suppose first that you add a small quantity of small stars with a large size asymmetry, q < 0.3 or so, to a glassy matrix of big stars. Here, the additives are small enough to pass through the holes left by the glassy matrix. Seen as a sub-system, they remain ergodic throughout and, once their concentration is sufficiently high, they have enough energy to kick around the cages of the big stars until they break up. Similarly to the glass melting induced by linear chains and discussed above, the small stars act as depletants that restore ergodicity to the big stars and bring the whole mixture to melting. For a sketch of the physical situation, see Fig. 3. As the depleting power of the additives grows with their size, one expects that the larger the qthe smaller the amount of additives necessary to melt the glass, and this is indeed the case for sufficiently small f_{1} which is confirmed both by experiment and by mode coupling theory.

However, the depletion mechanism does not act under all circumstances. As mentioned above, the additives have to be mobile enough (i.e. *small* enough) to go through the holes of the big stars. If this is not the case. the depletion picture breaks down altogether. In this case, a mode coupling theory approach in which the big stars are treated as the only possible glass formers in the system is not adequate any more. One has to incorporate into the theoretical treatment the possibility that the small stars will also become trapped in cages, since the big stars already restrict the amount of space available. Two competing mechanisms thus come into play: the smaller stars push the big ones more violently as they increase size but at the same time they are also rendered less mobile. So what happens at the end? It turns out that a novel state of glass appears, a double glass, in which both species are dynamically arrested in their mutual

Figure 4



cages, see Fig. 4. This reverses the trend mentioned above and pushes the glass region in the size ratio/additive concentration diagram to higher concentration values.

Finally, one can increase the additive concentration more and more in the high q-regime, thus asking the question of whether the double glass persists for ever. Here, the mixture has another surprise. It does not! At some additive concentration, the mutual cages start pushing each other so strongly that, in

combination with the fact that the stars are *soft colloids*, this leads once more to a restoration of ergodicity and a break up of the glass, see Fig. 5.



Fluidized state of a binary star mixture at high concentration of the depletant. The vectors suggest random motion of both big and small stars.

The overall kinetic phase diagram of soft star-star composites, displays, as a result, a nonmonotonic, U-shaped line separating the nonergodic (bottom) from the ergodic (top) region, as shown in Fig. 6.^[18,19]



Experimental (top) kinetic phase diagram of normalized depletant concentration ($\rho_2\sigma_1^{-1}$) vs. size ratio (q) for different functionalities of the depletant (f_2). Except where indicated, the big star has f_1 =267. The respective theoretical diagram is also shown (bottom). Taken from Ref. ^[18].



The Star Polymer Paradigm (continued)

The vitrification and melting scenarios we sketched above have no counterparts in hard colloids, as they crucially depend on the softness of the involved objects. Soft mixtures are indeed very promising in terms of the variety of their glassy states and the possibilities of modifying them and SoftComp offers an optimal research platform on which experiment and theory have the chance to come together in a fruitful collaboration. A collaboration which, in fact, is going on with undiminished energy.

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Acknowledgements

We are grateful to our colleagues at FORTH, Düsseldorf and Rome, and especially E. Stiakakis, C. Mayer and E. Zaccarelli for very fruitful collaborations. Figs. 1 and 3-5 were kindly provided by E. Stiakakis and C. Mayer, respectively.

About SoftComp

SoftComp is a Network of Excellence – a tool developed under the 6th Framework Programme of the European Commission dealing with the integra-

tion 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 selfassembly in polymeric, surfactant and colloidal matter prevail. This Network of Excellence will create 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.

SoftComp partners

www.eu-softcomp.net/about/part

Registration

More than 300 participants have already registered. If you would like to register contact: **f.h.bohn@fz-juelich.de**



triangle are, roughly

speaking, amphi-

abscissa and elongation or flexibility

as the ordinate. Let

me illustrate this by

following the left-

hand side of the tri-

angle from colloids

to flexible polymers.

Traditionally, colloids

are hard, spherical

particles. However,

there are also rod-

like colloids. As the

aspect ratio, the

ratio of rod length

to rod diameter,

as

the

philicity

International Soft Matter Conference 2007: A Review

Gerhard Gompper (Chairman of Program Committee) Institut für Festkörperforschung, Forschungszentrum Jülich

Why don't you organize a big international soft matter conference?

This is the question the SoftComp International Advisory Board (IAB) raised during its first meeting in Ancona in May 2005. The response of the Network Coordination Council (NCC) was that we were already organizing an annual international soft matter conference, the Jülich Soft Matter Days. The topic was then not discussed further. However, after thinking about this suggestion for a while, we had the feeling that such a conference would indeed serve the goal of European integration and dissemination of research results by a Network of Excellence (NoE) exceedingly well; furthermore, financial support from SoftComp would greatly facilitate the organization of such a conference. Therefore, in its autumn meeting, the NCC discussed the proposal of an International Soft Matter Conference in Aachen in 2007, and fully agreed to support such an endeavour and the conference finally



Announcement of the International Soft Matter Conference 2007



took place on October 1-4, 2007. The conference announcement is shown in Fig. 1.

