

Editorial

The two scientific articles in this newsletter present an exciting view of nanotechnology and soft matter research. While the article on nanotechnology provides a wide overview of the enormous contribution made by colloid chemistry to the broad field of nanotechnology, the article on soft matter research of applications gives an idea of what products and processes are considered under the heading soft matter research in industry.

Additionally fundamental differences in the methodological approaches in academia and industrial research – despite the similarities – become visible.

Future Newsletters will continue with similar overviews of the broad research spectrum of the SoftComp Network of Excellence.

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

Hugo Bohn & Dieter Richter 

Latest News

International Soft Matter Conference 2007

1-4 October 2007

Eurogress Aachen

www.soft-matter.net

...for more information see page **8**

New SoftComp Linux Cluster now operational

...detailed information see page **7**

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Colloid Science for Nanotechnology

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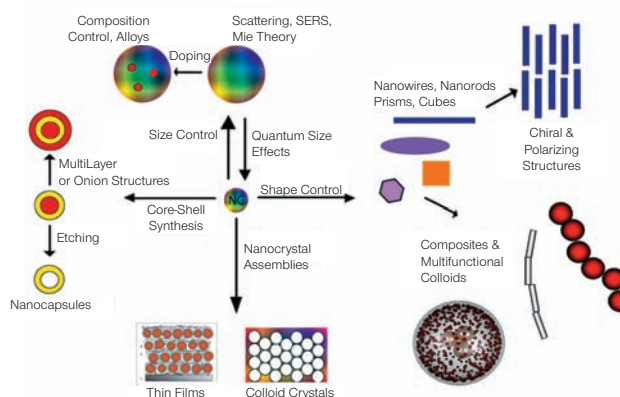
Introduction

There seems to be general agreement regarding the assignment of the birth of nanotechnology to the lecture presented by the Nobel laureate Richard Feynman at an American Physics Society meeting back in 1960. It was an unusual lecture entitled “There is plenty of room at the bottom,” in which Feynman predicted the existence of an unexplored area of research related to a scale just above the size of atoms and molecules, suggesting that if manipulation of matter on such a scale was achieved, the whole Encyclopaedia Britannica could be written on the head of a pin.¹ The idea of manipulation and assembly of atoms and molecules immediately became very appealing and the imagination of artists and science fiction

writers flew way faster than scientific developments in the area. Predictions were quickly made on the construction of nanobots to travel through the body and selectively attack or cure infected cells, or the fabrication of molecular machines *nanoengineered* to carry out work in very limited space.^{2,3}

These early predictions then gave rise to fears related to the self-replication of such nanomachines, which ultimately might achieve control over mankind, such as in the popular thriller by Michael Crichton, *Prey*.⁴ All this rapid popularization of nanotechnology did much more harm than good to the development of the field, since there was a high risk of it not being taken seriously. Fortunately, responsible scientists were able to convince politicians and funding bodies of the huge potential of

Figure 1



Schematic drawing summarizing the studies on synthesis, characterization and manipulation of nanoparticles that are possible using colloid chemistry.

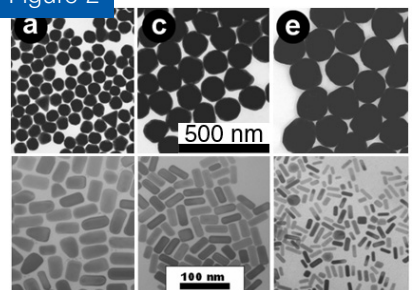
Colloid Science for Nanotechnology (continued)

