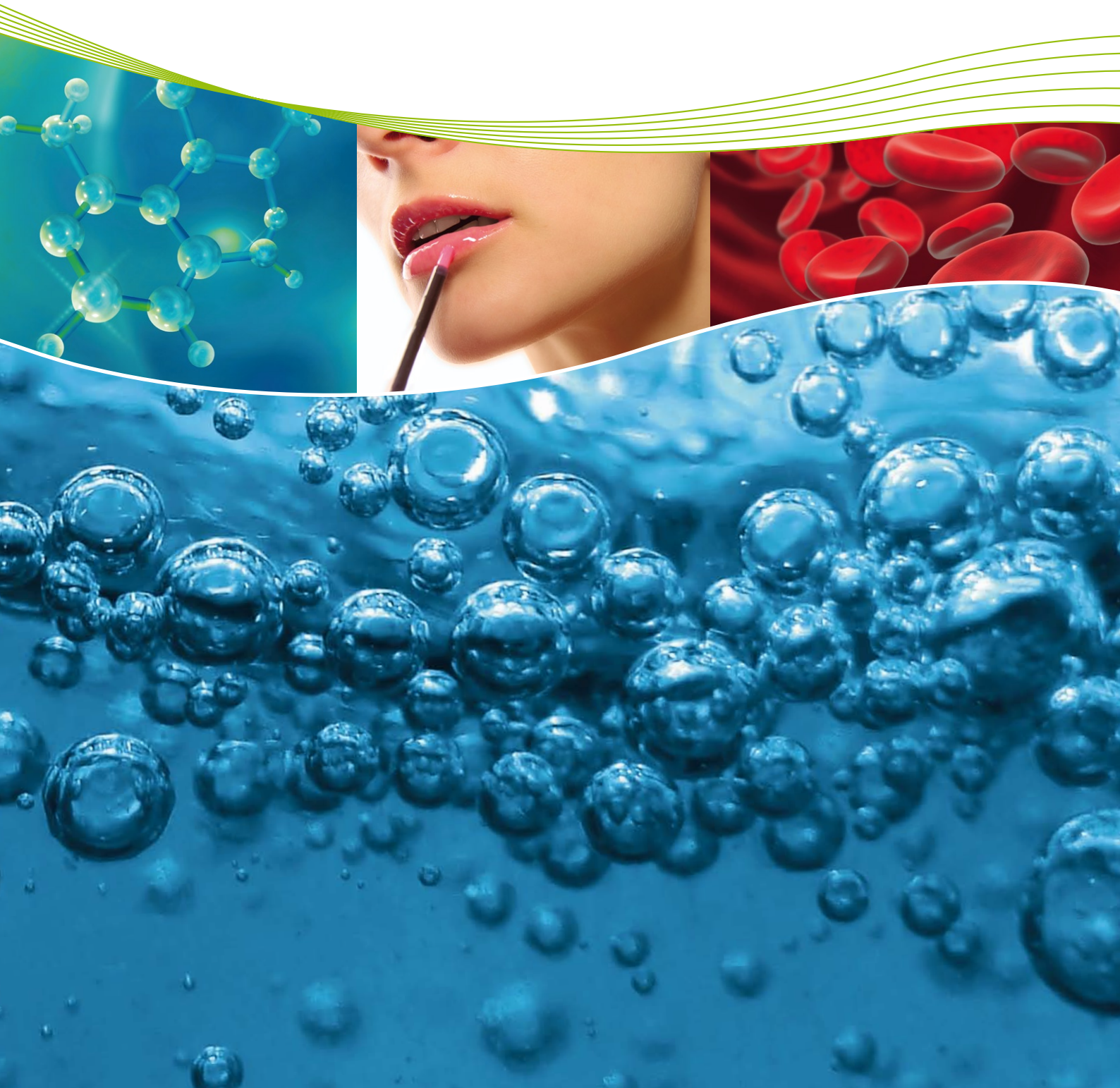


Soft-Matter Research for Society

The European Network of Excellence SoftComp





Foreword

Soft matter plays an important role in nearly every aspect of our daily lives and soft-matter research is a driving force for a broad range of innovation fields. You will find many examples of this on the following pages. Despite its undisputed importance, the soft-matter research landscape used to be fragmented. Its various subfields included surfactants, polymers, colloids, biomatter, etc., and different disciplines used to work on related topics such as physics, computational science, chemistry and biophysics.

In view of this unsatisfactory situation, a number of leading soft-matter groups in Europe decided to proactively work towards a change. For example, they organised regular workshops like the Jülich Soft Matter Days, which covered the entire spectrum of soft-matter science. To this end, the instrument of Networks of Excellence (NoE) within the EU Framework Programme FP6 proved very useful due to its similar objective, namely stimulation of the integration of European research with the goal of strengthening scientific and technological excellence in well-defined fields. In other words – bringing together a critical mass of resources and expertise to provide leadership.

With the founding of the NoE “Soft Matter Composites – An approach to nanoscale functional materials”, in the following referred to as SoftComp, in the spring of 2004, the strategic integration of soft-matter research in Europe was brought to a new level. Originally, 19 different academic institutions and five large European companies participated in SoftComp aiming at the creation of a knowledge base for the intelligent design of nanoscale soft-matter composites. A joint infrastructure was created enhancing the opportunities for each partner far beyond their own laboratory capabilities. This infrastructure provided access to the most advanced colloidal and polymer synthesis, and to experimental techniques such as state-of-the-art laboratories for spectroscopy, imaging and scattering

as well as a joint computer cluster for simulation work. The scientific work was organised according to five main priorities, each bringing together at least two soft matter fields and various disciplines. This endeavour was complemented by a focus on dissemination and the training of the next generation of soft matter scientists.

In due course, a number of further leading European groups in the field joined the Network and new European projects were initiated. The focus on education and dissemination generated numerous schools, workshops and conferences. The major event was the first International Soft Matter Conference in Aachen, Germany, which attracted more than 600 participants from all over the world. This great success stimulated a follow-up conference to be held in 2010 in Granada, Spain.

Looking back today, we are proud to say that the concept has developed extremely well. The integration created additional value, not only for the SoftComp members, but also for soft-matter research in general and therefore for society. You will find many examples of added value in this brochure.

With the EU funding coming to a close at the end of November 2009, the SoftComp partners agreed to maintain and finance the network for future activities. A consortium agreement was signed ensuring the continuation of SoftComp at least until the end of 2012. I am confident that also in the future major scientific results will emerge and that the joint activities will continue to provide further insights.

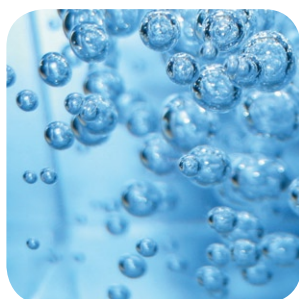
Contact

Professor Dieter Richter

Forschungszentrum Jülich

– SoftComp Coordinator –

 d.richter@fz-juelich.de



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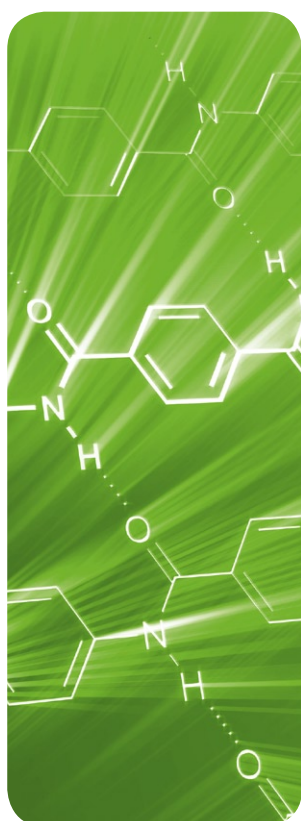
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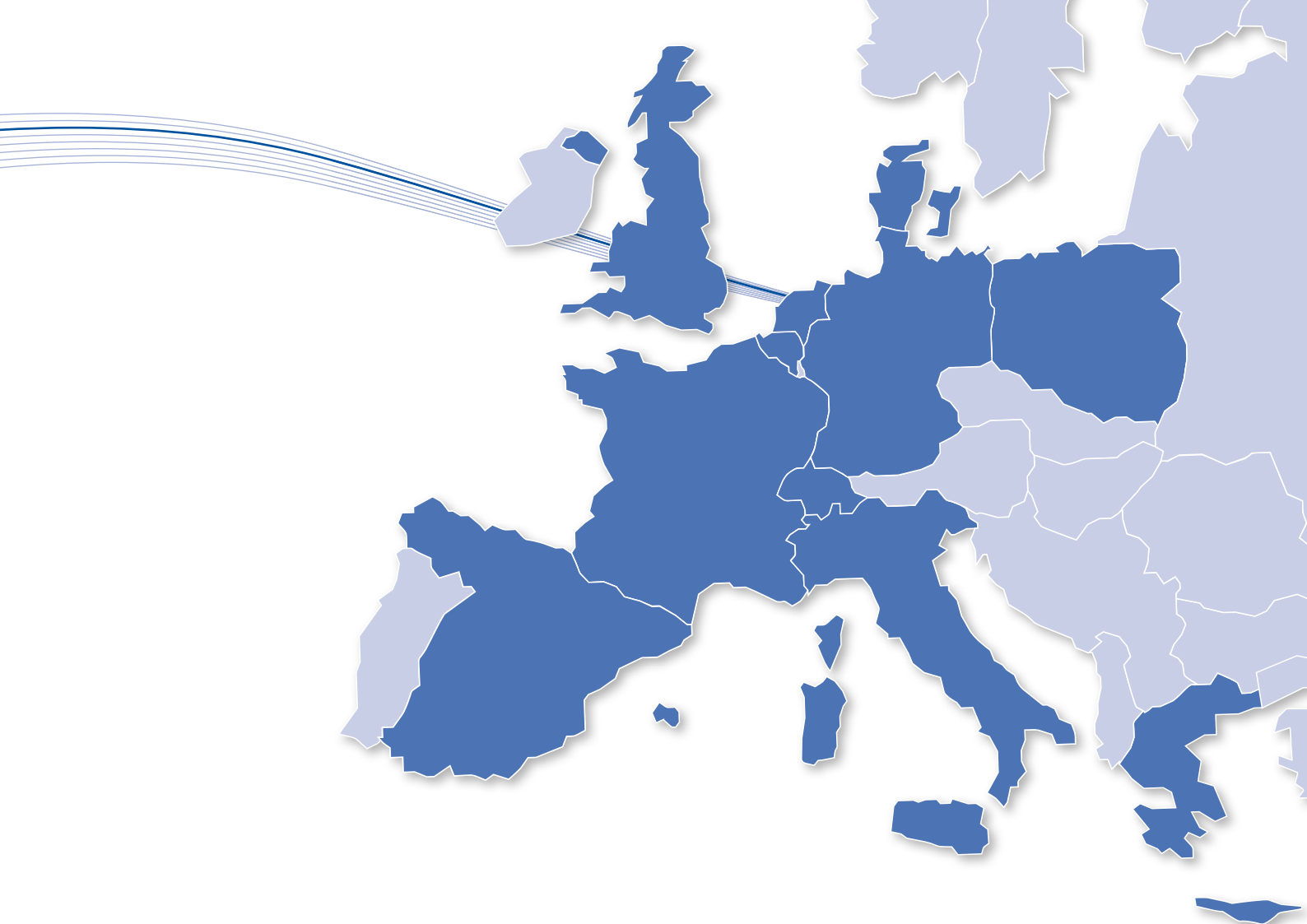
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SoftComp participants

Belgium

- Katholieke Universiteit Leuven
Leuven
- Université Catholique de Louvain
Louvain-la-Neuve

Denmark

- Danmarks Tekniske Universitet
Lyngby

France

- Centre National de la Recherche Scientifique (3 groups)
Bordeaux, Montpellier, Paris
- École Supérieure de Physique et de Chimie Industrielles
de la Ville de Paris (2 groups)
Paris
- Institut Curie
Paris
- Rhodia
Lyon

Germany

- BASF
Ludwigshafen
- Forschungszentrum Jülich (3 groups)
Jülich
- Georg-August-Universität Göttingen
Göttingen
- Heinrich-Heine-Universität Düsseldorf
Düsseldorf
- Johannes Gutenberg-Universität Mainz
Mainz
- Universität zu Köln
Cologne

Greece

- FORTH: Foundation for Research & Technology – Hellas
Heraklion

Israel

- Weizmann Institute of Science
Rehovot



All current participants, links to their respective homepages and contact information can be found on the SoftComp webpage:

www.eu-softcomp.net

Italy

- Università degli Studi di Roma “La Sapienza”
Rome

The Netherlands

- Dow
Terneuzen
- Universiteit Twente
Twente
- Universiteit Utrecht (2 groups)
Utrecht

Poland

- Adam Mickiewicz University
Poznań

Spain

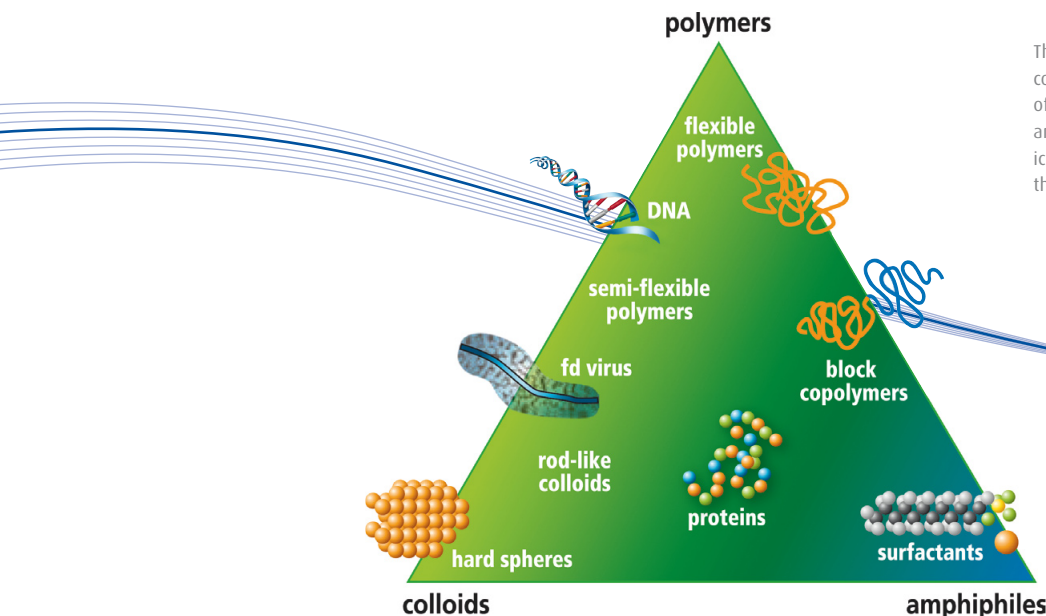
- Universidade de Vigo
Vigo
- Universidad del Pais Vasco
San Sebastián

Switzerland

- Université de Fribourg
Fribourg

United Kingdom

- Imperial College London
London
- Malvern Instruments
Malvern
- Schlumberger
Cambridge
- Unilever
Port Sunlight
- University of Leeds
Leeds
- University of Oxford
Oxford



The 'soft-matter triangle': it encompasses a broad, continuous range of materials, from colloidal suspensions of particles to flexible long-chain polymer molecules and amphiphilic, or soap-like, systems. Many biological systems such as proteins, DNA and viruses have the characteristics of all these soft-matter types

What are soft composites and why do we need to know about them?

