

Network of Excellence

www.eu-softcomp.net

Editorial

In 2013, interesting events took place in the SoftComp community, and some new procedures and features were implemented.

First, we modified the structure of the newsletter itself. Starting with the current edition, the newsletter will feature a selection of research highlights by the SoftComp network of the past year. Second, in the future, SoftComp will support a few topical workshops every year, focusing on topics of particular interest to the network, but open to all interested researchers. These workshops will be announced in the newsletter with a short description of their content.

In the current edition, the research highlights are followed by an outlook on the next-generation neutron-scattering facility for material research and life sciences, the European Spallation Source ESS, which is about to start its construction phase in 2014. This description is split into two parts. The first part describes the new frontiers for soft-matter-composites research. The second part provides a short look at the actual facilities.

A very important event this year was the 3rd International Soft Matter Conference, ISMC 2013, which took place in Rome in June. The conference brought together more than 800 scientists and provided an excellent overview of current and future research directions in Soft Matter science. A short summary of the conference can be found in this newsletter.

In addition to the print version of the newsletter, SoftComp plans to set up an internet microsite, aimed at interactive internal communication, picture animation, web links and faster actualization. The first version is planned to go online in spring 2014.

Finally, we would like to take the opportunity to wish you a Merry Christmas and a Happy and Successful New Year.

Hugo Bohn & Gerhard Gompper

In This Issue





SoftComp Network Research Highlights 2013

Plasmonic Mesoporous Composites as Molecular Sieves for SERS Detection

V.López-Puente, S.Abalde-Cela, P.C.Angelomé, R.A.Alvarez-Puebla and L.M. Liz-Marzán – Soft-Comp partner: CIC BiomaGUNE

Detection of small organic molecules in biological samples is often complicated because of the presence of other (larger) biomolecules such as proteins and nucleic acids. These biomolecules often interfere with the analysis methods by contaminating the transducer signal. The group headed by Luis Liz-Marzán recently reported the design and fabrication of a thin-film material that acts as a molecular sieve, filtering out the large molecules and allowing small ones through for detection by surface-enhanced Raman scattering spectroscopy. In SERS, the molecules to be analysed must be adsorbed onto the surface of the particles, so that they can be affected by the electromagnetic field enhancement related to localized surface plasmon resonances. Such field enhancement leads to huge Raman signals that are characteristic of each molecule. In biological fluids, large proteins and nucleic

acids can also adsorb onto the metal and their Raman signals can mask those from smaller molecules. In the new approach, a mesoporous material is grown on gold nanoparticles deposited on a glass substrate. The pores are then used as templates to grow thin tips from the nanoparticles so that they provide greater SERS enhancement. Additionally, the pores can act as molecular sieves to prevent the diffusion of large biomolecules and only allow smaller molecules to reach the metal underneath. The performance of the films was tested by using a simplified biological fluid containing bovine serum albumin (BSA) and 4-nitrobenzenethiol (NBT), as a model small molecule with a high Raman cross section. The results of SERS measurements indeed indicated that NBT could diffuse through the 6-nm-diameter pores of mesoporous titania, whereas BSA could not.



Transmission electron micrograph showing gold nanoparticles embedded in a mesoporous titania film. The nanoparticles were used as seed catalysts to grow thin branches for SERS enhancement. The inset shows a schematic view of the molecular sieving effect, where small MBA molecules diffuse through the pores but larger BSA do not because of size restrictions.



Skin – a Marvellous Functional Barrier

C.Das, M. Noro and P. Olmsted - SoftComp partner: Unilever, Univ. Leeds

The outermost part of the skin (the stratum corneum, SC) keeps us from drying up, protects us from dangerous chemicals, and is the first line of defence against foreign pathogens. While pliable, it resists mechanical and dehydration stresses [2]. New computer simulations show how the glue that holds the SC together is structured and gives skin its remarkable properties. The SC comprises water-retaining 'bricks' of proteinaceous dead cells (corneocytes) [3] surrounded by an impermeable 'mortar' made of roughly twenty solid layers of lipids (soap-like molecules, oils, and cholesterol) [4]. This mortar is responsible for the skin's extraordinary barrier properties.