nanotechnology in a large number of fields, so that it eventually was taken seriously enough to start investing specifically in this area, in such a way that it has become a priority area in most technologically advanced countries. As soon as funding was available, a definition was required to decide which proposals would qualify in this area. A useful definition is included "Research and technology development at atomic, molecular or macromolecular levels, in the length scale of approximately 1–100 nanometer range, to provide a fundamental understanding of phenomena and materials at the nanoscale and to create and use structures, devices and systems that have novel properties and functions because of their small and/or intermediate size."⁵ It thus seems clear that the main point is the change in material behaviour as a result of particle size. It is also interesting that the size range is somehow the lower end of the traditional size range of colloidal particles (typically 1 nm – 1 μm), which of course suggests that we should be able to profit from all the knowledge accumulated during the past century in the field of colloid science, which can now be applied to face the challenges of nanotechnology. The obvious link is the enormous increase in surface to volume ratio as particle size is decreased, so that interface properties soon become more relevant than bulk properties. An overview of the degree of manipulation in the nanoscale that can be achieved through colloidal synthesis and processing techniques is provided in Figure 1. Starting from particle size control with the objective of establishing a correlation between size and physicochemical properties, all aspects from doping, multilayer coating and capsule formation, nanoparticle shape control, to thin film, multilayer assembly and nanocrystallization have been extensively studied during the past few decades.

Metal Nanoparticles. Size and Shape Effects

What is the colour of gold? In this context it is obvious that the answer must be: *it depends on particle size*, and indeed it does! But size is not the only relevant parameter, since the optical response is also largely determined by the shape of the particles, interparticle distance, and the nature of the surrounding medium.⁶ Fortunately, the tremendous development of colloid chemistry has boosted the synthetic capabilities and a large number of papers have been published on the preparation of metal colloids of various sizes and shapes, so that the effect of all these parameters can be studied independently. Examples of size and shape control are shown in Figure 2 for gold spheres and rods. Relatively large spheres have been selected to demonstrate optical changes (see below) as well as size control over a wide range. Although one could say that in these samples each particle is different from all the others, we need to realize that macroscopically we see the average response, and therefore a narrow size distribution is already good news.

Figure 2



Transmission electron micrographs of gold nanospheres of various sizes⁷ (top) and of gold nanorods of varying aspect ratios⁸ (bottom).

In the visible spectra measured for these samples and shown in Figure 3, one can clearly see the large influence of both size and shape, but the

reasons for the colour changes derived from increasing particle size (Figure 3a) are rather different from those arising due to increasing particle anisotropy (Figure 3b), as will be briefly explained in the following.

We must bear in mind that the origin of the absorbance bands is the interaction of light with surface electrons, leading to collective oscillations which are known as surface plasmons.⁶ When

Figure 3a

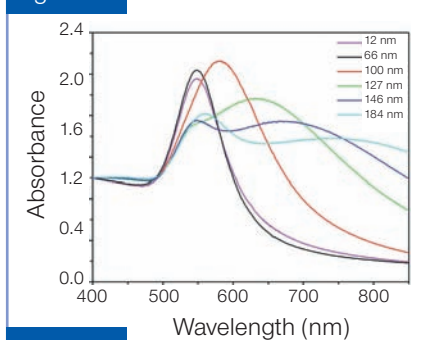
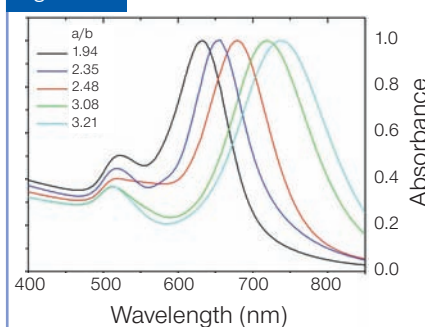


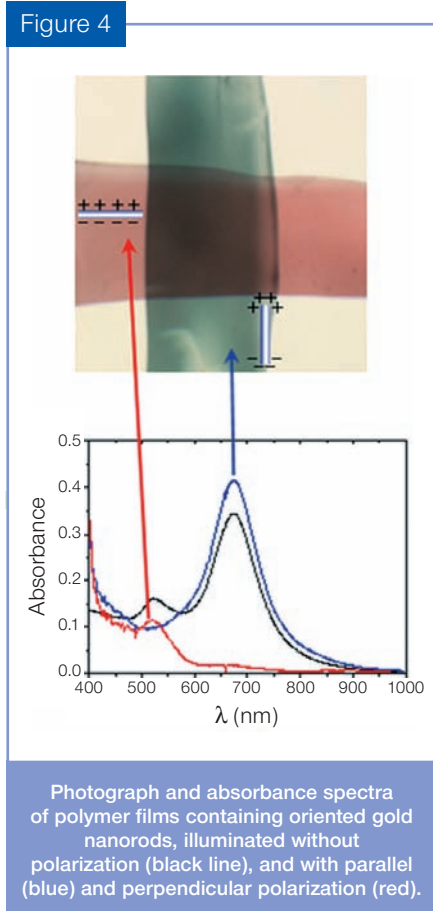
Figure 3b



UV-visible spectra of hydrosols containing gold spheres and rods as shown in Figure 2.