Research into the world of soft matter is crucial to the economic health of Europe

Many everyday materials – food, medicines, cleaning agents, paints and plastics – are highly complex at the microscopic and molecular scale, often consisting of several kinds of molecules or tiny particles, which are held together by weak electrostatic forces in a highly organised way. At room temperature, these forces are usually not strong enough to prevent the materials from deforming under stress – which is why they are 'soft'.

Soft-matter composites encompass an ever-widening range of materials. They are based on the following:

• Polymers

These are long-chain molecules which can have a variety of shapes and chemical properties. As well as having useful bulk mechanical properties, they may stabilise a material or provide a strong coating for a surface.

• Amphiphiles including surfactants

These are molecules with a water-loving (hydrophilic) component and a water-hating (hydrophobic) hydrocarbon tail. This means that they dissolve in both oil and water and also

act as detergents. In solution, they self-organise into intricate structures such as minute vesicles called micelles.

• Soft colloids

These are suspensions, usually in a liquid or soft solid, of minute particles, which can be metals, minerals, gas bubbles, micelles or polymers, or any combination of these. Colloidal composites often form glasses or softer gels, consisting of a network of randomly arranged particles.

• Biological materials

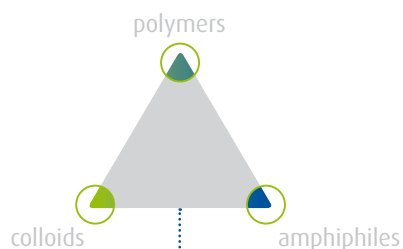
Living tissue represents the ultimate soft composite, with a hierarchical architecture composed of all of the above. Cell membranes are particularly interesting because they are composed of molecules that self-organise on the same principles as surfactants.

Not surprisingly, soft composites show complex behaviour. On gentle heating, or if subjected to shear forces (for example, by stirring), they may melt or change their molecular organisation – in other words 'change phase'. Even a small change in composition may

mean a big change in properties. Understanding this behaviour is important for several reasons: industry needs to know how to formulate and process soft materials, and what their long-term stability, or shelf-life is. Increasingly, soft composites are employed as self-organising biomimetic models for understanding biological processes. Furthermore, advanced functional composites with nanoscale and microscale structures, often inspired by biology, are now being designed for sophisticated applications in electronics and medicine. Finally, the subtle architecture and emergent properties of soft composites provide a fertile research area for understanding the organising principles of nature at the most fundamental scientific level.

Studying soft composites

The study of soft-matter composites is highly multidisciplinary, with physicists, chemists, biologists and engineers all involved. European institutes have had a long tradition in soft-matter research, which has been invigorated and consolidated through the outstanding theoretical advances made by the French Nobel Laureate Pierre-Gilles de Gennes and the



famous UK physicist Sir Sam Edwards. However, because of the broad nature of the investigations, in terms of experiment, theory and applications, research has been fragmented. For this reason, the leading European research groups, including those based in companies, decided in 2004 to submit a proposal to the EU Sixth Framework Programme to set up a Network of Excellence (see box) to integrate soft-matter research, with the aim of building up a knowledge base and enabling infrastructure for designing advanced soft-matter composites. "We wanted to establish a forum for discussion and a common infrastructure, upon which we could build the kind of synergic collaborations and cross-fertilisation of ideas that produce world-leading science," says SoftComp Coordinator Professor Dieter Richter of Forschungszentrum Jülich, Germany. The proposal was successful and SoftComp was born.

Organisation of SoftComp

The subject areas are divided into three Network Areas around which research collaborations, meetings and workshops are focused:

- Colloidal composites, gels and glasses
- Self-assembling and biomimetic systems
- Polymer-based complex systems

The integration of SoftComp resources is managed via an infrastructure based on three Research Platforms: synthesis; experimental techniques; and theoretical and numerical methods (p.29). These Platforms give all Network partners mutual access to the complete range of research tools needed to carry out the highest-quality research in the field of soft matter: well-characterised soft-composite materials for specific experiments; specialised instruments, which may be available only in certain

laboratories; and high-level computing facilities and theoretical methods.

Dissemination and education are also key parts of Network activities (p.32). SoftComp organises conferences, meetings, laboratory courses, and schools. Links with industry are actively fostered, with all interactions kept confidential as required.

Through the Research Visits Programme, SoftComp encourages student and scientist exchanges and interlaboratory visits.

Gender equality is promoted through child-care offers for women going to conferences, as well as travel allowances for invited female speakers and scientists visiting other SoftComp laboratories.

SoftComp has a Network Governing Board, consisting of one representative from each partner, which is advised by

an International Advisory Board of scientists from industry and academia. The running of the Network is managed by a Network Coordination Committee. Annual meetings facilitate strategic planning and foster scientific collaboration through round tables, workshops and cooperation meetings.

The future

The SoftComp Network will have almost ended its final year of EU funding at the time this brochure is published. It has been extremely successful, as the examples given in the following pages will show. It has about 30 partners, including six companies, with some having joined at a later stage. The Network plans to continue, with funding based on subscriptions from the partners. This will ensure that Europe has a thriving, well-coordinated scientific community working in this rapidly expanding area of science and technology for the years to come.

The EU Network of Excellence (NoE) scheme

The Network of Excellence (NoE) is a tool developed under the EU Sixth Framework Programme (FP6) aimed at strengthening excellence by tackling the issue of fragmentation in European research. The main deliverable is the durable structuring and shaping of the way that research is carried out in a well-defined scientific field. Each NoE aims to strengthen scientific and technological excellence by bringing together European research groups to form a world-leading partnership.

NoE partners also have the mission of spreading excellence outside the Network, training and educating scientists within the field and beyond, and encouraging knowledge-transfer to industry and other disciplines. NoEs are related to the specific thematic areas of FP6, which depend upon assembling a critical mass of expertise and resources to accomplish FP6 goals.

The NoE is based around a Joint Programme of Activities (JPA), which includes a Joint Programme of Integration (JPI), a Joint Programme of Spreading and Dissemination of Knowledge (JPS), a Joint Programme of Research (JPR) and Management. In addition, special attention is paid to promoting gender equality.



Soft matter and people

Soft matter is everywhere

Look around the house and you will see that you are surrounded by many kinds of soft matter: toiletries and medicines in the bathroom, plastic containers, cleaning materials and food in the kitchen, and soft furnishings, toys and clothes in the living room and bedroom. The modern equipment and components in your car and workplace are often made of, or coated with, soft-composite materials. Today, traditional materials such as metal, ceramics and wood have partly been replaced by synthetic soft materials, which may be stronger, lighter and cheaper, and which, through scientific research, can be tailored to specific requirements.

Fantastic plastic

It is hard to imagine life without modern synthetic plastics and rubbers. These polymers (p.6,10) can be moulded into almost any shape, extruded into thin films and fibres, applied as coatings, and given bright colours or made transparent. New polymer composites are continually

being developed, including reinforced rubbers that are more hard-wearing (p.12).

A clean sweep

Supermarket shelves are bursting with specialist cleaning agents for washing clothes, dishes, and household surfaces. They generally contain surfactants (p.6, 18) which loosen and bind oily dirt. A huge amount of basic research goes into synthesising and formulating detergent products with just the right properties, such as chemical activity, viscosity, foaming power and pH. A simple-looking laundry liquid, for example, actually has a highly complex structure at the microscopic scale or below.

Food, glorious food

Many foods such as yoghurt, sauces, spreads and cream desserts are typical emulsions – minute droplets of oil suspended in water or vice versa – stabilised by a surfactant. These products are formulated to have exactly the right flow

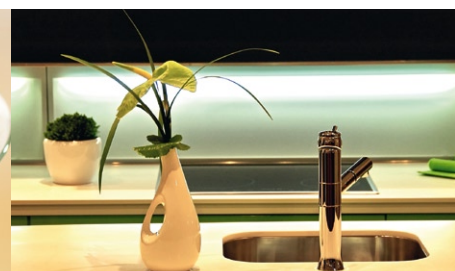
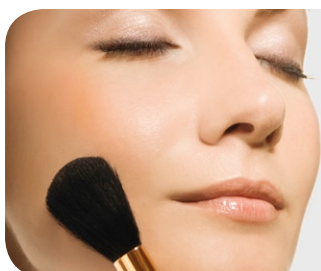
properties, a pleasant mouth feel, which depends on microstructure, and a long shelf-life – and of course they must taste good!

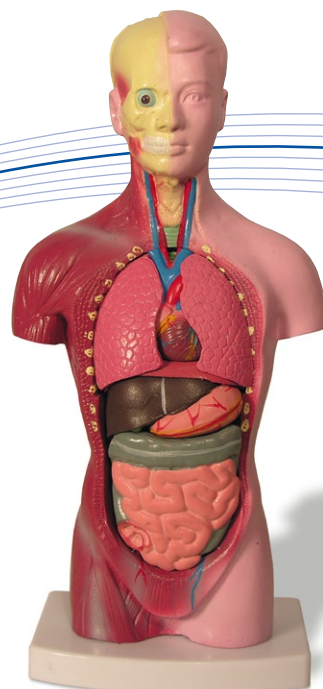
Secrets of beauty

Cosmetics and toiletries encompass a wide variety of soft-composite materials, from shampoos and toothpaste to skin creams and eye shadow. Formulations can be highly sophisticated, and may contain mineral particles, pigments and perfume suspended in a gel or emulsion. They are often designed to leave a coating on the skin or hair.

Ideal home

Home-improvement products are just as complex. Paints are usually designed to be 'non-drip', which means that they are gel-like in the tin but become liquid under shear stress when applied (p.16). The surface properties of coatings, fillers and glues may also be tailored so that they age in a certain way, or are water-repellent.





Soft materials and society

Everyday items and high-tech applications

Because soft composites are so versatile, constructed from relatively inexpensive, readily available raw materials, and capable of being processed under mild conditions of temperature and pressure, they are increasingly being exploited in advanced technological applications.

Soft on the environment

Soft materials are helping us to source and use energy efficiently. They are considerably lighter than metals, and are increasingly being used in the bodywork of vehicles, which improves fuel efficiency. Polymers incorporated in fuels themselves inhibit the formation of soot, thus reducing pollution (p. 18). The amount of oil that can be recovered from an oilfield can be increased considerably by injecting polymers or surfactants into an oil well to help force the crude out of the rocks (p. 22).

Better health for all

Because soft matter is largely constructed

from molecular building blocks similar to those in living tissues, it can be designed to mimic the self-organising and molecular-recognition characteristics of biological systems. Using this approach, minute surfactant vesicles called liposomes, or coated metal nanoparticles can be used to deliver anti-cancer drugs to tumours, for example. Scientists are also developing novel methodologies for fabricating artificial tissues or biomimetic soft materials for clinical and therapeutic applications.

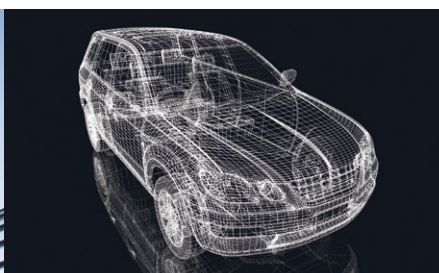
Technology innovation

Soft-matter composites are generally structurally organised at the micro- or nanoscale and offer amazing potential for new technologies. The first step in this direction was liquid crystals – fluids in which molecules change their orientation in response to a voltage. Liquid-crystal displays are now the device of choice for TV screens and computer monitors. Increasingly, the properties

associated with soft matter are being explored in the emerging technology of microfluidics, whereby fluids are manipulated at the millimetre scale, in devices employed as sensors and used for analysis.

The future

The prospects for soft-matter composites are promising. With the experimental and computer techniques that are available through SoftComp, researchers can investigate and start to predict how the many forms of soft matter behave. They can design new materials and structures, which have the potential to display the same diversity as the most complex form of matter we know of – living matter.

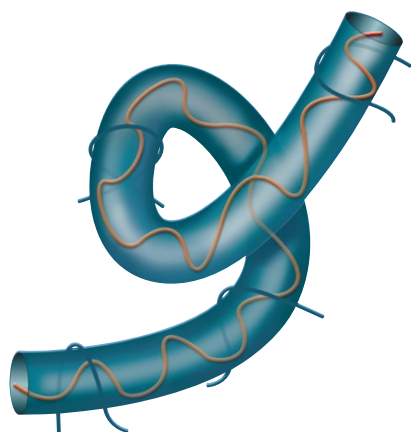




How do real polymers flow?

Polymer scientists are beginning to be able to predict the behaviour of commercial plastics under processing conditions

Plastics are the archetype of soft matter: they bend and soften when heated – complex behaviour that emerges from their special molecular structure. Industrial processing involves melting the material, which is then extruded, moulded or turned into films. Understanding what happens at the molecular level as the molten plastic flows is essential in optimising production, since bulk behaviour is deeply influenced by the length and branching of the entangled constituent polymer chains and how they move.



The tube model of polymer movement

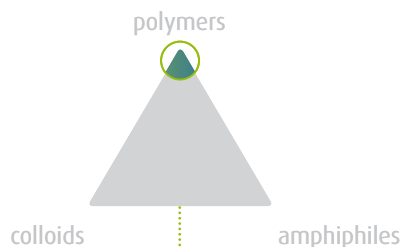
Over the past decade, polymer physicists have built up a good understanding of polymer dynamics, thanks to a highly successful theoretical picture in which each polymer chain is considered to slide through a tube created by the spatial confinement imposed by neighbouring chains. The tube theory can predict what the bulk flow properties of polymers should be, and it works well for simple model polymers consisting of linear chains. The theory can also be applied to branched chains but requires modifications.

Branched polymers

Tom McLeish, working first at the University of Leeds and then at Durham University, UK, is keen to apply the theory to real polymers of industrial significance; commercial plastics such as polyethylene consist of a mix of many thousands of different molecules with complex, branched chains of different lengths. The first step was to take the simplest branched structure, an H-shaped polymer with just two branch points, and model the changes after it

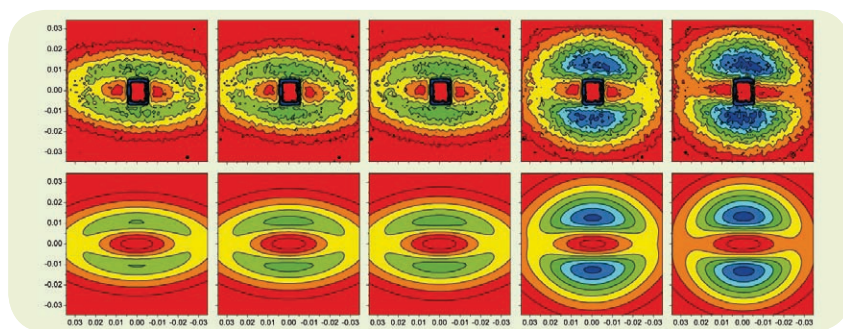
had been stretched as would happen in an extruder, for example. How would the arms and cross-bar of the H-polymer relax back to their original state and how long would it take?