We have run massive computer simulations on realistic SC lipid mixtures. We find that the spontaneous phase of SC lipids in water is not layered; rather, the lipids encase water droplets in a so-called 'inverted micelle' structure, matching electron microscopy observations from larger irregular spaces between corneocytes. However, the simulations show that adjacent SC corneocyte walls actually induce layers, through an envelope of covalently-bound lipids whose molecular corrugation encourages the low-permeability 'mortar' layers between the 'brick' faces. These simulations relate the sometimes paradoxical biochemical pathways for lipid synthesis to the physical lipid structures found in the SC, and shed light on the reason for the relatively long time required for skin barrier healing. The simulations also suggest how the lipid mixture provides plasticity and allows the skin to absorb energy, as well as enabling three-dimensional packing of corneocytes without compromising the barrier. Hence, this work can assist future efforts to make, heal, and nourish skin; moreover, the fundamental physics is relevant for making new functional nanomaterials based on self-assembly.

Figure 1



Simulation of a the evolution of a hydrated double bilayer, showing that an unconstrained layered state is unstable to the formation of water drops encased within inverse micelles. The bilayer is a polydisperse mixture of ceramides, free fatty acids, and cholesterol, which is representative of lipid bilayers in the stratum corneum.

Patterning Polymer–Fullerene Nanocomposite Thin Films with Light

H.C.Wong, A.M.Higgins, A.R.Wildes, J.F.Douglas, J.T.Cabral – SoftComp partner: Imperial College London and ILL

Trace amounts of nanoparticles, including fullerenes, can impart stability to thin polymer films against dewetting by the combined effects of pinning the contact lines of dewetting holes and by effectively altering the polymer-substrate interaction. Polymer nanocomposite thin films stable to dewetting eventually yield well-defined morphologies from uniform to spinodal-like, via spontaneous polymer-nanoparticle phase separation and crystallization. In this paper, we show that UV-visible, and even background, light exposure, can finely tune the morphology of dewetting and phase separating polymer-fullerene thin films. Neutron reflectivity allows us to locate the various constituents within the film. We find a coupling of fullerene photosensitivity and both self-assembly processes, which results in controlled pattern formation, and we illustrate the potential with a model polymer-fullerene circuit pattern. We believe this approach opens new opportunities in soft matter lithography via the directed

assembly of polymer nanocomposites and underscores their photoactive nature, an effect of great interest to material performance and stability of organic photovoltaics (OPV) and aerospace materials under long-term radiation exposure.





Capillarity-Induced Ordering of Spherical Colloids on an Interface with Anisotropic Curvature

D.Ershov, J.Sprakel, J.Appel, M.A.Cohen Stuart, and J.van der Gucht SoftComp partner: Univ. Wageningen

Objects floating at a liquid interface, such as breakfast cereals floating in a bowl of milk or bubbles at the surface of a soft drink, clump together in space-saving hexagons to minimize the disruption of the liquid interface. Micrometre-sized colloidal particles embedded in a liquid interface normally do not disrupt the interface, so that such clustering does not occur. Here, we show that this is different when the interface has a curvature that is anisotropic. We find that in this case the condition of constant contact angle along the three-phase contact line can only be satisfied when the interface is deformed. We present experiments and numerical calculations that demonstrate how this leads to quadrupolar capillary interactions between the particles, giving rise to organization into regular square lattices. We demonstrate that the strength of the governing anisotropic interactions can be rescaled with the deviatoric curvature alone, irrespective of the exact shape of the liquid interface. Our results suggest that anisotropic interactions can easily be induced between isotropic colloids through tailoring of the interfacial curvature.



Square lattice organization of colloids on a droplet with anisotropic curvature. Particles are labelled with a fluorescent dye to make them visible.