With the large number of conferences organized every year on topics like polymer chemistry and polymer physics, colloid chemistry and colloid physics, surfactants in solutions, etc., the aim of an international soft matter conference clearly had to be to bring together a balanced mixture of scientists working on all kinds of soft materials – such as polymers, colloids, surfactants, membranes, biomaterials and their composites.

The need for a unified view of soft matter systems is threefold.

First, it has been recognized over the past years that colloids, polymers and surfactants are by far not as such distinct materials as previously assumed. Indeed, there is essentially a continuum of molecules and systems, which fills the triangle of materials illustrated in Fig. 2. The two main axes of this

becomes larger, rods typically become more flexible. An example is the fd-virus shown in Fig. 2. For even larger aspect ratios, the length exceeds the persistence length; this is the regime of semi-flexible polymers, of which DNA is an example of enormous importance. Finally, in the limit of very small persistence lengths, we arrive at the classical, flexible synthetic polymers.

Second, mixtures of several components of colloidal, polymeric or amphiphilic character are becoming increasingly important, because they provide the opportunity to adjust and control material properties. Well-known examples are the depletion interaction between colloidal particles induced by polymers in solution, the intriguing mesophases in mixtures of spherical and rodlike colloids, the tuning of membrane properties by anchored polymers and amphiphilic block copolymers, or the modification of the properties of polymer melts by the addition of colloidal



International Soft Matter Conference 2007 (continued)

particles to form nano-composites. Finally, biological and biomimetic systems share many macromolecules and properties with soft matter systems. Indeed, the application of physical concepts and ideas to biological systems has become one of the most intense fields of activity in soft condensed matter in recent years.

With more than 600 participants from about 35 countries (see Table I), 8 plenary talks, 42 invited talks, 85 contributed talks, and about 400 posters, the amount of information provided during the conference was much too large to be summarized in a few lines here. Instead, I hope that the list of the plenary speakers and the titles of their talks will give a feeling of the exciting atmosphere and the intensity of the discussions during the conference:

M. Cates (University of Edinburgh, UK) Lattice Boltzmann simulations of nonequilibrium complex fluids.

6

- W. Gelbart (University of California, Los Angeles, USA)
- *Physical aspects of viral infectivity.*L. Leibler (ESPCI, Paris, France)
- Supramolecular plastics and rubbers.
- G. Maret (University of Konstanz, Germany) · Elasticity, phonons and melting of colloidal crystals.
- D. Nelson (Harvard University, USA) Neutral mutations and gene surfing in microorganisms.
- D. Roux (Saint-Gobain, Courbevoie, France) • Glass technologies: colloids and active surfaces.
- H. Tanaka (University of Tokyo, Japan) · Mechanical instability in phase separation, fracture, and cavitation.
- D. Weitz (Harvard University, USA) Dripping, jetting, drops and wetting: Structuring new soft materials with microfluidics.

Due to the great interest and overwhelming participation in the conference, the program committee came to the



conclusion that it would be a good idea to organize an international soft matter conference every three years in the future. Participants were therefore asked for proposals to host the the next conference. These proposals were presented in a plenary session. A vote showed the greatest support for the proposal from Granada (Spain), which will therefore be the location of the International Soft Matter Conference 2010. I am very much looking forward to this meeting of the soft matter community.

First Anniversary of the SoftComp Cluster



One year ago, the opening ceremony for the SoftComp cluster was held at the Jülich Supercomputing Centre (JSC), the former ZAM.

In the meantime, 27 scientists have access to the cluster and all of the eight funding member groups are represented. In 2007 about 25,000 jobs with an overall cpu time consumption of 1.5 million hours were run.

Some events in the course of the year:

May: An express queue was established, allocating four nodes for small jobs requiring less than 4h of cpu time and 4 GB of memory.

July: The standard switch was replaced by a separate Cisco switch, thus improving the net-

work performance. The data transfer was considerably accelerated, e.g. copying data from a local disk on the frontend to all 66 nodes can now be done at a speed of 40 MB/s. The limiting factor is now the local disk on the nodes.

September: Capacity problem with the */home filesystem*. As a result filesystems had to be re-configured and a disk quota was introduced for each user group.

November: Quota arrangement was

enforced with respect to both disk space and compute time.

The prospects for 2008 are promising. Procurements have been launched to extend the cluster. At the beginning of 2008 an upgrade to 126 nodes in total is scheduled, resulting in a peak performance of nearly 2.5 TFLOPS.