Through a SoftComp collaboration with another eminent research group at the German research centre Forschungszentrum Jülich led by Wim Pyckhout-Hintzen, Professor McLeish and his colleagues were able to test the predictions experimentally. The Jülich researchers were experts in synthesising well-characterised H-polymers (p.30) and also in the technique of neutron scattering (p.30), which could be used to explore real-time molecular changes in the materials when they were put under strain. "Small-angle neutron scattering is ideal for probing structure at the length scales of polymers," notes Dr Pyckhout-Hintzen. The samples were warmed up until just molten and quickly frozen at a series of selected times. Successive neutron 'snapshots' were then taken to give a 'movie' of the chain arms as they relaxed. Labelling the arm ends



The SoftComp advantage

The UK and German research teams are leaders in the field of polymer dynamics. "SoftComp really brought us close together to make the most of our strengths," says Dr Pyckhout-Hintzen. "The Leeds team was strong on theory, while we had a readily accessible neutron-scattering facility for experiments." Professor McLeish agrees: "They had a beautiful rig for making neutron movies, with sharp timeframes, of the stretched polymer chains. The Network helped me to internationalise the fundamental work on model polymers, whilst also enabling me to engage at a deep level with industrial scientists who really know about the much more complex materials they are making and processing."



Two-dimensional neutron scattering images of polymer melts after being stretched and then allowed to relax. Top: experiment, bottom: theoretical prediction

or the central H-bar with deuterium, so that they were highlighted in the resulting neutron-scattering pattern, revealed that the arm ends got rid of the polymer tube completely before the H-bar relaxed – just as predicted.

More recently, the Jülich team, working with Dimitris Vlassopoulos at FORTH in Crete (p.20), have turned their attention to ring-shaped polymers, which, on the contrary, have no arm ends and so present somewhat of a theoretical challenge for the tube model of chain relaxation. This polymer architecture will be one of the model systems to be studied by DYNACOP (Dynamics of Architecturally Complex Polymers), a new EU-funded network that has arisen entirely out of SoftComp collaborations.

The physics of polythene bags

Meanwhile, Professor McLeish has gone further in his ambitious goal of predicting the behaviour of industrially

produced polymers at the molecular level. With help from Dow Polyethylene Product Research in the Netherlands, also a SoftComp partner, scientists at LyondellBasell in Ludwigshafen, Germany, and colleagues Daniel Read and Chinmay Das in Leeds, he has developed a series of connected models that relate the factors affecting the initial polymerisation process for low-density polyethylene (LDPE) to the final viscoelastic and processing properties of the melt. "This was where our collaboration with industry really paid off, because Dow and Basell were able to supply us with a whole series of beautiful long-chain branched polymers that had been carefully characterised," says Professor McLeish. The samples represented levels of complexity that were in between the very clean H-polymers and the ill-defined LDPE.

The first model uses the chemistry of the polymerisation reaction to provide

data on 100,000 representative polymer molecules. The data file is then read by another program that applies all the physics of the H-polymers, using the tube model, to predict the flow behaviour. "Amazingly, we found that the combined computer programs gave the correct predictions," remarks Professor McLeish. "It is a dream come true. I did not think that we would ever achieve this in my lifetime." This work will enable industry to tweak both the synthesis and processing conditions so as to ensure that they obtain the product they want, as well as predicting the processing behaviour of new plastics.



Soft-matter research can help improve the processing of industrially produced polymers such as polythene

Contact

Professor Tom McLeish

Durham University, UK
✉ t.c.b.mcleish@durham.ac.uk

Dr Wim Pyckhout-Hintzen

Forschungszentrum Jülich, Germany
✉ w.pyckhout@fz-juelich.de



Car tyres get greener

Tyres made of rubber containing nanostructured silica aggregates need less energy to roll and so save on fuel

During the past two decades, composite materials structured at the nanoscale have been the core focus of much materials research in both academic institutes and in industry. An important goal has been to develop novel materials that are more resilient. For example, there are active research programmes to develop materials using nanostructured aggregates – clays, silica and carbon – in plastics, with the aim of imparting properties such as fire or scratch resistance. According to one SoftComp partner, the leading chemicals manufacturer Rhodia, this has been more challenging than expected, since although nanostructuring the material

effectively increases hardness, it also makes the material more brittle.

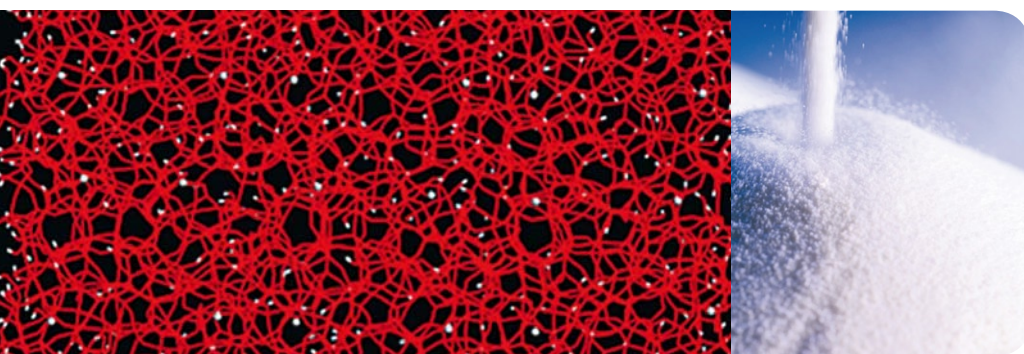
Nevertheless, one area where introducing nanostructured mineral fillers into bulk polymers has been highly successful is in the development of reinforced synthetic elastic polymers, or rubbers, for car tyres. Incorporating particles of silica, which are 30,000 times stiffer than the average rubber, into a rubber matrix through chemical coupling improves the wear and tear resistance. This is particularly effective in tyres for heavy-goods vehicles. A key aim has been to develop 'green' tyres that have low rolling

resistance, and so increase fuel efficiency, as well as having a longer life and better road grip in wet weather.

Rhodia is the main supplier of highly dispersible silica fillers for tyres manufactured for the domestic car market in France. To design the ideal products requires understanding exactly how the size and dispersion of the aggregates in the rubber impact on the tyre performance (rolling/wear resistance and wet/dry grip). To achieve this aim, the company has developed specific know-how on how to fine-tune its production methods to make silica aggregates with the required characteristics. The filler is produced in a precipitation step between a sodium silicate solution and an acid such as sulphuric acid.

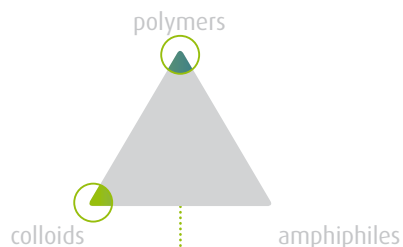
The effects of rolling

To establish what morphology and/or aggregation scale the silica particles should have, Ludovic Odoni and colleagues at Rhodia in Lyon and Collonges au Mont d'Or in France investigated how their properties affected what is known as the Payne effect, which describes the material's physical response



Molecular modelling of a silica surface with hydroxyl (OH) groups in grey and silicon-oxygen bonds in red; there are roughly six to eight OH bonds per square nanometre

Silica as a raw material (typical particle size of 100 micrometres)



The SoftComp advantage

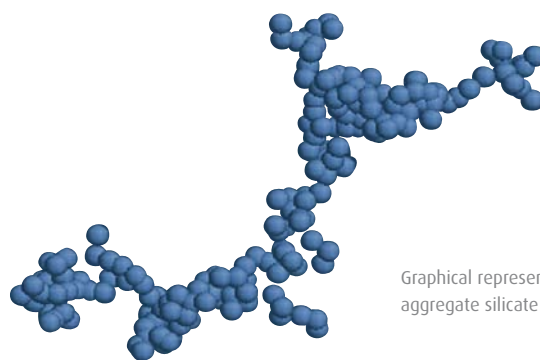
Rhodia is one of the industrial partners of Softcomp collaborating on polymer and composites research. "We have joint projects with teams at the University of the Basque Country in San Sebastián, Spain, and the KU Leuven, Belgium. The SoftComp connections help to better our knowledge of science," says Dr Odoni, who heads up a joint research institute between Rhodia and CNRS, a French government-funded research organisation. He has been able to interact with Dr Oberdisse and collaborators through the specialist Network workshops, which have helped forge successful links between industrial and academic scientists.

to moderate stress. When a tyre rolls along, the shearing force from the road deforms the rubber. With increasing rolling speed and shearing stress, the stiffness of the rubber compounds decrease with the appearance of a dissipative effect – the Payne effect. This causes more movement in the component particles so that the tyre expends more energy; keeping the Payne effect to a minimum means that the rubber remains more rigid under stress, and less energy is used to move forward.

The researchers carried out tensile measurements on a series of silica-reinforced rubber samples prepared with different coupling agents at various concentrations. Using microscopy, X-ray, neutron and light-scattering methods, they compared the results with the levels of silica dispersion. In this way, they could show that the softening of rubber was influenced by the nature of the coupling and the total area of contact between the polymer chains and the aggregates. The team concluded that to get the best product, the silica filler needed to be evenly dispersed, with optimum cohesion with the polymer. "The objective is to have a filler with silica objects of about 200 nanometres in size and with a carefully tuned interface that can even immobilise the rubber at the vicinity of the filler," says Dr Odoni.

Particles in films

Julian Oberdisse at the University of



Graphical representation of an aggregate silica structure

Montpellier, France, has also been studying the behaviour of silica nanoparticles in polymers, working with Michelin, as well as with academic groups within the SoftComp network. He has been studying the reinforcement effect in detail, in model latex films in which nanoscopic silica beads were embedded. These kinds of basic studies have broad applications to many nanocomposite systems including coatings.

Dr Oberdisse was particularly interested in seeing exactly how clustering of the particles affected the mechanical properties of the film. The films were prepared by evaporating a colloidal mixture of the polymer and silica particles. The degree of clustering could be controlled simply by altering the pH of the precursor solution. The films were stretched and the mechanical properties measured, while their structure was explored with small-angle neutron scattering, which is Dr Oberdisse's speciality. This technique, which is used extensively by scientists

within SoftComp (p. 10, 18, 30), is ideal for probing structure at the length scale of nanoparticle clusters. He found that the level of aggregation has a strong effect on mechanical strength, with larger aggregates giving the strongest reinforcement. This is probably because an aggregated, possibly volume-spanning, structure tends to dissipate any applied stress. Dr Oberdisse believes that controlling aggregation is as important as controlling the interface between the particles and polymer. "Industry is beginning to think that having controlled clusters is a good idea," he says.

Contact

Dr Julian Oberdisse

University of Montpellier II-CNRS,
France

✉ oberdisse@lcvn.univ-montp2.fr

Dr Ludovic Odoni

Rhodia Europe, Saint-Fons, France

✉ ludovic.odoni@eu.rhodia.com



Making the perfect nanoparticle

Understanding what controls the formation of nanoparticles is key to many products, from detergents to cosmetics

Minute particles ranging from 10 to a few hundred nanometres in size turn up everywhere. They are found in your body, your water supply, the air, and in many modern products such as paints, cosmetics and the highly specialised catalysts used to make chemicals. Nanoparticles can be minerals such as calcium carbonate, metals, organic compounds, or even biological molecular entities such as protein assemblies and viruses. Many natural processes such as the formation of biominerals, for example shells, or the deposition of limescale in your washing machine, involve the initial formation of nanosized crystallites.

Nanoparticles often have physical characteristics such as optical and mechanical properties uniquely related to their size which are increasingly being exploited in the expanding field of nanotechnology. Understanding how shape and size affect these properties, and how to control their synthesis is thus an active area of research.

Controlling crystallisation

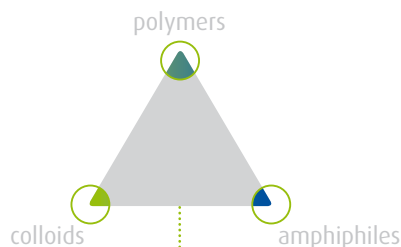
Several research groups within the SoftComp network are interested in making and characterising nanoparticles for industrial and technological purposes, often combining them with other materials such as polymers to control their production and behaviour (p. 12). Understanding how particles form and grow is extremely important in many practical processes, for example, the precipitation of salt crystals during sea-water desalination, or in the setting of concrete which involves complex recrystallisation processes that affect its strength.

Germany, are interested in studying how to limit the growth of calcium carbonate crystals, which cause the fouling of water pipes, with the aim of developing new limescale inhibitors for laundry detergents and other products. The standard picture of the crystallisation process was that spherical nanosized particles in the saturated water solution act as critical nuclei around which the crystals grow, but this had not been experimentally studied in detail. Electron and X-ray microscopy studies revealed that the crystallisation process is much more complicated: the particles can, for example, re-dissolve or cluster together into flocs. "We are interested in understanding the whole story of crystallisation with the idea of controlling particle formation," says Dr Rieger. Studies of precipitation in the presence of polycarboxylate, which is a standard detergent additive, showed that the polymer wraps around the nanoparticles and stabilises them against further growth. Calcium carbonate represents a generic example, and the same principles can be applied to the growth of other nanoparticles, such



Companies such as BASF test the effectiveness of new limescale inhibitors in laundry detergents, based on a better understanding of particle formation

Jens Rieger and colleagues working at the chemical company BASF in Ludwigshafen,



The SoftComp advantage

BASF has been a keen supporter of SoftComp from the start, having links with several research groups in the Network. Dr Rieger comments that SoftComp offers a coordinated, structured approach to bringing together diverse activities across Europe that enhances BASF's own strong research effort. "The Network gives us direct access to the forefront of soft-matter research," he notes. "The SoftComp meetings also give us the opportunity to let our academic partners know of the scientific problems that are important to industry." Professor Liz-Marzán enthuses about collaborations enabled by SoftComp. His group supplies silver and gold nanoparticles to several other groups for specialised studies including phase behaviour in composites, and his students are able to visit other laboratories to carry out specialised measurements such as dielectric spectroscopy. "This is something that we would never do ourselves," he says. "Through the SoftComp collaborations, we have now applied to start a new European project," adds Dr Pastoriza-Santos.

as pigments in paints or even in natural dyestuffs used in food and drinks.