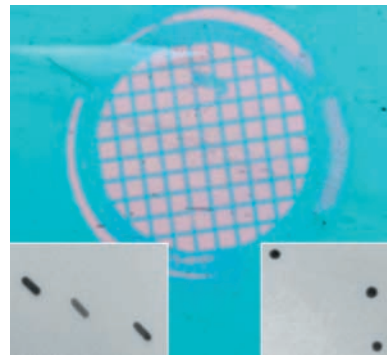
the particles are very small compared to the incident wavelength, only a dipole resonance is possible (black spectrum in Figure 3a), whereas when the spheres become larger, losses due to surface scattering decrease the resonance efficiency, so that the band shifts to lower energies and becomes broader. Above roughly 100 nm, quadrupolar plasmon resonances are possible, leading to a second absorbance band at lower wavelengths, as can be seen in the figure. Thus, if we are restricted to sizes below 50 nm, the surface plas-

mon frequency of gold nanoparticles remains basically constant (although for sizes below about 5 nm strong changes are observed due to quantum effects). However, the situation is completely different for non-spherical particles, such as nanorods (Figure 3b). First of all, the spectra of gold nanorods display two distinct bands because oscillations both along and across the rods are possible and require different energies (both are present in the spectra of colloidal dispersions because the rods are randomly oriented). Second, while the so-called *transverse* plasmon band (at lower wavelength) varies only marginally, tiny



changes in nanorod aspect ratio (length over width) are responsible for large shifts of the *longitudinal* plasmon band, quickly reaching the near-IR and thus promoting drastic colour changes.

Figure 5



Optical micrograph of a nanorod-containing polymer film upon irradiation with a nanosecond laser. Transmission electron micrographs show the morphology of the particles in non-irradiated (rods) and irradiated (spheres) areas.

The ability to tune the absorption frequency as well as the orientation-dependent optical response opens up a whole new range of practical applications for these systems.

Orientation Effects. Patterning and Encoding

Let us now return to the anisotropic response of gold nanorods. As a direct consequence of anisotropy, if we are able to fabricate samples containing nanorods aligned with the same orientation over macroscopic distances, we should be able to observe different colours when changing the polarization of the incident light. This is demonstrated in Figures 4 and 5, which include a photograph of two polymer films containing gold nanorods that were aligned by stretching the polymer. In this photograph, the incoming light is polarized parallel to the blue film (exciting the nanorod longitudinal plasmon mode) and perpendicular to the red film (exciting the rod transverse plasmon mode). The corresponding extinction spectra confirm the correspondence between the absorption bands and the

electron oscillation modes.

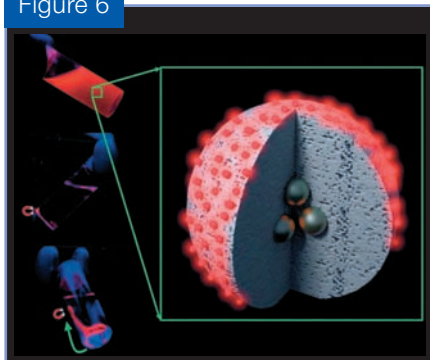
Another interesting property of gold nanorods is related to a rather high sensitivity to heating, meaning that, even though the melting point for gold has been reported to only depend on particle size below 10 nm, nanorods are observed to reshape into spheres at much lower temperatures (of the order of 200 °C).⁹ This thermal reshaping seems to be related to a higher mobility of surface atoms, and to a higher thermodynamic stability of the spherical geometry as compared to the cylindrical one. In a more sophisticated experiment, localized heating of the nanoparticles was achieved using intense, ultrafast laser beams.¹⁰ The right-hand photograph in Figure 4 shows the effect of irradiating a polymer film containing aligned nanorods with a single pulse of an intense nanosecond laser beam through a TEM copper grid, which acts as a shadow-mask. As a consequence, rod-to-sphere conversion occurs only in the areas actually irradiated, so that the grid pattern is perfectly reproduced on the film with a colour contrast derived from the different spectral response of rods compared to spheres. Additionally, since the frequency of the transverse plasmon band for rods is very close to that of the single band for spheres, just by changing the polarization of incident light the contrast between irradiated and non-irradiated areas can be drastically changed. Applications of this effect can be foreseen for security printing.