This extension is partly funded by a SoftComp group member now starting to invest in the cluster. The major fraction of the costs is financed by an initiative of the German Federal Ministry of Education and Research (BMBF) to promote applications in economics and science using grid infrastructures. In this context, a fast InfiniBand switch as a fast network interconnect will be installed for the additional nodes offering the chance to run parallel programs efficiently. *W. Homberg*





Clock Explosion by Salvador Dali. Sometimes art can also express physical concepts

In the spirit of SoftComp, looking for universal features of different classes of soft materials is one of the major goals. This inter-area (topical) workshop aimed at discussions of the properties of the slow dynamical processes taking place in different systems including polymers, colloids, biological molecules, micelles, liquid crystals. The main properties of the dynamics related to the glass transition, functionality of proteins, yielding mechanisms, reptation in polymers of different architectures, ageing etc. were addressed. A very rich variety of systems and phenomena were thus considered; also noteworthy was the number of experimental techniques involved in the papers presented (dielectric and mechanical spectroscopy, NMR, neutron scattering, tracer diffusion, dynamic light scattering including novel developments with laser-speckle imaging, microscopy). From a theoretical point of view, the tremendous progress made in the last few years in this direction was obvious as well. We can say that the workshop was very worthwhile, giving a broad idea of the state of the art of this subject in the different areas of SoftComp. Arantxa Arbe 5

The SoftComp Research Road Map

Novel and fascinating research areas are emerging at the interface between physics, chemistry and biology. SoftComp research investigates the properties of macromolecules, colloids and surfactants in solution and in the bulk, their interactions and aggregation, and their cooperative behaviour on nano-to-micrometre length scales. The goal of the SoftComp partners is to establish a quantitative and theoretical understanding of the complex structures and mechanisms governing soft matter composites and related biological systems. The SoftComp research themes are highly complex and require great instrumental efforts and close cooperation between different academic disciplines and between theoreticians and experimentalists.

The medium-to-long-term prospects for SoftComp research are discussed in detail in the Research Road Map, an Annex to the new Consortium Agreement.

Three main research directions are identified there:

1. Molecular engineering and flow rheology

In the quest to optimize and control materials formulations and/or processing, viscoelasticity and flow-induced structure appear to be of foremost importance. This research direction attempts to elucidate the microscopic origin of the rheological response of soft matter, in connection with the interactions. This is needed for the rational design of novel composite materials with optimized properties, which can be used in a wide range of applications from plastics to cosmetics and from food to pharmaceuticals.

2. Self-assembly and structure formation

The structural properties of soft matter systems are determined by the mesoscopic building blocks and the weak interactions between them. Soft matter composites offer a new, unique possibility of modifying and controlling this structure, and thus the mechanical, thermal, optical, rheological and dynamical properties of these materials. There are different ways of organizing soft materials: self-assembly of specifically designed building blocks, non-equilibrium structure formation by external fields, or by active biological processes. Self-assembly is mainly important in amphiphilic and biological systems. Non-equilibrium structure formation occurs in colloids or polymers in flow, but also in wormlike micelles and network-forming polymer-surfactant mixtures. Dispersing colloids in polymer matrices or at liquid interfaces is an important approach for tailoring nanocomposite properties. Soft matter concepts are also essential for understanding the complex machinery of biological systems at the cell level, in particular their non-equilibrium behaviour.

3. Slow dynamics

Both the size of the mesoscopic objects as well as their interactions give rise to slow dynamics. Particularly interesting are gelling and glass transition phenomena, which are common themes for many soft matter systems. Apart from soft matter the nature of the glass transition is one of the most important and challenging open questions in condensed matter science and is also investigated in many other contexts. Also geometric or topological interactions lead to slow dynamics which are relevant for the rheological and mechanical properties of soft matter systems. As a major result, a big step towards a basic understanding of glass transition and gelling phenomena is expected relating them to molecular properties with important consequences for the other two research directions. Constitutive equations based on microscopic insights will provide predictive tools for controlling the state of a composite mixture and its flow. The increasing complexity of an environment and its impact on the slow dynamics will help to create new materials with new rheo-mechanical properties.





Vacancies

Postdoc 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. www.fz-juelich.de/iff/e_ins_stellen **Contact:** neutronscattering@fz-juelich.de

Position available ...

... in a joint research project between ESPCI (Paris) and FORTH (Heraklion) on ageing of soft colloids. This collaborative experimental investigation will address the effects of interactions on ageing and will attempt to elucidate the microscopic mechanisms of the evolving slow dynamic processes. The use of fluorescence microscopy, dynamic light scattering and rheology is planned. Duration: 1 year, with the possibility of an extension for another year. **Contact:** ESPCI: Michel Cloitre

(michel.cloitre@espci.fr) · FORTH: Dimitris Vlassopoulos (dvlasso@iesl.forth.gr)

Postdoc position (Slow dynamics and ageing of star-like micelles and mixtures) ...