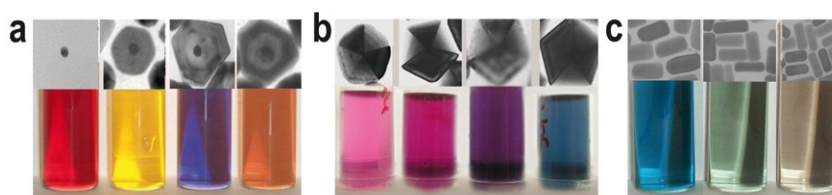
Multicoloured silver and gold

Another type of particle that is exciting interest is silver nanoplatelets and gold nanorods, which have unusual optical properties. Light impinging on the metal causes electronic surface oscillations called plasmons, which control how the light is reflected from the particle and thus their colour. The exact hue depends on the shape, size and composition of the particles. Luis Liz-Marzán and his colleague Isabel Pastoriza-Santos at the University of Vigo, Spain have been developing methods to make particles with a controlled shape – triangles, rods, decahedra, octahedra, spheres and even star shapes, so that the colour can be tuned.

Dr Pastoriza-Santos has developed a highly successful chemical method of fabricating the particles from a gold or silver salt, and using a polymer stabiliser to control the formation. "It is known that adding polyvinyl pyrrolidone induces the formation of nonspherical nanoparticles, but the mechanism is still not really clear," she says.

Gold and silver nanoparticles have several exciting applications. One is for biosensors. The particles are of the right size for attaching single molecular bio-receptors that bind with a target molecule such as a protein in the blood. Plasmons are accompanied by very high electric fields at the nanoparticle surface, which in turn enormously enhance the characteristic

properties such as a negative refractive index, with intriguing applications as 'invisibility cloaks'. Metamaterials, so far, have been composed of arrays of microstructures responsive to microwaves, but the use of much smaller metallic nanoparticles is predicted to lead to similar results in the visible part of the spectrum.



Aqueous dispersions of gold and silver nanoparticles with the corresponding electron micrographs of the particles

light scattering from the attached molecule – an effect called surface-enhanced Raman scattering (SERS). When the probes recognise their target, it can be detected through its specific vibrational signature. The researchers are already working with other groups to optimise biosensors based on this technology. "We are trying to find the perfect nanoparticle," explains Dr Pastoriza-Santos.

Another application can be found in the so-called metamaterials. These are composite materials with peculiar optical

Contact

Professor Luis M. Liz-Marzán

University of Vigo, Spain

✉ lmarzan@uvigo.es

Dr Isabel Pastoriza-Santos

University of Vigo, Spain

✉ pastoriza@uvigo.es

Dr Jens Rieger

BASF, Ludwigshafen, Germany

✉ jens.rieger@basf.com



Worms, onions and bands on the run

Composite liquids can show unusual organised behaviour when put under stress

Many everyday materials such as paints, cosmetics, cleaning products and even foods consist of a complex dispersion of minute particles in a liquid – a colloid. These may be fine powders, long polymer chains, or surfactant micelles (p.22) or some combination of all of them. Emulsion paints, for example, contain pigment particles, film-forming polymers, as well as surfactants to stabilise and maintain the paint's integrity. Not surprisingly, the physical behaviour of such complicated materials, especially when put under shear stress by stirring or spreading on a surface, is rich in variability and can be unpredictable. Some soft-composite materials will suddenly change from a mobile liquid to a gel-like solid when sheared, while others will become thinner. Such phase transitions can be a nuisance in processing, causing blockages in equipment, but can also be used to advantage in, say, squirting tooth-

paste out of a tube or applying paint to a surface.

Despite the complexity, soft-matter physicists are making progress in understanding some of the surprising changes that can happen, and this will help industry to design products that are easy to process and are fit for purpose. One particular set of phenomena that intrigues the SoftComp community was first noted in the 1950s in polymer extrusion, when, at a high enough shear rate, the polymer melt would suddenly thin and 'spurt' out. This flow instability, not surprisingly called the 'spurt effect', can be due to the threadlike particles, whether polymer chains or worm-like surfactant micelles, suddenly untangling and stretching out, or breaking up, to form a differently organised phase.

This kind of mechanism can also result in curious banded structures, and this has been revealed using the standard piece

of equipment employed to study shear flow – the Couette cell. This is a narrow container with concentric cylindrical walls, where the inner wall can rotate. This creates a velocity gradient in the flow of a sample in the cell, from the outer to the inner wall. In a simple liquid, the stress increases directly with the shear rate. However, in complex liquids like polymer and micelle solutions, the material can suddenly 'give way' at a given shear rate, separating into a new phase with a lower viscosity, creating distinct bands in the direction of the flow gradient. Jan Dhont at Forschungszentrum Jülich, Germany, has been studying such band phenomena experimentally and theoretically to understand this kind of behaviour.

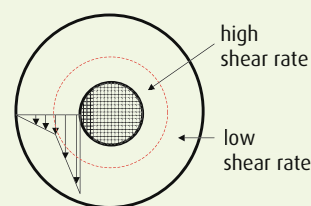
Rolling with the flow

A more unusual type of banding can occur in the direction perpendicular to the flow, which is more difficult to explain. Professor Dhont has studied this so-called vorticity banding and believes it is related to



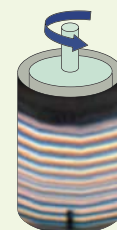
A Couette cell (left), routinely employed to study shear flow in soft materials. The sample is placed between the inner and outer cylinders, which rotate independently. The resulting shear flow can cause the sample to separate into bands of material with different viscosities, either in the direction of the flow gradient (middle), or more unusually perpendicularly to the flow (right)

Gradient banding

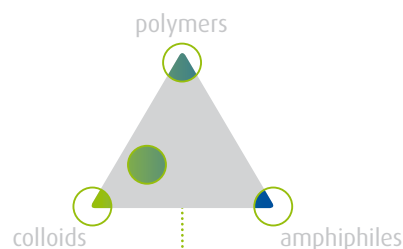


Top view of a Couette cell with a gradient-banded stationary state

Vorticity banding



Schematic of a Couette cell

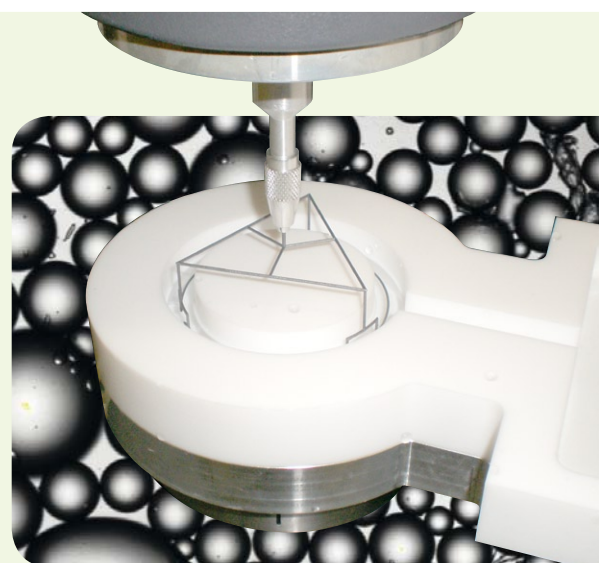


The SoftComp advantage

Experiments on flow in complex liquids depend on highly specialised equipment. Through SoftComp, Professor Dhont's laboratory, for example, makes available unique light-scattering facilities to the Network partners. "I was able to send my PhD student to Jülich, and elsewhere, to make flow measurements. The opportunity to learn new expertise was invaluable for the student, who could not have done her PhD without it," says Professor Olmsted. Professor Vermant concurs: "SoftComp gave us access to a range of advanced techniques that we had not used before."

Flow in two dimensions

Jan Vermant at the Catholic University (KU) Leuven, Belgium, has been studying the flow of colloidal materials at liquid interfaces. Many products found in the home, whether ice cream or shaving foam, consist of a suspension of bubbles or droplets in a liquid. Their performance is strongly influenced by their flow behaviour and stability, which in turn depends on the elasticity of the interface between the particles and liquid. Through SoftComp, the Leuven team has improved an experimental technique that allows them to measure the elastic response of such an interface. It uses a double-walled ring that lies on the surface of the material of interest. An attached motor applies stress by rotating the ring back and forth such that it is deformed by the viscosity of the surface material. Measurement of the deformation then gives information about the mechanical properties of the interface. These kinds of studies can then be applied in the design of new emulsions and foams as well as for membranes of biological significance. The team also measures the flow of material interfaces. "We have particularly focused on particles in viscoelastic liquids. Using light scattering and microscopy techniques, we can obtain information not available from studying the bulk material," says Professor Vermant.



A special piece of equipment designed to measure the elastic response of a material's surface or its interface with another material, as found in bubbles or droplets shown in the micrograph

a phenomenon called the Weissenberg effect in polymer solutions. Near the top of the sample, normal stresses force the liquid up to the rotating inner cylinder. This is therefore also referred to as the 'rod-climbing effect'. "You get the same stresses – even in colloidal solutions that are not polymers, for example in a solution of self-assembled rod-like viruses, where the role of the polymers is now played by the self-assembled structures. In bulk, away from the top of the sample, the normal stresses lead to bands with an internal rolling flow," says Professor Dhont.

Peter Olmsted and colleagues at the University of Leeds, UK have also been

studying vorticity banding. They are experts on phase-separation phenomena in emulsions containing surfactant molecules. The surfactant can form layered structures, which act as an interface between the oil and water phases. Under flow, these low-stress stacked structures can roll up into more viscous onions. Recent experiments using light scattering, combined with measurements of flow velocities and stress, revealed something more complicated. The two phases of the low-stress layers and more viscous onions coexisted and could be seen as dark and light bands under the microscope. "We were able to show that the phenomenon really exists and had the experimental signatures that we predicted

theoretically," says Professor Olmsted. Whether the mechanism is the same as that seen by the Jülich group is still under discussion.

Contact

Professor Jan K. G. Dhont

Forschungszentrum Jülich, Germany

✉ j.k.g.dhont@fz-juelich.de

Professor Peter Olmsted

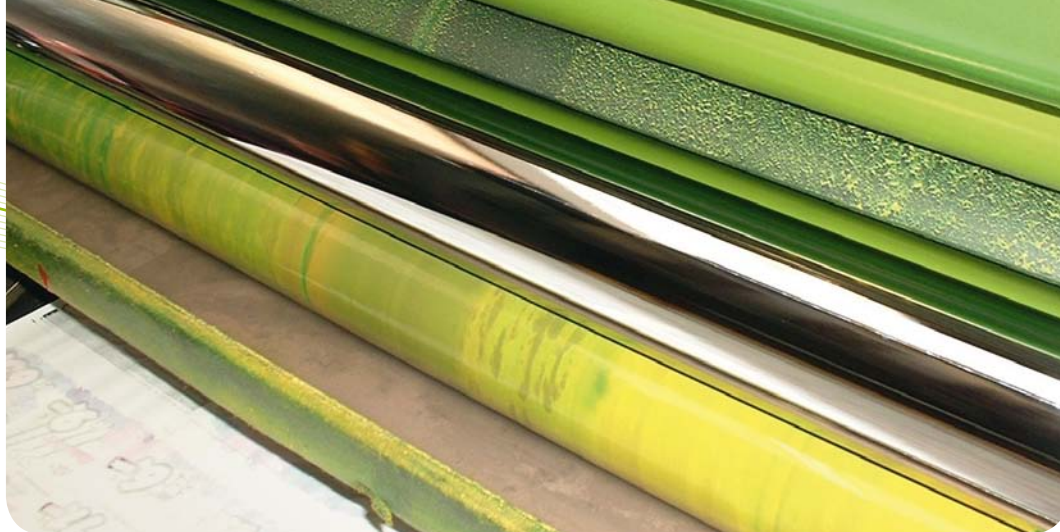
University of Leeds, UK

✉ p.d.olmsted@leeds.ac.uk

Professor Jan Vermant

KU Leuven, Belgium

✉ jan.vermant@cit.kuleuven.be



Cleaning gets a turbo-boost

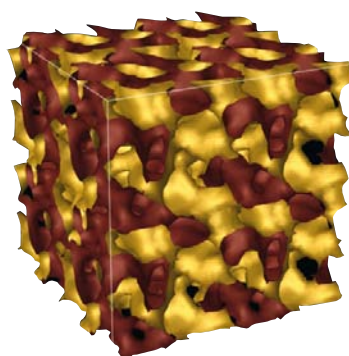
A new type of polymer-based additive makes detergents superefficient, leading to safer, greener cleaning as well as pollution-free fuels

One of the most intriguing types of soft composite is the microemulsion – a finely dispersed mixture of water and oil, brought into intimate contact by a surfactant, or detergent, which loves both of these normally immiscible liquids. Microemulsions differ from ordinary emulsions, such as mayonnaise for example, in that the dispersion is on the nanoscale. This results in an elegantly transparent material which is extremely stable – compared with even the most expertly made mayonnaise which eventually separates back into olive oil and vinegar.

The staying power of a microemulsion arises from the special properties of the particular surfactants used. Traditional surfactant molecules contain both a water-loving component such as a positively charged metal ion or groups of atoms and an oil-loving hydrocarbon tail. They line up in ordered arrays, creating thin membranes separating the oil and water phases. In microemulsions, these membranes can form a range of intricate structures: they can roll up into nanosized water or oil-containing vesicles called micelles, or form layers, or spongy networks which create bicontinuous oil and water phases throughout the material.

Soft-matter scientists are interested in understanding all the factors that affect

the kind of microemulsion structure formed and its properties – for example, the concentration, chemical composition, geometry and membrane flexibility. Since these composites also make excellent cleaning agents, absorbing both oily and water-based dirt – although they are expensive – one aim of researchers is to establish the design rules for making microemulsions, in the hopes of developing cheaper, more efficient materials of commercial interest.



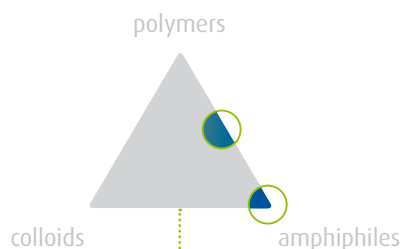
A computer simulation of a microemulsion showing a continuous fine network of oil and water phases

A surprising discovery

In pursuing these goals, one highly successful SoftComp collaboration, involving teams led by Jürgen Allgaier at Forschungszentrum Jülich and Reinhard Strey at the University of Cologne, Germany, has made a breakthrough in

microemulsion technology. Dr Allgaier, a chemist, had what seemed like a great idea – that of making a potentially powerful surfactant composed of blocks of two kinds of polymer, one hydrophobic and the other hydrophilic. Unfortunately, the diblock copolymer turned out not to have the anticipated surfactant properties, so he asked the Cologne group, who were experts in microemulsions, to take a look at the material. “We have a tool for studying the properties of unknown surfactants,” explains Professor Strey. “Using a well-understood standard surfactant system that produces microemulsions, we add trace amounts of the new surfactant and study the phase behaviour at various concentrations and temperatures. We measure the efficiency of the system as the least amount of surfactant needed to solubilise equal amounts of oil and water.”