Multifunctional Colloids. Magnetic and Optical Response

A final example of the versatility of colloid chemistry for the design and fabrication of functional nanomaterials is the possibility of incorporating more than one functionality into a single

Colloid Science for Nanotechnology (continued)

Figure 6



Schematic showing the structure of composite silica colloids with magnetic cores and luminescent dots on the surface. The photographs of the dispersed colloid (top), after the particles accumulate near a magnet (middle) and upon displacement of the magnet (bottom) were taken under UV illumination.

colloidal particle, which will certainly increase the potential for practical applications. If we are able to synthesize nanoparticles which simultaneously display magnetic and luminescent properties, they could be dragged under the influence of an external magnetic field and their movement could be easily monitored through the photoluminescent signal. If such particles are designed to carry encapsulated drugs, they can almost be seen as a primitive version of the medical nanobots described in the introduction.

The fabrication of multifunctional materials will typically require various synthetic steps to incorporate the necessary, independent ingredients. The design shown in Figure 5 involves the synthesis of magnetic (Fe_3O_4) nanoparticles, which are then embedded within a spherical silica (SiO_2) matrix, onto which luminescent quantum dots (CdTe) are homogeneously assembled. This has been recently accomplished¹¹ by a combination of sol-gel and electrostatic self-assembly techniques. Figure 6 also demonstrates that the particles can be dragged by a weak external magnetic field by showing photographs (with UV illumination for excitation of the CdTe

luminescence) of the dispersed colloid, the particles agglomerated near a hand-held magnet, and how the concentrated particle phase follows the magnet when this is displaced near the walls of the container. In a future step, similar experiments will be performed in biological media, including drug encapsulation and release.

Conclusions

In this short article it was intended to provide a general overview of the enormous contribution that colloid chemistry can make to the broad field of nanotechnology. In fact, colloid scientists have been working on nanoscale objects for over a century, with important applications in various areas, such as the food or detergent industries, to name but two. However, all the knowledge accumulated on synthesis and surface properties is a valuable background that will find even more numerous applications when it is applied to fabricate and manipulate objects with size-dependent properties, as required by the concept of nanotechnology.

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About SoftComp

SoftComp...

...is a Network of Excellence – a tool developed under the 6th Framework Programme of the European Commission dealing with the integration of European research, with the intention of strengthening scientific and technological excellence. In particular, SoftComp aims to establish a knowledge base for intelligently designing functional and nanoscale soft matter composites.

It will do so by overcoming the present fragmentation of this important field for the development of new materials at the interface of non-living and living matter, where the delicate principles of self-organization in polymeric, surfactant and colloidal matter are ubiquitous.

This Network of Excellence has created an integrated team able to activate the European potential in soft matter composite materials and thus to disseminate excellence through extensive training and knowledge transfer schemes. Presently about 260 SoftComp members have registered at SoftComp's web portal.