Emergence of Metachronal Waves in Cilia Arrays

J.Elgeti and G.Gompper – SoftComp partner: FZJ-Gompper

Propulsion by cilia is a fascinating and universal mechanism in biological organisms to generate fluid motion on the cellular level. Cilia are hair-like organelles, which are found in many different tissues and many uni- and multi-cellular organisms. Assembled in large fields, cilia beat neither randomly nor completely synchronously - instead they display self-organization in the form of metachronal waves (MCWs). The main questions are how the individual cilia interact with the flow field generated by their neighbours and synchronize their beats for the metachronal wave to emerge, and how the properties of the metachronal wave are determined by the geometrical arrangement of the cilia, such as cilia spacing and beat direction. We address these issues by large-scale computer simulations of a mesoscopic model of two-dimensional cilia arrays in a three-dimensional fluid medium. We show that hydrodynamic interactions are indeed sufficient to explain the self-organization of MCWs, and study beat patterns, stability, energy expenditure and transport properties. We find that MCWs strongly increase both propulsion velocity and efficiency - compared to all cilia beating in phase. This can be a vital advantage for ciliated organisms, and may be interesting to guide biological experiments as well as the design of efficient microfluidic devices and artificial microswimmers.



Cilia beat by alternating power and recovery strokes, which are characterized by nearly extended and curled-up shapes, respectively. Hydrodynamic interactions lead to the formation of metachronal waves.

About SoftComp

SoftComp is a Network of Excellence – a tool developed under the 6th Framework Programme of the European Commission dealing with the integration of European research, with the intention of strengthening scientific and technological excellence. In particular, SoftComp aims to establish a knowledge base for an intelligent design of functional and nanoscale soft matter composites. It will do so by overcoming the present fragmentation of this important field for the development of new materials at the interface of non-living and living matter, where the delicate principles of self-assembly in polymeric, surfactant and colloidal matter prevail. This Network of Excellence has created an integrated team that is able to activate the European potential in soft matter composite materials and thus disseminate excellence through extensive training and knowledge transfer schemes. Since December 2009, when EU funding came to an end, Softcomp has been a self-supporting consortium consisting of 38 research groups belonging to 33 different institutions.

SoftComp partner details

www.eu-softcomp.net/about/part

Network coordinator

www.eu-softcomp.net/about/part E-mail: g.gompper@fz-juelich.de

Registration

If you would like to register for the SoftComp portal, please contact: E-mail: f.carsughi@fz-juelich.de



Effect of Nanoconfinement on Polymer Dynamics: Surface Layers and Interphases

M. Krutyeva, A. Wischnewski, M. Monkenbusch, L. Willner, J. Maiz, C. Mijangos, A. Arbe, J. Colmenero, D. Richter – SoftComp partner: FZJ-Richter, Univ. Basque Country

The presence of a solid surface reduces the number of possible conformations of a polymer chain and influences the dynamics, in particular for those macromolecules which are close to the surface. In this work, we demonstrate that the attractive polymer-surface interaction leads to the formation of the frequently discussed interphase in a confined linear polymer melt using neutron spin-echo (NSE) spectroscopy. The dynamics of polydimethylsiloxane (PDMS) confined in cylindrical nanopores of anodic aluminium oxide is strongly affected by the confinement and is characterized by two phases, one that is fully equal to the bulk polymer and another that is partly anchored at the surface. By topological interaction, the anchored part confines further chains with no direct contact to the surface. They form the frequently mentioned interphase.

The confined phase is internally highly mobile and not glassy, unlike current opinions in the literature. These results are inferred from the space-time dependent chain dynamics observed in terms of the single chain dynamic structure factor and represent the first direct and quantitative observation of the interphase.



Left figure: The NSE results for confined PDMS. Solid lines show fitting to the two-phase model. In the insert, the sketch of the two-phase model is shown. Right figure: Schematic representation of the artificial surface-induced entanglements in the confined polymer melt. Black line represents the chain adsorbed on the surface of AAO nanopore, red lines show entangled chains in the confined phase.