The researchers were in for a surprise. Adding very small amounts of the block copolymer greatly enhanced the surfactant efficiency, reducing the amount needed by more than a factor of ten. “I coined the term efficiency booster,” says Professor Strey. This meant that microemulsions could be achieved using much less of the expensive surfactant – which is music to the ears of any detergent manufacturer.



The SoftComp advantage

The Jülich and Cologne teams have been working closely together through the SoftComp network. "The collaboration has been an ideal combination of different capabilities," says Dr Allgaier. "Our competence is polymers and neutron scattering and Cologne's is microemulsions and their phase behaviour."

Why did the block copolymer work so well? To find the answer required analysing the emulsion at the microscopic scale. The technique of neutron scattering, in which the Jülich researchers are experts, is the ideal method for uncovering structure over a range of scales, from those of atoms and molecules to micelles. A neutron beam is passed through a sample and the resulting scattering pattern taken at small angles gives information about the polymer structure and the geometry of the water and oil domains. Of crucial importance is the technique of 'contrast matching', whereby the hydrogen atoms in selected components of the system are replaced by deuterium. This heavier hydrogen isotope scatters neutrons differently from its lighter brother, so the deuterated component then stands out. The water or oil phases can be partially deuterated such that their scattering properties match those of the chosen surfactant components, thus rendering them invisible. In this way, just one specific component can be highlighted.

"We looked mainly at the bicontinuous emulsion phase with equal amounts of water and oil," says Dr Allgaier. "The diblock copolymer sits at the oil-water interface with the surfactant molecules. The scattering patterns showed that adding the polymer increased the size of the oil and water domains. We found that there is a kind of repulsion between the polymer blocks and the surfactant interface, which tended to make the membrane more rigid, giving larger domains," he says.

Commercial applications

Both research teams have taken out patents on versions of the efficiency booster. In conjunction with the small German company Schwegmann, the Jülich group has been developing water-based agents for cleaning the inks and dust from printing machines. They employ much less organic solvent than conventional cleaners. Organic solvents are harmful to health and not very friendly to the environment. The new water-soluble material is based on a new polymer additive with a very small hydrophobic polymer block, and is biodegradable, as required by EU legislation. "It works very nicely but we still need to make it cheaper," notes Dr Allgaier.



The effects of adding a booster

Each of the four containers above has equal amounts of oil and water. Starting from the left, the first container has no surfactant, so there is no mixing; the next one has only enough surfactant to mix a small amount of the water and oil as a microemulsion (the middle phase); the third sample has the same amount of surfactant but also a small quantity of block copolymer, which greatly increases the emulsification capacity so that the middle phase expands; and in the far right sample, yet more polymer has been added, which increases emulsification even further.

Meanwhile, the Cologne team has also been looking at applications, in particular as diesel fuel additives. Adding a microemulsion, with a surfactant booster based on nitrogen-containing polymers, makes the engine run soot-free, thus increasing efficiency and reducing pollution. Car companies such as Daimler are already interested in testing it, and the additive could be used in diesel formulations powering ships and trains. Again, the hunt is on for cheaper additives that exploit the same principle which made the original – but rather expensive – block copolymers so effective.



Such a system has been developed as an environmentally friendly agent for cleaning printing machines

Contact

Dr Jürgen Allgaier

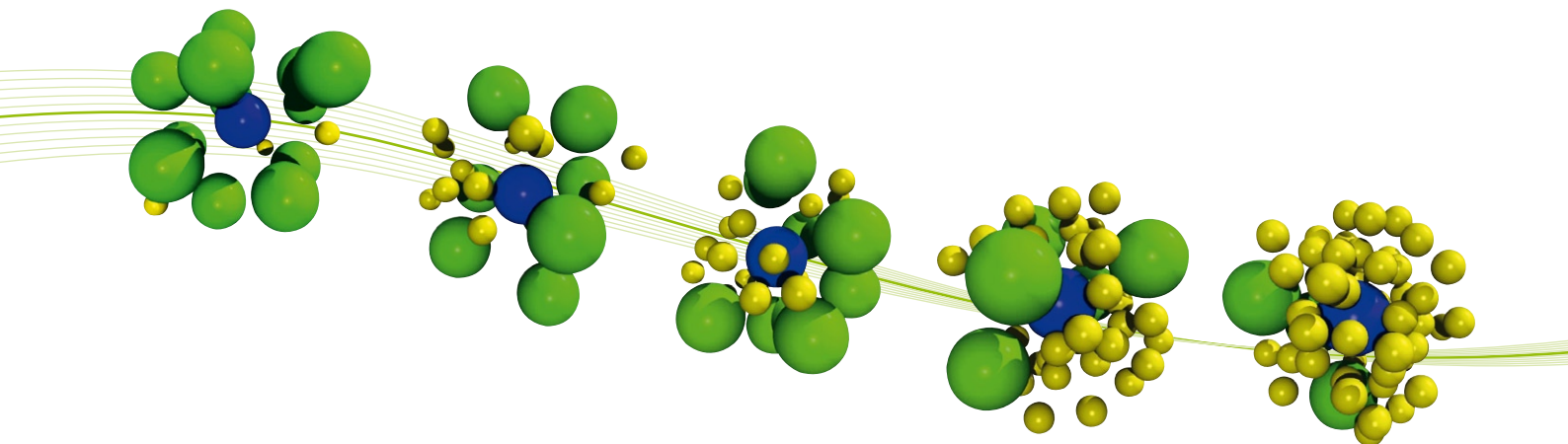
Forschungszentrum Jülich, Germany

✉ j.allgaier@fz-juelich.de

Professor Reinhard Strey

University of Cologne, Germany

✉ rstrey@uni-koeln.de



Soft glasses become a star attraction

An unusual colloidal system based on star polymers shows some very complex behaviour

Soft glasses and gels represent one of the most intriguing forms of soft matter. They are usually colloids – dispersions of particles randomly crowded together, such that their individual movement is restricted by their neighbours, as though trapped in a cage. Glasses are truly dense particle suspensions, in which the particles typically repel each other, whereas in gels the particles occupy a lower volume fraction and attract each other. In a colloidal glass, above a certain volume fraction, the particles do move slowly, resulting in a variety of changes over long periods of time – in other words, they age. Like us, the exact changes that happen depend on their history. However, the particles can escape from their confines if given enough mechanical energy, in which case the material becomes a liquid. Adding other components can also alter the local environment of particles and change this ‘glass transition’.

Not surprisingly, these materials can behave in unusual ways. We may see the unexpected results in products such

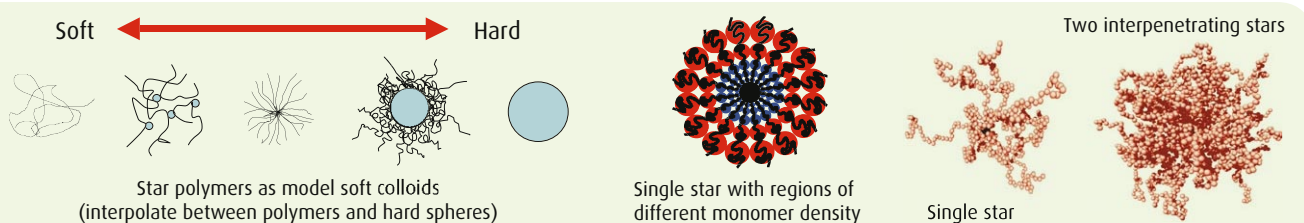
as food and toiletries bought from the supermarket – for example, a dessert or cosmetic that starts to separate. Trying to predict and explain what happens is a challenge for both theorists and experimentalists. They would like to establish the rules that govern the glass transition and stability. This would enable industry to determine or extend the shelf life of products and engineer their processing more effectively.

Theorists start out with the simplest model of a colloidal glass, which treats the particles as hard spheres that mutually repel each other, and then calculate the kinetic evolution of the system. Of course, real colloidal glasses are not simple spheres, and SoftComp partner Emanuela Zaccarelli and colleagues at the Sapienza University in Rome, Italy, have been working on extending the theory to more complex systems. In particular, in collaboration with Christos Likos and his team at the University of Düsseldorf, they have been carrying out calculations on an unusual set of

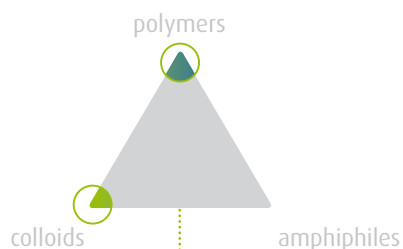
colloidal glasses prepared and studied by Dimitris Vlassopoulos and colleagues at FORTH and the University of Crete, Greece.

A model system

Professor Vlassopoulos and colleagues design and use star-shaped particles, in which a series of linear polymer chains is anchored to a central core. These materials were originally synthesized by Nikos Hadjichristidis at FORTH and the University of Athens, Greece and other groups. The star polymers do not behave exactly like hard spheres but are more flexible; each particle has arms which can interpenetrate those of another particle. “I love these systems because they lie between the two extremes of hard colloidal particles and soft polymeric coils,” enthuses Professor Vlassopoulos. They are also very versatile: their properties can be tuned by altering the number and length of the chains. Several SoftComp research groups work on different aspects of star polymer systems (p.23).



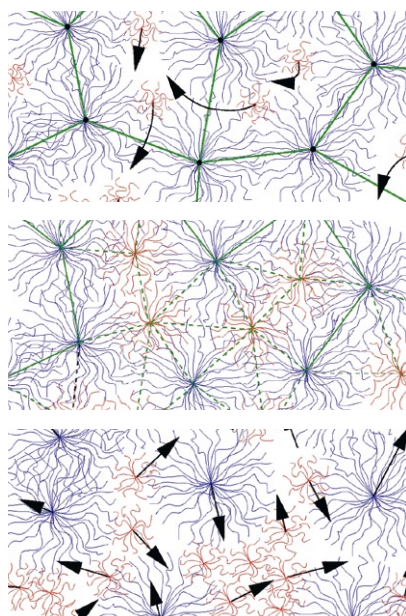
Star polymers as model soft colloids; they have microscopic properties between soft flexible polymers and hard spheres



The SoftComp advantage

Professor Vlassopoulos' group in Crete is very active within the SoftComp Network. Research groups such as his, with limited national funding available, depend heavily upon EU grants, which often involve international collaboration. "SoftComp is particularly important to us as it provides a grid for working with a number of different groups," he comments.

Dr Zaccarelli and colleagues in Rome have also benefited from SoftComp: they were carrying out theoretical work on glasses and colloidal systems but did not collaborate with experimentalists such as the Crete group. "This was a weakness for us, but through SoftComp, we now work very closely with experimental groups," she explains.



Mixtures of varying concentrations of large and small polymer stars behave differently. The top graphic shows how a few small stars can move around the immobilised big stars. However, larger small stars immobilise both components into a 'double glass' (middle graphic), while high concentrations of the smaller stars completely melt the system and all the stars can then move (bottom)

It turns out that star-polymer glasses show some remarkable behaviour. If smaller, but chemically identical, star polymers are added to a glass composed of big stars, they first move around the immobilised larger stars. When the volume fraction of the small stars is high enough, however, they start to knock the cages of the big stars until they break, and the glass melts into a liquid. There is also a competing scenario: using larger

stars, albeit still smaller than the big ones, they can get trapped in the cages of the large stars to form a so-called double-glass system, in which both star types are immobilised. The system has yet more surprises. On adding further small stars, the cages start to push each other and the system melts again. And for the finale, on adding even more small stars, a new type of glass appears in which the cages are asymmetric.

Computer insights

Using computer simulations, the Rome team calculated the glass-transition line – where the system should become liquid – for the different concentrations of small stars and showed that it followed a U-shaped curve. The advantage of simulations is that they can easily explore more extreme conditions. "It turns out that if you keep on increasing the concentration of small stars, you get this asymmetric class of glasses. The experimentalists then added as many small stars as was feasible, and in this way they confirmed the simulation results," recalls Dr Zaccarelli. The team also showed that the second glass that formed was more robust. "It suggests that playing with simple parameters such as concentration of additives you can really tune the properties of the resulting material," she says.

Recently, the Rome team has focused more on gels, which differ from colloidal

glasses in that the particles are more spread out, giving a less dense material. They are often held together by transient weak attractions or entanglements in an open network to create the typical elastic, jelly-like texture. Their behaviour is much less well understood and is not so easy to model. Nevertheless, the team hopes to apply their theoretical approach to gels composed of colloidal particles with directional 'sticky' patches, which would act as models for many systems of nanotechnological and biomedical relevance.



Star-polymer research is relevant to studies of drug-delivery systems

Contact

Professor Dimitris Vlassopoulos

FORTH: Foundation for Research & Technology – Hellas, Heraklion, Greece
✉ dvlasso@iesl.forth.gr

Dr Emanuela Zaccarelli

Sapienza University, Rome, Italy
✉ emanuela.zaccarelli@phys.uniroma1.it



The ever-changing world of micelles

Surfactants and polymers both form complex structures in solution; when they come together new properties can arise

Surfactants are fascinating because of the way their constituent molecules neatly organise themselves into intricate microstructures in oil and water mixtures. One type of structure that has excited great interest is very long flexible cylinders, dubbed worm-like micelles. They behave a little like polymers, which also have long flexible shapes, forming viscous, elastic solutions (p. 10). However, there are differences: while polymers are single long-chain molecules held together by chemical bonds, worm-like micelles are molecular assemblies which continually break up and reform.

Recently, Wim Briels, a theoretical physicist at the University of Twente, The Netherlands, became interested in worm-like

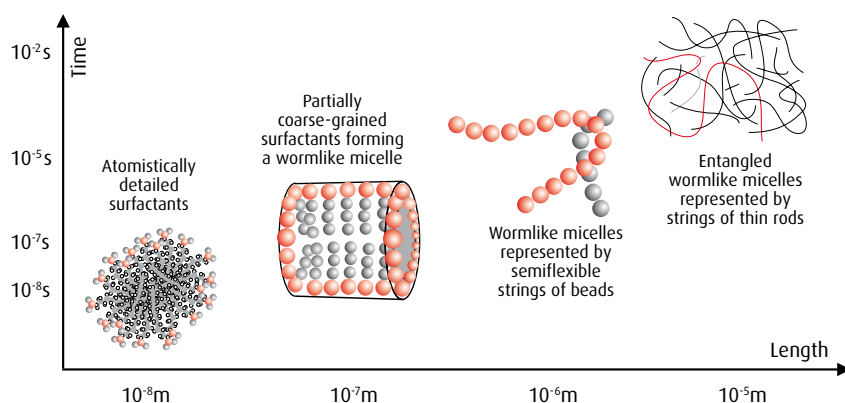
micelles as a result of collaborating with Edo Boek at Schlumberger in Cambridge, UK. The company had been using a polymer-based fluid pumped at high pressure to fracture rocks so as to recover the last dregs of oil from a well. However, the highly viscous polymer then had to be removed with chemicals, which was environmentally undesirable. The researchers therefore turned to fluids containing worm-like micelles to perform the same function. Once these come into contact with the escaping oil, they break up into spherical micelles; the material becomes runny and is easily pumped to the surface.