... the Institute of Solid State Research, (IFF, Forschungszentrum Jülich, Prof. Dr. D. Richter, www.fz-juelich.de/iff/e_ins) in collaboration with the Foundation of Research and Technology Hellas, (FORTH, Heraklion, Greece, Prof. Dr. G. Fytas), is offering an 18-months postdoctoral position, which will be equally distributed between the two sites Jülich and Heraklion. The applicant should have a PhD in experimental physics/ physical chemistry, experience with scattering techniques: a well-founded theoretical background in soft matter science will be advantageous. **Contact:** j.stellbrink@fz-juelich.de

Tel. +49-2461-61-6683

Postdoc position Structure Formation and Rheology of Active Gels ...

... available for a joint research project between Juelich and Twente. The goal of the project is to apply two different mesoscopic simulation techniques to investigate the behavior of gels of semi-flexible polymers (like aktin), which are crosslinked by motor-proteins. A background in statistical mechanics and familiarity with simulation techniques is be advantageous. For more information see www.fzjuelich.de/iff/d_th2_dipdoc **Contact:** FZ Juelich: Gerhard Gompper (g.gompper@fz-juelich.de).

Twente: Wim Briels (w.j.briels@tnw.utwente.nl)

Coming Up...

SoftComp Conferences & Workshops	Date
International Workshop on Computational Physics and Materials Science Progress in Computational Electronic Structure Theory - Gustav- Stresemann-Institut, Bonn, Germany http://i2cam.org/conference/cpest/	10-12 Jan 08
39th IFF Spring School Soft Matter - From Synthetic to Biological Materials - Jülich, Germany www.fz-juelich.de/iff/fs2008	03-14 Mar 08
CODEF II - Colloidal Dispersions in External Fields Gustav-Stresemann-Institut Bonn, Germany www.codef.de	31 Mar - 02 Apr 08
Collective Effects in Cell Biophysics Les Houches School, France Contact: P. Bassereau and J.F. Joanny http://houches2008.curie.fr/	06-11 Apr 08
Annual SoftComp Meeting Riva del Garda, Italy • NA Meetings • Industrial Meeting • EU Report Meeting • NGB04 Meeting • NCC14 Meeting	05-08 May 08 05 May 08 06 May 08 06-07 May 08 08 May 08 08 May 08
Annual Meeting of the American Crystallographic Association Knoxville; Tennessee http://neutrons.ornl.gov/conf/aca2008	31 May - 05 Jun
9th European Summer School on Scattering Methods Applied To Soft Condensed Matter Bombannes, Gironde, France www.ill.eu/bombannes/	07-14 Jun 08
8 th International Meeting on Thermodiffusion Gustav-Stresemann-Institut Bonn, Germany www.fz-juelich.de/iff/IMT8	09-13 Jun 08

Coming Up (continued) ...

SoftComp Conferences & Workshops	Date
The XV th International Congress on Rheology Monterey; California, USA http://www.rheology.org/ICR2008	03-08 Aug 08
Gordon Research Conference Magnetic Nanostructures Centre Paul Langevin Aussois, France http://www.grc.org/programs.aspx? year=2008&program=magnano	31 Aug - 05 Sep 08
Jülich Soft Matter Days 2008 Gustav-Stresemann-Institut Bonn, Germany www.fz-juelich.de/iff/jsmd2008	12-14 Nov 08

Personalia



SoftComp, and in particular the Jülich Soft Matter Groups, congratulate **Prof. Peter Grünberg** on being awarded of the Nobel Prize 2007. **Prof. Peter Grünberg** (Jülich) and Albert Fert (Paris) were honoured for the discovery of the giant magnetoresistance (GMR).

Leibfried Prize for Sperm and Tiny Rowers

Jens Elgeti was awarded this year's Günther Leibfried Prize of Research Centre Jülich for communicating scientific findings in a comprehensible way – with prize money of € 3000 – on the basis of his particularly lively lecture presenting the topic of his PhD thesis: *The Swimming Behaviour of Sperm*. Dr. Elgeti works in the Theoretical Soft Matter Group at Jülich.

For more frequently updated information, please see also the SoftComp web pages... Vacancies: www.eu-softcomp.net/news/jobs · SoftComp News: www.eu-softcomp.net/news/ SoftComp Events: www.eu-softcomp.net/news/cal

SIXTH FRAMEWORK

PROGRAMME

Credits/Disclaimer

Acknowledgements: This research project was supported by the European Commission under the 6th Framework Programme through the Key Action: Integrating and Strengthening the European Research Area. Project title: SoftComp, Soft Matter Composites – An approach to nanoscale functional materials

Contract Type: Network of Excellence · Contract: NMP3-CT-2004-502235

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