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 SoftComp Web Portal: www.eu-softcomp.net 

Soft Matter Research in the Chemical Industry

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Introduction

Shampoos, plastic bags, detergents, vitamins, adhesive tapes, concrete, paint, saltwater desalination – this short list, which could go on and on, gives an idea of what products and processes are considered under the heading of *Soft Matter Research* from the industrial point of view. Polymer materials, like polystyrene and polyamide, are familiar in everyday life as typical products of the chemical industry. What is less well known, however, is that polymers make a substantial contribution to the quality of life in non-visible forms, as so-called *active materials*, such as cosmetics, pharmaceuticals, and detergents. Supramolecular structures (**soft matter**), on a scale ranging from nano to micrometres, and combinations of ingredients (**composite matter**) determine the physical characteristics and, therefore, the process-related characteristics of polymer raw materials as well as active materials. For this reason, understanding the relationships of the structural characteristics of soft matter composites is a precondition for paving the way to innovations.

Structure Property Relationships

One of the goals in industrial research is to acquire sufficient understanding of which structures, ranging in length scales from the atomic to the macroscopic, have which effects in applications. The term *application* is not only related to classical aspects like strength or transparency, but also to traits like the fluidity of colloidal systems, workability, adsorption tendency, paintability, bioavailability etc. In all cases, the characteristics resulting from structural connections on the molecular and mesoscopic levels must be understood. A question of particular importance is how the structures are formed during the production/application of the system and how the structural formation can be controlled. On the basis of this understanding, market conditions or direct client requirements can be converted into physical questions and solution proposals. To give an idea of the typical physical problems in the chemical industry, the following two examples will show where physics is involved with some of the terms mentioned at the beginning of the article.

Particles and Paints

In the case of commercial paints, for example, a typical question is: what does a certain paint have to be composed of so that it can be applied properly, is long-lasting, is sufficiently permeable to water vapour, and also looks good? In addition to the many specifically chemical questions pertaining to the composition of paint made from polymer nanoparticles and pigments, one of the many problems facing the scientist is how a homogenous film is formed from polymer globules that are about 100 nm in size, see Figure 1. We gained particular insight from experiments with small-angle X-ray and neutron scattering. We could see that the polymer globules arranged themselves in a crystalline superstructure – an effect that could be recorded with electron-microscopic methods and that is of current interest in connection with the development of optical switch units (*photonic crystals* [1]). We were also able to discover the range in which the polymers – of which the nanoparticles consist – become interdiffused and give the film its stability.

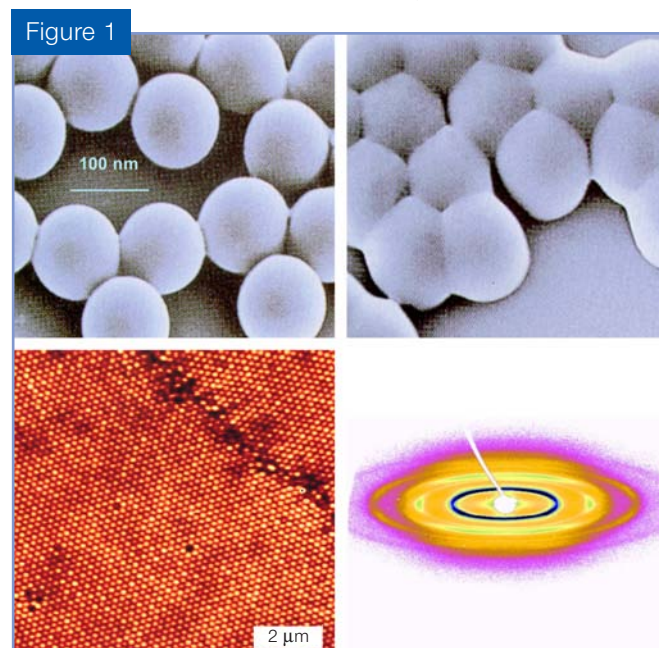


Figure 1
 Polymer dispersion made of compact polymeric particles of around 100nm (top left) that fuse when the water evaporates (top right). Upon suitable preparation the particles pack in crystalline structures that can be used for colour effects or in the development of photonic crystals. Bottom left: AFM image taken on a colloidal crystal; bottom right: small-angle X-ray scattering data from a dried and stretched film made from a polymer dispersion [2].

Soft Matter Research in the Chemical Industry (continued)

The dispersion data also show how water is stored in the moist films in wedges between the packed globules and in the empty cells. Understanding these mechanisms makes it possible to optimize water and water vapour permeability.