To understand the flow behaviour better, Professor Briels and his team developed

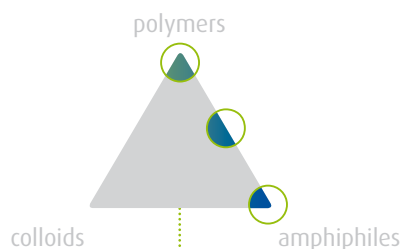
a novel type of computer simulation in which the micelles were treated as chains of rods including properties such as the stiffness, and the breaking and fusion energies of the entangled micelles. He then simulated what would happen to the particles under shear flow. The coarse-grained approach adopted allowed simulations of meaningfully large groups of micelles. At first, the computer predictions did not appear to support Schlumberger's experimental results. However, when the experiments were extended over the same length and time scales as for the simulations, they matched exactly. "It was a spectacular result," says Professor Briels, "which excited my team and Dr Boek for a long time."

Living networks

The simulations that Professor Briels found most challenging related to a type of exotic complex fluid in which the micelles are linked by a network of a polymer with 'sticky ends' – so-called telechelic polymers. These materials are extremely viscous but also very 'stretchy'. The transient networks that form therefore represent an excellent model system for studying complex soft matter especially under shear forces. Christian Liguore at the University of Montpellier, France, has been pioneering studies of these materials for several



Particle-based computer simulations of worm-like micelles carried out at different length and time scales. 'Coarse-graining' the surfactant molecules greatly accelerates the calculations



The SoftComp advantage

Coming into soft-matter research from a background of physical chemistry, Professor Briels found that the Network gave him contacts within the broader community. "Participating in the SoftComp network has been a fantastic experience for me," he explains. "My specific way of modelling soft matter, which is halfway between the chemist's and the physicist's approach, has been much appreciated and has resulted in many collaborations." Industry has also profited in unexpected ways. Malvern Instruments in the UK, which recently joined SoftComp, has been able to use Professor Ligoure's bridged worm-like micelle systems to test the performance of a new high-frequency rheometer. "This was a very interesting collaboration for us," confirms Professor Ligoure.

years. His team designs network-forming systems, in which small amounts of telechelic polymer are added to aqueous micelle solutions. The hydrophilic polymers have hydrophobic ends which then anchor onto the surfactant assembly to

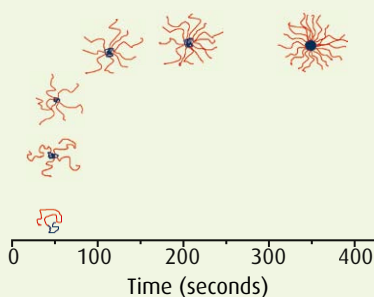
form bridges and loops. Exploring their properties using neutron-scattering techniques and rheometry, they found that worm-like micelles and polymers formed a double transient network. Carrying out simulations they also showed

that longer polymer chains created more bridges which increased the liquid's elasticity. Theory and experiments also showed that under shear stress some of these living networks can suddenly 'fracture' like a brittle solid. Industry is very interested in these systems, according to Professor Ligoure. Worm-like micelles, on their own, feel slimy to the touch, so are not used in cosmetics, for example. However, adding a second, more rigid network can improve the material's feel. They could also provide an interesting model of actin cytoskeletons, the protein microfilaments involved in muscle contraction and sperm motility. "Our studies are providing a better understanding of real systems," comments Professor Ligoure.

The life and times of micelles

How do surfactant molecules spontaneously assemble into micelles? Until recently, no one had studied their formation and growth in quantitative detail. The experiments are hard to do because the process happens so quickly. However, Reidar Lund at the Donostia International Physics Centre in San Sebastián, Spain, in collaboration with an international team, has succeeded by using X-ray diffraction. In experiments at the European Synchrotron Radiation Source, which generates very bright X-rays, the team could follow the micellisation process. The material that they worked with was composed of alternating blocks of two polymers, one of which prefers to be in water while the other is insoluble in water. When dissolved in another solvent laced with water, the diblock copolymer assembles into star-shaped micelles. "It took us a couple of days to get the conditions right. We made measurements every few milliseconds, and systematically changed the concentrations," says Dr Lund. The researchers found that the micelles grow quickly at first, as single molecules are inserted into each micelle. The smaller micelles then shrink and larger ones grow, as molecules are expelled and re-inserted into other micelles.

The team hopes to develop a predictive framework for tailoring micelles used in controlled drug release and other reactions. "We want to be able to control the shape and size of stable micelles by understanding the kinetic pathways by which they are formed and use them as nanoparticles," says Dr Lund.



A graphic showing the growth of star-shaped polymer micelles as more polymer molecules are added

Contact

Professor Wim Briels

University of Twente, Enschede,
The Netherlands

✉ w.j.briels@utwente.nl

Professor Christian Ligoure

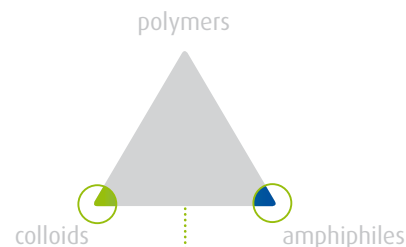
University of Montpellier II-CNRS,
France

✉ ligoure@icvn.univ-montp2.fr

Dr Reidar Lund

Donostia International Physics Centre –
University of the Basque Country,
San Sebastián, Spain

✉ reidar_lund@ehu.es



Towards a better drilling mud

There is more to oil and gas recovery than just drilling a hole

Drilling an oil well might seem to be a well-established engineering procedure – but, as oil and gas companies seek to extract deeper and less accessible hydrocarbon reserves, developing new technology becomes increasingly important. Of critical significance are the ‘drilling muds’ used. They lubricate the drill, keep it cool, remove the drilled ‘cuttings’ and keep the borehole under pressure to prevent it from collapsing. The mud is pumped down the drill pipe, sprays out around the drill bit, and is then pushed back up to the surface with the cuttings.

Drilling muds are typical soft composite materials, consisting of a suspension of mineral particles and surfactants, in water or oil, depending on application. Getting the formulation right speeds up the extraction, reduces the pumping power and avoids damaging the surrounding rock. With this aim in mind, SoftComp scientists have been collaborating to explore the properties of different combinations of model drilling-mud ingredients.

One of the most common materials is based on an aqueous suspension of clay particles such as bentonite (an aluminosilicate), which is cheap and environmentally friendly. The micron-sized plate-like particles form a network, which creates

a solid gel structure. When pumped under pressure, the gel collapses and flows as a fluid down the drill pipe, but reforms when the pump is turned off. This thixotropic behaviour is essential because it prevents the cuttings from settling out at the bottom of the well and clogging up the pores of oil-bearing rock.

Faster, stronger gelling

However, the reformation of the gel is slow, taking up to several hours, but can be made to happen almost instantly by adding a tiny amount of much smaller particles of magnesium aluminium hydroxide. The particles have an opposite electric charge to bentonite, and being smaller can rapidly squeeze around the lumbering bentonite particles to create electrostatic cross-links in the particle network. The result is a stronger, faster-reacting gel. There is a snag though: because the gel-enhancing interaction depends upon charge, the effect is lost when drilling through salty rock, for example under the sea. Typical salts, like sodium or calcium chloride, consist of positively and negatively charged atoms (ions) which screen out the residual charge on particles and so reduce these electrostatic attractions. The ideal would be a product that does not rely on electrical charge for fast gelling. To find a better

product requires understanding how the microscopic structure affects gelling and gel strength. Geoffrey Maitland from Imperial College London, UK, together with teams from Utrecht University, The Netherlands, and the oil-field engineering company, Schlumberger based in Cambridge, UK, systematically investigated the effects of adding small amounts of mineral particles of different shapes and sizes – rods, platelets and spheres – with controlled surface charges to a well-characterised model clay (hectorite). In a range of experiments to establish how the gel properties and performance changed under various stresses, silica spheres came out on top.

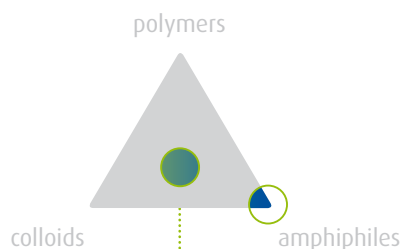
“Once we understand the rules from the model system, we can go back to cheaper, commercially available materials,” says Professor Maitland. “We are continuing the work within SoftComp, and hope to extend the studies to other components beside clays.”

The SoftComp advantage

Professor Maitland, who first worked at Schlumberger, says that SoftComp provided an ideal way to allow industry to collaborate with academic groups. “SoftComp enabled short-term exchanges of researchers between laboratories which broadened the range of research done,” he says.

Contact

Professor Geoffrey Maitland
Imperial College London, UK
✉ g.maitland@imperial.ac.uk



The SoftComp advantage

Scientists working on soft matter have started to apply their knowledge and methods to complex processes in biological membranes. SoftComp has provided a focus for discussion at the Network meetings and workshops and in research collaborations.

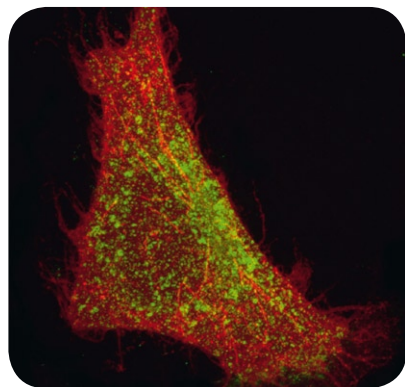
Bending biological membranes

Physics is providing powerful new insights into dynamic cellular processes

The living cell represents the ultimate soft-matter system, with self-organising molecular assemblies that also form larger-scale architectures. Because cells are dynamical objects, they show the same strain and flow behaviour as any polymer or surfactant solution put under stress. A better understanding of these biophysical changes can lead to new therapeutic treatments for disease and to novel biomimetic technologies.

Artificial cells

To study such complex behaviour experimentally, biophysicists employ simplified artificial cells called giant unilamellar vesicles (GUVs). These structures comprise a spherical lipid bilayer filled with water, which can vary from 20 to 100 micrometres across, and so match the dimensions of cells and organelles.



The Shiga toxin (red) causes a cell membrane to bend inwards, forming tubules by means of which it can enter the cell

Patricia Bassereau and colleagues at the Curie Institute, Paris, France, have been using GUVs to develop new physical models of cellular function. In particular, they have turned their attention to understanding the transport of biomolecules between organelles. Long tubular lipid vehicles are thought to form, pulled by molecular motors called kinesins along fixed protein rails. The researchers showed that when these motors are bound to a GUV in contact with microtubules, the GUV is locally deformed into a long tube, just as in a real cell. "We were able to test our model of this mechanism by varying the parameters, showing it was correct," says Dr Bassereau.

The team has also used GUVs to study changes in the shape of cell membranes triggered by protein binding. They demonstrated how the Shiga toxin, a protein produced by *E. coli*, binds to a specific membrane receptor, forming clusters and inducing a local spontaneous curvature. This causes the membrane to bend into tubules, which then provides a conduit for the toxin to enter the cell. Dr Bassereau is already collaborating with other SoftComp groups to design drug-delivery systems based on this principle.

Forces of nature

A biological cell membrane is supported by a cytoskeleton of actin filaments (p. 23), and several SoftComp partners

are interested in measuring the mechanical properties of a membrane anchored to an actin network. Theoretician Nir Gov at the Weizmann Institute of Science in Rehovot, Israel, has proposed a model that explains how the shapes of cells are determined by forces generated through coupling between the cytoskeleton and membrane. His colleague Sam Safran has looked at the orientation of cells in response to applied stresses, which is a factor in directing tissue growth and healing. He has also been modelling cells on curved substrates, as are found in blood vessels and bones. "These systems are extremely difficult to model because you have to take into account that the cell is consuming energy and can exert its own forces in addition to mechanistic and thermal effects," says Professor Safran. This kind of work is relevant to a type of tissue engineering called organ printing, where cells are literally printed layer by layer in a gel so that they organise into new tissue.