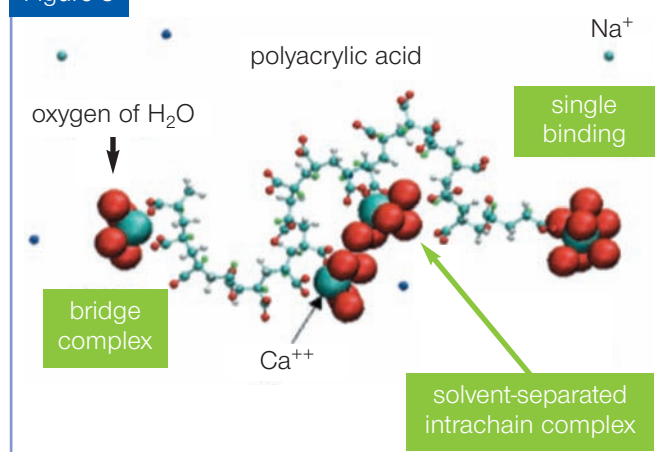
Polymers and Crystallization

The incrustation (scaling) in domestic appliances as well as in seawater desalination plants is caused by the deposition of inorganic salts like CaCO_3 , CaSO_4 , Mg(OH)_2 , etc. which become insoluble at elevated temperatures. The formation of scale is due to the precipitation and crystal growth of such substances. In order to control these processes several approaches are conceivable, one of which is the reduction / prevention of scaling by the introduction of polymers – as is evidenced by the successful use of polycarboxylates in seawater desalination plants and laundry detergents.

In order to further improve polymeric incrustation inhibitors it is essential to understand the physicochemical mechanisms on a molecular level. However, crystallization of inorganic (and organic) matter often proceeds via intermediate stages [3] – rather than by simple nucleation and growth mechanisms. These precursor stages not only comprise crystal modifications that are less stable than the final one, but amorphous, hydrated (nano-)particles and emulsion-like precursors have also been observed. These

precursors tend to aggregate or restructure before being dissolved and entering the next structural stage. Structural information on all these intermediates – and the mechanisms by which they form – is essential for the development of additives to control crystallization processes.

Figure 3



Example of the result of a molecular dynamics simulation of the interaction between polyacrylic acid and Ca^{2+} ions [4]. The water molecules that are included in the simulations are not shown for the sake of clarity.

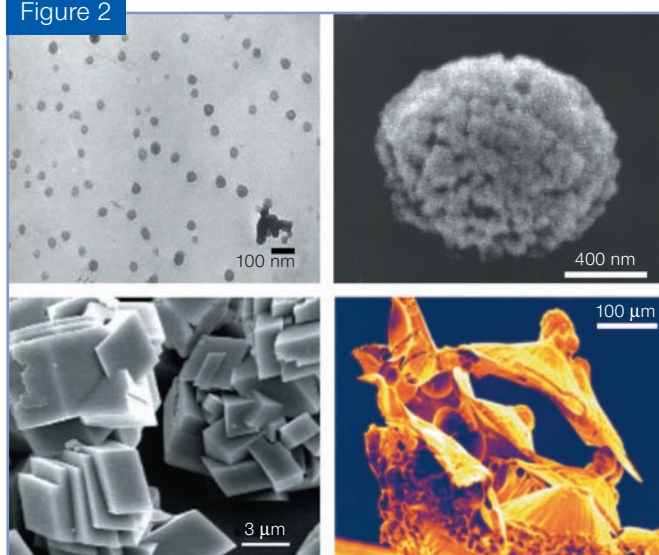
This information is obtained by combining various scattering and microscopy methods and special equipment to obtain access to time-resolved data. A typical example is given in Fig. 2 showing the various morphological stages during the precipitation / crystallization of CaCO_3 .

Since charged polymers, like proteins and synthetic polycarboxylates, not only interact with inorganic precursors and crystals but also with cations right from the beginning of the precipitation / crystallization reaction it is essential to understand the details of this interaction. Recent molecular modelling experiments on the complexation mechanisms of calcium to polycarboxylates unravel an unexpected richness in the binding process – for binding states, see Figure 3, and their time evolution [4].