Contact

Dr Patricia Bassereau

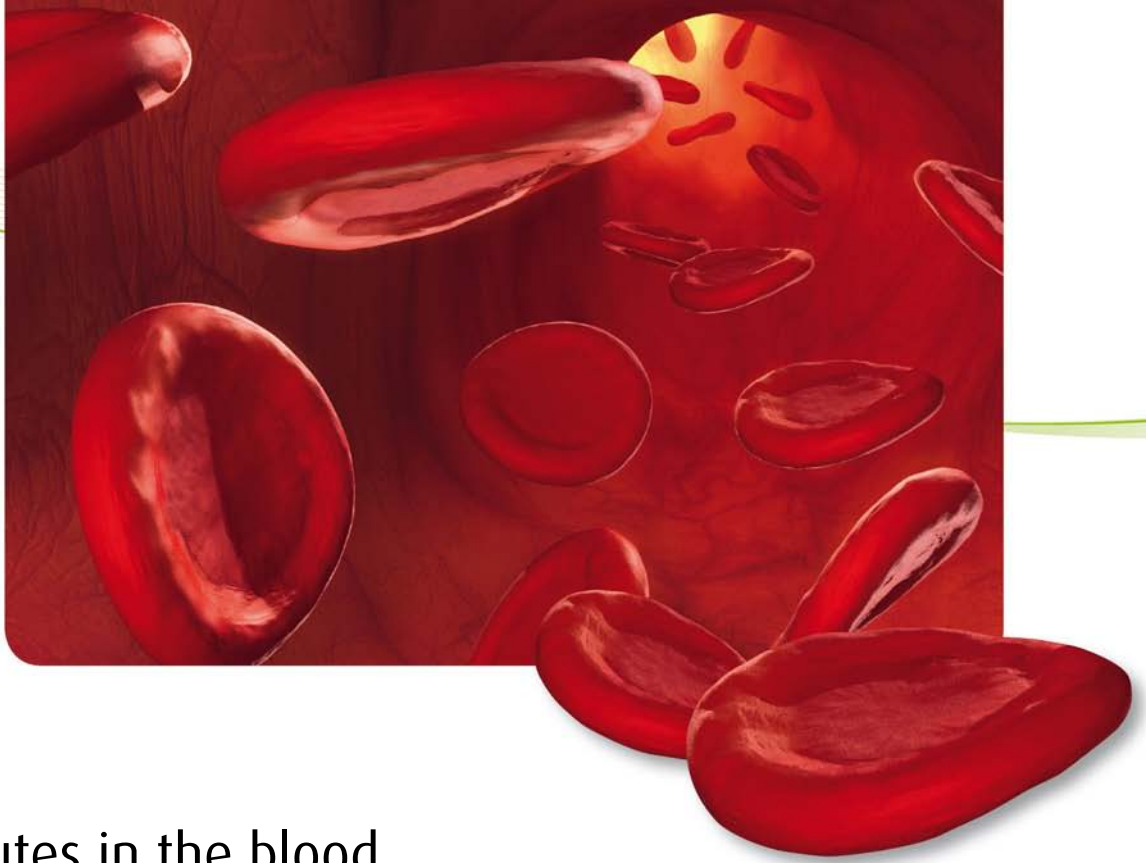
Curie Institute, Paris, France

✉ patricia.bassereau@curie.fr

Professor Sam Safran

Weizmann Institute of Science, Rehovot, Israel

✉ sam.safran@weizmann.ac.il



Parachutes in the blood

Red blood cells are just flexible enough to maintain a healthy blood circulation

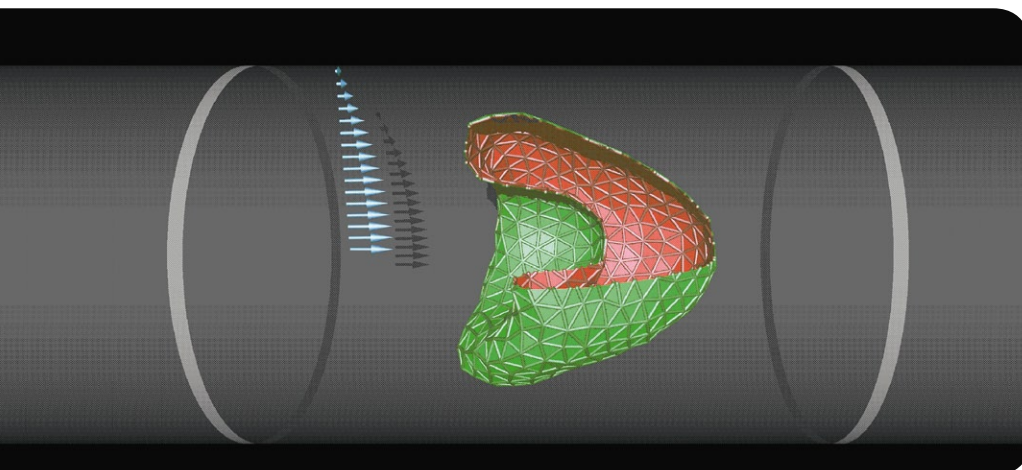
The blood coursing through our veins, arteries and capillaries literally keeps us alive. It is a highly complex system, consisting of a fluid plasma which transports the oxygen-carrying red blood cells, the protective white blood cells, blood platelets and a myriad of essential molecules including proteins. Blood is, in fact, a typical soft composite – and, not surprisingly, how it flows through finely branched vessels has a critical effect on our health.

A key influence is the micron-sized red blood cells, which account for 45 per cent of the volume of blood and are by far the dominant cellular component. Physicists find their flow behaviour intriguing because they are not spherical but shaped like biconcave discs which deform under stress. Unlike the vesicles contained in many synthetic complex fluids, which have very fluid membranes, red blood cells have lipid membranes supported by an internal protein network which

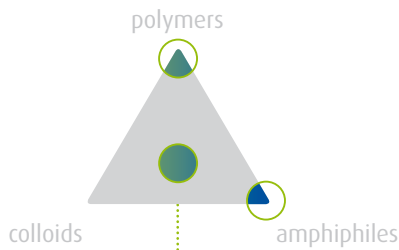
makes them more elastic, like soft rubber. Some diseases, however, such as diabetes and sickle cell anaemia, render them more rigid. This is thought to increase the flow resistance of blood, which then affects circulation. Understanding the link between the deformability of the blood cells and their motion, especially in the confines of capillaries, is thus of interest to clinicians as well as soft-matter scientists.

Cluster power

Gerhard Gompper, a theorist at Forschungszentrum Jülich, Germany, has been interested in the flow of red blood cells for several years. Using the SoftComp supercomputer cluster (p. 31), he has been developing advanced simulation techniques to predict how the shape of red blood cells changes when they flow in a very narrow tube. Observational studies on flowing red blood cells had already shown that they deform into parachute shapes, and computer simulations enable this behaviour to be probed in more detail. “With the increased computer power made available, we were



Disc-shaped red blood cells become parachute-shaped when they flow (the arrows show the velocity profile)



The SoftComp advantage

Professor Gompper works with a number of research groups in the SoftComp network who are interested in microemulsions and polymer flow, as well as those working on biologically based problems. "The advances in computer methods achieved through SoftComp mean that we can start to answer questions that we could not address ten years ago," he says.

able to study the system taking into account the full hydrodynamic interactions and the deformability," says Professor Gompper.

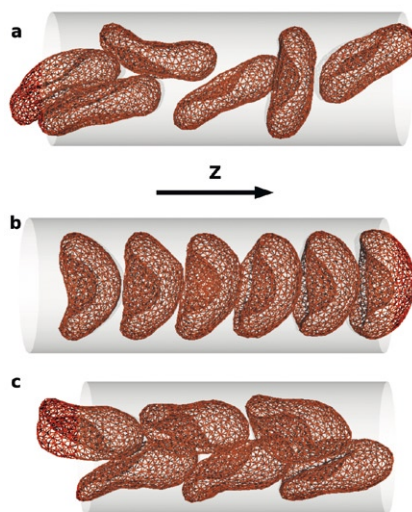
By calculating the deformation energy due to the curvature and shear elasticity of the cell membranes, and treating the surrounding liquid as a stream of moving, colliding particles, the simulation confirmed that above a certain flow velocity the cells do, indeed, bend back in the shape of a parachute. In comparison, a simple, more fluid lipid vesicle just elongates into a rugby-ball shape aligned in the direction of the flow. Professor Gompper believes that the transition to the parachute shape limits the flow resistance in a way that maintains a healthy blood circulation, and regulates oxygen delivery around the body.

Modelling real blood

In the real system, the red blood cells tend to cluster and they also interact with other components in the bloodstream. Professor Gompper is now working on simulations of how groups of red blood cells move together in microvessels. Starting with up to six cells, and assuming no attractive interactions between them, he showed that they go through a series of complex manoeuvres, first forming a chaotic array of discs which then deform and stack into parachutes as the flow rate increases. At the

same flow rate but higher density, the sides of the cells nearest the tube walls elongate forming 'slipper' shapes in a zigzag arrangement.

These results have aroused the interest of the biomedical community, and Professor Gompper is now planning collaborations with medical research groups to take the work further. He hopes to look at more complex systems, including the large-scale flow of red blood cells in wider vessels or in those with more complex, branching geometries. "We will also mix in other components," he says. "For example, it would be interesting to



Computer snapshots of elastic vesicles at increasing flow rates and densities, moving randomly at first, and then stacking up as parachutes, and finally forming a zigzag of slipper shapes



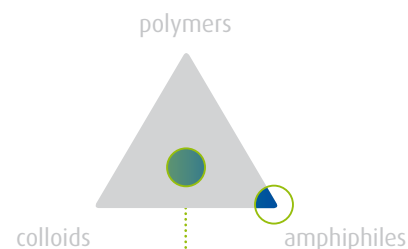
Manipulating the flow of cells is important in the new technology of microfluidics

simulate how red blood cells interact with blood platelets, because this will help us to understand blood clotting," he adds.

A commercial area that should benefit from this research is microfluidics, whereby minute volumes of liquids are manipulated in geometrically constrained environments at the microscale. Microfluidics is revolutionising clinical diagnosis and biological research, and often involves separating and manipulating cells under continuous-flow conditions in microfabricated channels. Computer simulations could provide data on how to control the flow in relation to cell properties.

Contact

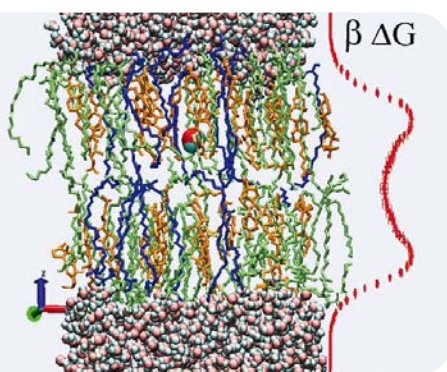
Professor Gerhard Gompper
Forschungszentrum Jülich, Germany
✉ g.gompper@fz-juelich.de



Science goes skin deep

The way to a soft and healthy skin starts with fundamental research into its molecular and mechanical properties

Walk into any department store and the first thing you see is the beauty counter displaying creams and lotions proclaiming how they care for your skin. Backing up those claims is vital, and companies producing personal-care products are increasingly investing in basic research on how the skin works and what kind of ingredients can promote a healthy skin. As an active partner in the SoftComp network, Massimo Noro and his colleagues at Unilever, Port Sunlight, UK, have been collaborating with several university research groups on experiments and computer simulations on model lipid systems that mimic the properties of human skin.



A computer model showing the diffusion of a water molecule (the sphere) through a lipid bilayer

The outermost layer of the skin is a composite biomaterial of protein-rich cells embedded in organised double layers of various lipids in a 'bricks and mortar' arrangement. The main lipid component is the ceramide molecule, which has two hydrophobic hydrocarbon tails of different lengths and a very small hydrophilic head. These long, thin, flexible molecules pack together, grasping each other in a tight embrace through hydrogen bonding, to form an excellent barrier protecting the body.

A computer model

"We decided to build, first, a simple model of the skin on the computer, based on a lipid bilayer of pure ceramide, and then simulate how water would penetrate it, using a molecular dynamics program," says Dr Noro. Using a classic penetration enhancer, the simulations showed that this molecule nudged its way between the hydrophilic ceramide heads thus breaking the lipid-lipid hydrogen bonds to form its own hydrogen bonds with ceramide. The result was that the rigid gel-like structure of the lipids loosened into a more liquid state, which became softer and more permeable to water. "Combining the simulations with atomic force microscopy and

scattering measurements, we can couple the penetration mechanism with changes in mechanical properties. No-one had done this before, so it was very exciting," says Dr Noro.

With theorist Peter Olmsted of the University of Leeds, UK, the Unilever researchers then simulated the diffusion of water molecules through more complex, more realistic lipid layers also containing cholesterol and free fatty acids, and compared the results with measurements made on real skin. The team went on to carry out simulations of how these special lipids help improve the effectiveness of the membrane barrier. Professor Olmsted is interested in phase changes in lipid solutions and is now applying his expertise to transitions in biological membranes such as skin.

Contact

Dr Massimo Noro

Unilever, Port Sunlight, UK

✉ massimo.noro@unilever.com

Professor Peter Olmsted

University of Leeds, UK

✉ p.d.olmsted@leeds.ac.uk

The SoftComp advantage

Dr Noro says that SoftComp gave Unilever the opportunity to send its scientists to academic institutes to be trained in specialised and advanced techniques: "They came back with a lot of useful hands-on knowledge." Through the SoftComp links, a subgroup was set up to study the skin, which has led to a new UK-funded collaboration. "It would not have happened without SoftComp," adds Professor Olmsted.



SoftComp partners can make use of large-scale facilities such as neutron scattering through the Network's Experimental Platform

Strengthening scientific excellence

The SoftComp Network has set up an infrastructure aimed at bringing together a critical mass of resources and expertise that will underpin European leadership in research on soft-matter composites

Research into soft matter requires diverse resources, including the skills required to create complex and sometimes exotic materials, combined with a wide range of experimental equipment to characterise them. In order to achieve a quantitative understanding at the deepest level, it is also essential to model the behaviour of materials theoretically or numerically on a computer, or both.

Individual research groups working on soft matter often specialise in particular aspects. They may have developed a novel instrument or methodology for measuring properties, or, if theorists, they may have a particular simulation method that can then be applied to a wide range of problems. They may make new materials with model structures that are ideal for testing fundamental properties predicted by theory, or for exploring attributes of commercial interest, or even for validating the performance of commercial equipment.

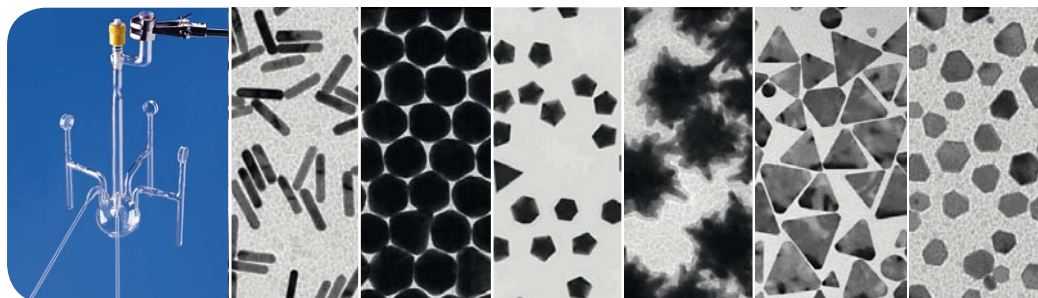
Three Research Platforms

The SoftComp Network of Excellence has been able to integrate all these activities by establishing three Research Platforms, through which scientists can access the resources available in partner laboratories. These are:

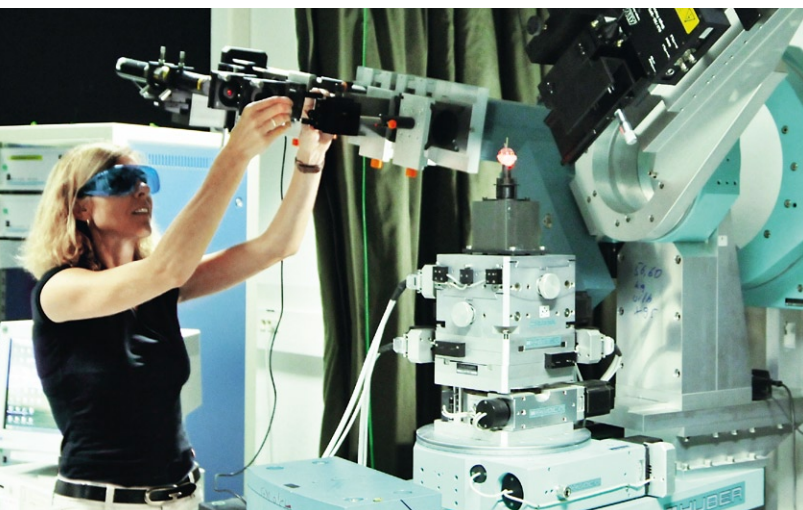
- Synthesis
- Experimental techniques
- Theoretical and numerical methods

The aim of this infrastructure is to strengthen research capabilities within

the SoftComp community by providing the means to ensure that the outcomes of research are fully optimised in an efficient and economic way. Each platform is coordinated by a designated scientist, through whom research teams can make appropriate arrangements for access to materials and equipment, as well as any necessary training. Although research groups rely on their existing SoftComp funding arrangements to make use of the Platforms, they can apply to the Network's central budget if additional support is required.