Research in Industry, Research in Academia

Although the same instruments are used in both industrial and university research (diffractometer, spectrometer, microscope etc.), there are still fundamental differences, despite similarities concerning methodological approaches – both in terms of manner of working and how the data are handled. These differences can be summed up in an imper-

Figure 2



Micrographs taken on samples prepared at various stages during the precipitation of CaCO_3 . Top left: after some seconds amorphous CaCO_3 nanoparticles form; they aggregate (top right), and recrystallize via the liquid phase to calcite (bottom left). By adding water-soluble polymers to the reacting system it is possible to prevent the crystallization step or to control the crystallization to obtain specific crystal morphologies (bottom right).


ative that a successful industrial scientist must consider: **Research should be performed as thoroughly as necessary, and with an application in mind.** This means, in many cases, a fundamental understanding is sought for the relationships of structural characteristics at the molecular level, but that the structural connections do not always have to be calculated *to the third decimal place*.

We believe that basic research is the domain of universities because they are in a precompetitive field. As a result, it is the industrial researcher's task to recognize quickly which approaches for basic research can be transferred into products or processes. For this reason, BASF has established more than 1200 alliances with academic institutions around the world.

Challenges

Finally, we come to the question which areas of physics we think, are in need of more intensive research. The problems listed below can be solved on a case-by-case basis using experimental screening in the relevant parameter range. But, basically, the emphasis is on unsolved matters in a physical sense. Though not exhaustively listed, the issues are: computer simulation of structure-forming processes on all levels of length – from the atomic to the mesoscopic and to the macroscopic level, formation and structure of foams, formation mechanisms of (organic) nanoparticles in water, optimization of surfaces (scratch-resistance, adhesive ability), combined materials research (including high-throughput screening) with adapted physical methods, and finally, *formulations*. Formulations are systems with two or more components that are used by the consumer such as shampoos, medications, paints, cosmetics and cleaning agents (*soft matter composites*). Formulations are also synthetic additives like pigments and nanoparticles. These products, almost without exception, have been developed empirically (*optimization by trial*). For the specific development of new products or the improvement of existing products, it is clearly necessary to understand the physical interaction of components.

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New SoftComp Linux Cluster Now Operational



New Linux cluster

On 8 November 2006 an opening ceremony for the new SoftComp cluster was held at the Central Institute for Applied Mathematics (ZAM) of Research Centre Jülich. The computer cluster was financed in a joint effort by eight member groups of the Theory & Simulation Platform with strong support by the focused funding initiative of the SoftComp Network of Excellence. The cluster was installed by ZAM and the soft- and hardware delivery companies Transtec and ParTec and will be administered by ZAM.

The members of the Theory & Simulation platform and ZAM will cooperate in using this computer as a competitive large-scale computing facility for soft matter simulations. The cluster has a peak performance of 1 Tflop, significantly enhancing the computing capabilities within the network. It serves as focal point for integration activities within the Theory & Simulation Platform. It is expected that the cluster will contribute to grow both in installed CPU power and number of contributing groups. 



Opening of the Linux cluster

Vacancies

Postdoctoral position in soft matter and biomaterials theory...

...available in the summer/autumn of 2007 at the Weizmann Institute. The postdoc will have the opportunity to work on theoretical studies of charged membranes, cell shape, adhesion and self-assembly, membrane rafts and other problems in both soft matter physics and biological physics. In addition, he/she can interact with the broad range of activities in biological physics and soft matter physics at the Weizmann Institute.

www.weizmann.ac.il/fluids/Safran/positions.htm
Contact: sam.safran@weizmann.ac.il

Postdoc or PhD position...

...available in the field of mesoscale hydrodynamics simulations of polymers in flow, in the theory group at the Institute of Solid State Research (IFF) in Jülich.

www.fz-juelich.de/iff/e_th2
Contact: g.gompper@fz-juelich.de
r.winkler@fz-juelich.de

Post doctoral position in the adhesion group at CRPP, Pessac, France...

...for details see:

www.eu-softcomp.net/news/jobs
Contact: fabre@crpp-bordeaux.cnrs.fr

Postdoctoral position in soft matter and biomaterials theory...

www.weizmann.ac.il/fluids/SafranGroup
 Postdoctoral fellows benefit from interaction with the wide variety of research conducted at the interface between physics and biology and physics and materials science in other groups at Weizmann, as well as the opportunity to travel to conferences in Europe and the US.

www.weizmann.ac.il/feinberg/postdoc_fell/
Contact: sam.safran@weizmann.ac.il

Postdoctoral fellowship for computer simulations of skin lipids...

...available at Unilever, to work on the structure and dynamics of skin lipids, using computer simulation techniques, part of a joint project between Unilever R&D Port Sunlight and Leeds University.

Contact: massimo.noro@unilever.com

SoftComp Events related to PhD Education

Date	Conference/Place	Contact
12-23 Mar 07	Summer School Probing the Nanoworld Jülich · Germany	K. Urban
Apr 07	Soft Condensed Matter & Advanced Colloid Systems Utrecht · The Netherlands	A. van Blaaderen
Sep 07	European School on Rheology: Rheological Measurements Katholieke Universiteit Leuven/Louvain · Belgium	P. Moldenaers
03-14 Sep 07	11th JCNS Laboratory Course on Neutron Scattering Jülich/Munich · Germany	D. Richter
Autumn 2007	Lab Course on Broadband Dielectric Spectroscopy Methods in Polymers and Related Materials Donostia/San Sebastián · Spain	J. Colmenero

...more information on International Soft Matter Conference 2007

In recent years, the various disciplines of soft matter – investigating the behavior of polymers, colloids, surfactants, membranes and biomaterials – have increasingly converged.

To a large extent, this is due to the increasing interest in composite materials which combine several components of a polymeric, colloidal or amphiphilic character.

The application of soft matter concepts to biological and biomimetic systems is among the grand challenges for the next decades.

Therefore, the time is ripe for a large international conference bringing together scientists from all disciplines of soft matter.

This conference will take place at the Eurogress Conference Centre in Aachen from 1-4 October 2007. It will emphasize the interdisciplinary approach in this field by connecting theoretical, computational and experimental physics, physical chemistry, material science, and biology. The conference will also cover the full range of investigations from basic science to modern technological applications, and is thus intended to foster the exchange between academia and industry.

Coming Up...

SoftComp Conferences & Workshops	Date
SoftComp Topical Meeting "Biomimetics" Paris (Curie) · France Coordinators: G. Gompper · P. Bassereau	15-16 Jan 07
Network Area 2+3 Meeting Paris (Curie) · France Coordinator: G. Gompper · P. Bassereau	16 Jan 07
SoftComp Topical Meeting "Micro (or nano-)scopic Engineering of Rheological Properties" Leuven/Louvain · Belgium Coordinator: D. Vlassopoulos	01 Feb 07
Network Area 1 Meeting Leuven/Louvain · Belgium Coordinator: D. Vlassopoulos	31 Jan 07
Annual SoftComp Meeting Erice Sicily, Italy	02-05 May 07
<ul style="list-style-type: none"> • NA Meetings • Industrial Meeting • EU Report Meeting • NGB04 Meeting • NCC14 Meeting 	02 May 07 03 May 07 03-04 May 07 05 May 07 05 May 07
Mainz Materials Simulation Days 2007 Mainz · Germany Contact: W. Paul	13 Jun - 15 Jun 07
Length Scales and Heterogeneous Dynamics in Glassy Materials Oxford · United Kingdom Contact: L. Cipelletti	Summer 07
International Soft Matter Conference 2007 Aachen (Eurogress) · Germany Contact: J.K.G. Dhont	01-05 Oct 07
FIT: French-Israeli Trends in soft matter, biophysics and microfluidics. 4th French-Israeli Soft Matter Meeting Biarritz · France · Contact: P. Fabre	04-07 Oct 07

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