Specialised materials for experiments, such as nanoparticles, are synthesised and made available through the Synthesis Platform



The Synthesis Platform

Several research groups have expertise in synthesising specialised materials for experiments, and an inventory of available samples has been placed on the SoftComp website. "The inventory helps people to broaden and enrich their research, exploring composite materials they would not have thought of using before" says Luis Liz-Marzán of the University of Vigo, Spain, who organises the Synthesis Platform.

Samples available include polymers with different architectures. Jürgen Allgaier at Forschungszentrum Jülich, Germany, for example, synthesises well-characterised polymers, not only for colleagues in Jülich but also for other SoftComp partners. "It is important to characterise the material extremely well, in terms of chain length, molecular weight distribution and branching, for experiments," he explains. "We have made H-branched polymers for flow experiments (p. 10), which had precisely two, well-defined arms, no more and no less," he adds. In addition, Dr Allgaier prepares polymer samples for neutron-scattering experiments, in which hydrogen atoms have been selectively replaced by the heavier isotope deuterium (p. 19). Polymers with well-defined star shapes are also supplied by Dimitris Vlassopoulos and his colleagues at the University of Athens, Greece (p. 21).

Another important group of materials essential for studies of soft composites are colloids; some are available through

Professor Liz-Marzán and his group. They supply not only metallic nanoparticles – gold nanorods and spheres and silver platelets (p. 15, 29) – but also more sophisticated materials such as latex spheres coated with carbon nanotubes. "We supply nanospheres with fluorescent tags for studies of the transport of viruses through biological membranes, for example. We have also collaborated on developing complex nanocomposites prepared from polymers and nanoparticles. The Synthesis Platform has led to many more connections between research areas than expected; it has been really successful," he explains.

The Experimental Platform

Soft matter research requires a diverse range of experimental tools, from large central facilities such as the Jülich Centre for Neutron Science at Garching near Munich, Germany, which provides neutron beams for scattering experiments, to smaller specialised equipment belonging to individual partners, which is specifically designed to make measurements relevant to soft-matter research. Many of the instruments are not available commercially, and are often unique, having been developed by a research group with a certain experiment in mind. The Experimental Platform maintains an inventory of where such equipment is located, which is then made available to visiting partner groups, including PhD students and postdoctoral researchers, who are given training in its use. "This infrastructure, which is perhaps the most sustainable and enduring element in

the SoftComp Network, is unique in the world and has been a real success," says Peter Schurtenberger of the University of Fribourg, Switzerland, who leads the Experimental Platform.

Equipment includes novel light-scattering instruments and specialised microscopes, which are used to investigate structure at the microscopic length scales typical of soft-matter composites. Professor Schurtenberger's own laboratory has a suite of such instruments which are suitable for studying samples relevant to industrial applications. Other research groups such as the team at the University of Leuven, Belgium, can offer specialised rheometers for measuring properties related to processing conditions (p. 17). Characterisation at smaller scales can be done using neutron and X-ray scattering, spectroscopy and nuclear magnetic resonance. "We now have the framework to create a virtual large-scale facility with an absolutely outstanding and unique instrument suite that allows the Network partners to make measurements over all necessary length and time scales for complex systems. That is one of the outstanding features of SoftComp," says Professor Schurtenberger.

The Theory and Simulation Platform

Because soft-matter composites have complex hierarchical structures and dynamical properties, especially under non-equilibrium conditions, statistical and numerical techniques requiring large amounts of computer power are essential to describe their behaviour.



An advantage of SoftComp is that novel and unique light-scattering instruments developed by one research group can be used by other partners in the Network (far left)

Small-angle neutron scattering is one of the main techniques for studying molecular and larger soft-matter structures (centre, right)

The SoftComp partners therefore agreed to set up a dedicated computing infrastructure for the Network. Eight research groups invested 50 per cent of the funds needed, while the other 50 per cent came from the central budget. The Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich agreed to host and operate the facility.

A Linux computer cluster with a processing power of one teraflop was installed in 2006. Then, with additional funding from the German Government, the size of the cluster was doubled in 2008. The intention was to embed the SoftComp cluster users as a working group – a so-called virtual organisation – into the German D-Grid. In a grid, resources like computing power and storage are distributed among a number of locations. “The partners contribute their own resources and using the appropriate software particular jobs can then be run on the most suitable computer in the grid,” says Willi Homberg of the JSC.

Within the Theory and Simulation Platform, theorists develop algorithms to tackle physical problems pertinent to soft matter, such as thermodynamic properties, structure, or flow behaviour. “We are constantly improving existing algorithms to find the best way to solve a particular problem. Computer simulations complement experiments because they can explore the underlying physical processes and mechanisms in more detail or over a wider range of conditions,” says the Platform leader, Wolfgang Paul of Martin Luther University in Halle, Germany, who worked at the University of Mainz, Germany, until 2009.

The SoftComp computing grid has funding for another two years. Professor Paul would like to see it expand and become the nucleus of a broader European grid for soft-matter research. “It works very nicely for the participating groups but we would like to see it grow into a more permanent institution,” he comments.

Contact

Dr Jürgen Allgaier

Forschungszentrum Jülich, Germany

✉ j.allgaier@fz-juelich.de

Willi Homberg

Forschungszentrum Jülich, Germany

✉ w.homberg@fz-juelich.de

Professor Luis M. Liz-Marzán

University of Vigo, Spain

✉ lmazaran@uvigo.es

Professor Wolfgang Paul

Martin Luther University,
Halle, Germany

✉ wolfgang.paul@physik.uni-halle.de

Professor Paul Schurtenberger

University of Fribourg, Switzerland

✉ peter.schurtenberger@unifr.ch



The SoftComp Theory and Simulation Platform has a dedicated computing infrastructure based on a Linux computer cluster. The partners hold regular meetings to discuss theoretical approaches in soft-matter research



Spreading the word

Dissemination of knowledge and training of the next generation of scientists are key components of SoftComp

One of the roles of the SoftComp network is to disseminate knowledge of both techniques and results among the partners and others, and to provide the means to support the training and education of research students. This is implemented through a stimulating programme of conferences, combined with workshops, laboratory courses, schools, and inter-institute visits.

Education and training

• Exchange visits

Through SoftComp, all researchers, from PhD students to senior scientists, have

been encouraged to make exchange visits with other partner laboratories, where they are given the opportunity to use specialised equipment not available in their home laboratory, along with additional training. Academics with expertise on specialised topics visit other institutions to give lecture courses to PhD students and postdocs.

• Eurothesis programme

To train PhD students in working with various different types of soft-matter systems and techniques, SoftComp set up the Eurothesis programme, whereby

a student at one institution can spend at least six months in the laboratory of another SoftComp group. In this way, students not only broaden their expertise but also have the opportunity to experience a different research environment in another country.

• Schools and laboratory courses

Educational opportunities for students have also been made available through laboratory courses and schools hosted by various partner institutions. These include a two-week spring school held each year at Forschungszentrum Jülich,

Researchers at the 2009 Annual SoftComp Meeting held in Venice, Italy, were also able to enjoy the city's historic surroundings (right)

SoftComp partner institutions host laboratory courses for students in experimental techniques such as neutron scattering (p. 33)



Germany, covering advanced experimental techniques and applications, and theoretical and computer simulation methods, at both an undergraduate and graduate-student level. More specialised schools have included courses on neutron scattering, rheology and its application to different soft-matter materials, nuclear magnetic resonance, and light-scattering techniques.

"SoftComp contributes to these activities, encouraging as many students as possible to take them up," says SoftComp Educational Officer, Peter Olmsted of the University of Leeds, UK.

Dissemination

• Conferences

The main scientific conference for SoftComp is the Jülich Soft Matter Days. This meeting is organised once a year and brings together scientists, including researchers who are not necessarily

SoftComp members, working in all the soft-matter areas, including biophysics. More than 200 people regularly attend. In 2007, a larger conference, the first International Soft Matter Conference, was held and was attended by more than 600 scientists. SoftComp plans to organise further similar conferences every three years.

Once a year, all members are invited to attend the SoftComp Annual Meeting, which for many young academics often offers the first international platform for the presentation of their results.

• Workshops

Small focused workshops are regularly held that explore topics of mutual interest in two or more of the network research areas within SoftComp. Industrial workshops are also held, where the industrial partners can discuss scientific issues relevant to their R&D programmes

with their academic colleagues, and in the process strengthen academic-industrial contacts.

• The SoftComp Newsletter

SoftComp produces a newsletter once a year, which contains articles written at a popular level on all aspects of the SoftComp programme and subject areas, with special emphasis on applications. All past issues of the newsletter can be accessed on the internet: www.eu-softcomp.net/news/news

Contact

Professor Jan K. G. Dhont

Forschungszentrum Jülich, Germany

✉ j.k.g.dhont@fz-juelich.de

Professor Peter Olmsted

University of Leeds, UK

✉ p.d.olmsted@leeds.ac.uk



Achievements of SoftComp

The SoftComp Network of Excellence started in 2004, and is now in its sixth year at the time that this brochure is published in autumn 2009. The following information gives some idea of the breadth, uptake and output of the programme.

Membership

Membership of SoftComp extends across Europe, covering twelve countries from the UK to Israel, and involves scientists with a diverse disciplinary background (physics, chemistry, biology, computer science and process engineering). 35 academic groups in 29 institutions are participating, including most of the main European research teams working on soft matter (p. 4). The Network also provides an opportunity for smaller groups, often with specialised expertise but limited resources, to maximise their output. Six companies are members, including major multinational organisations able to provide invaluable information on applications and industrial

process techniques, while benefiting from fundamental research carried out by academic groups. SoftComp was financed by an EU grant until 30 November 2009. A new consortium agreement has been set up for the SoftComp future, which foresees an annual fee from each participant. Only five SoftComp partners have decided not to continue membership in the next phase, while new ones will be joining.

Organisation and financing

During its 66-month lifetime, SoftComp received € 6,200,000 in funding. About 60 to 65 per cent of the funding was allocated to SoftComp partners for activities. These activities included, for example, a focused funding programme for strengthening the Research Platforms, with eight instruments and twelve joint positions funded.

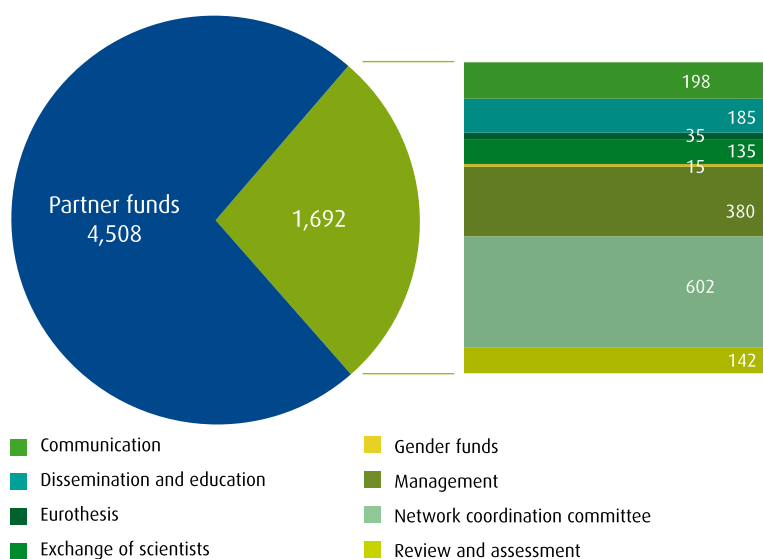
The remainder was used to support the central budget. This covered

administration and communications costs such as the website, the dissemination and education programme, the Annual Meeting, or exchanges of scientists and visits to research platforms (p. 32). A gender fund was set up to help with childcare costs for women going to conferences.

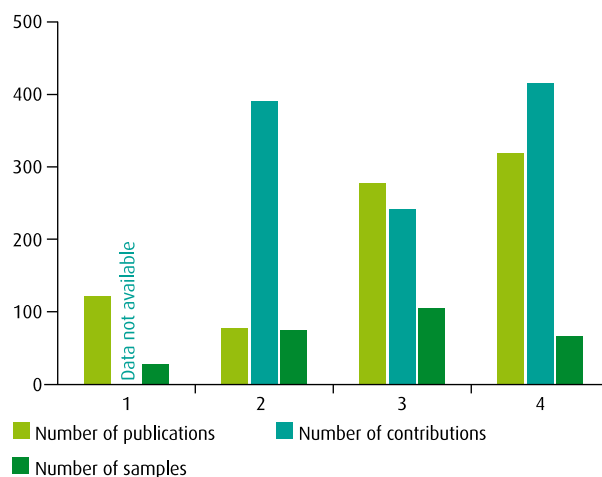
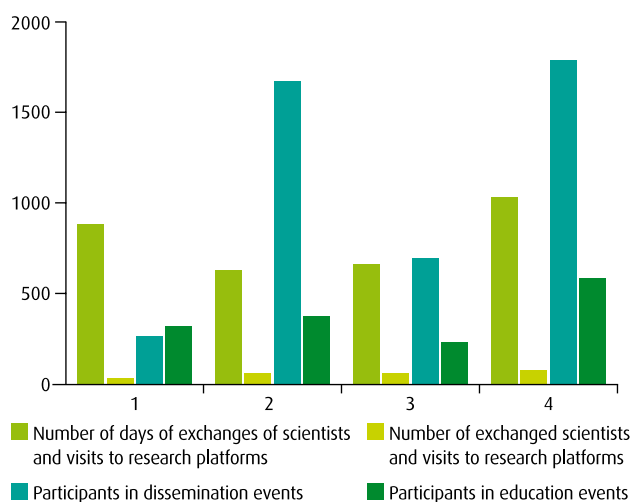
Delivery

The following data are for the first four years.

- **Exchange of scientists:** 43 scientists for a total of 2,038 days (5.6 years), on average 47 days per exchange
- **Visits to Research Platforms:** 203 scientists for a total of 1,180 days (3.2 years), on average 6 days per visit
- **Samples exchanged between partners:** 273
- **SoftComp contributions to conferences (invited, oral, poster):** 1,047
- **Dissemination events supported (workshops, conferences, topical meetings):** 30 with 4,437 participants
- **Education events supported (schools, lab courses):** 19 with 1,525 participants
- **Total number of research papers:** 794 (of which 152 publications are joint publications by two or more SoftComp members)
- **Papers published in leading journals:**
 - Nature journals* 11
 - Science* 3
 - Phys. Rev. Lett.* 78
 - Biophys. J.* 31
 - Macromolecules* 70
 - J. Phys. Chem. B* 31
 - Langmuir* 52
 - J. Chem. Phys.* 94



Distribution of the SoftComp budget according to activity (in 1,000 euros)



SoftComp activities over four years: (left) visits and exchanges, education and dissemination; (right) publications, samples provided and contributions (invited, oral, poster)

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Concept and editing: Angela Wenzik

Editing: Angela Wenzik, Dieter Richter, Hugo Bohn, Flavio Carsughi

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