3rd International Soft Matter Conference ISMC 2013: A Review

Francesco Sciortino and Emanuela Zaccarelli Dipartimento di Fisica and CNR-ISC, Sapienza Universita' di Roma, Rome, Italy

The 3rd International Soft Matter Conference (ISMC2013) was held in Rome from 15 to 19 September 2013. Following previous meetings in Aachen (2007) and Granada (2010), the conference was organized jointly by Sapienza University of Rome and the European Consortium SOFTCOMP. Eight topics were selected by the Program Committee: Biological Soft Matter, Colloids, Dynamics of Complex Fluids, Membranes, Polymers, Self-Assembly, Surfaces and Interfaces, and Soft Nanotechnology.

The conference featured eight plenary talks, twenty-five keynote talks and one hundred contributed oral presentations, selected from more than 700 abstracts. The final number of posters was 720, displayed in four lively sessions. In total, about 840 participants from 45 different countries took part in ISMC 2013. Of those, 194 were from outside Europe, with a very large contingent from Japan. The unprecedented number of submissions of scientific contributions and of participants demonstrate how active, lively and interdisciplinary the soft-matter community is.

During the conference, the EPJE – Pierre Gilles De Gennes Lecture Prize – reserved for outstanding scientists for their contribution to Soft Matter research – was awarded to Prof. Julia Yeomans of the University of Oxford (UK) for her profound contribution to the dynamical behaviour of complex and active liquids. Further, the conference hosted the 2013 edition of the Soft Matter Lectureship, an annual award to honour a young soft-matter scientist. The recipient was Professor Eric M. Furst of the University of Delaware (USA).

ISMC 2013 was also supported (besides SOFTCOMP and Sapienza) by the Italian National Research Institute (CNR) through the Department of Physical Sciences and Technologies of Matter and its institutes CNR-ISC and CNR-IPCF. Several sponsors contributed to the success of the conference, including Soft Matter World; American Chemical Society; European Physical Journal; IOP Publishing; RSC publishing; LS instruments.

Proceedings will be published in Soft Matter as regular articles and highlighted through a dedicated website. Dr. Kantorovich and Dr. Zaccarelli will act as guest editors.





The European Spallation Source – the Next-Generation Facility for Soft Matter, Materials Research and Life Sciences

F. H. Bohn, P. Schurtenberger

ESS and SoftComp – a happy couple

Scientific activities in SoftComp have always been driven by a research philosophy where soft matter is seen as a rapidly expanding area of fundamental and highly interdisciplinary research, but at the same time also as being at the core of industrial and technological applications in materials science, personal care, pharmaceutical and food industries, to name but a few. The underlying structure and composition of SoftComp directly reflects the ultimate challenge for contemporary soft matter research: to understand the equilibrium and non-equilibrium properties not only of well-defined model systems, but also of those that we experience in everyday life and industrial and technological applications. With its focus on complex soft matter systems, SoftComp will thus strongly profit from the exciting research opportunities offered by ESS.

Designing, manipulating and processing complex materials requires a comprehensive understanding of the roles of the constituent components and their interactions. This is a task for which neutrons with their high penetration depth and sensitivity to isotopic labelling are ideal probes. Many of the research projects conducted within SoftComp focus on often highly complex samples under non-equilibrium conditions, and thus need investigations that cover a large range of length scales with high spatial and temporal resolution. At present, this often fails due to the current limitations in neutron flux, temporal and spatial resolution. This is exactly the area in which ESS will excel, thus creating the potential for major breakthroughs in fundamental and applied soft matter research that is at the heart of SoftComp. While the final instrument suite is not yet fully defined, it is already clear that many of the instruments at ESS will have unique properties that directly address the requirements of current and future activities of SoftComp. The key techniques for addressing soft matter at ESS will undoubtedly include small-angle neutron scattering (SANS), reflectometry and neutron spin-echo spectroscopy (NSE). They will be able to

fully profit from the unique properties of ESS, and, for example, allow us to investigate significantly smaller gauge volumes than currently feasible, while covering an extended range of scattering vectors for time-resolved in situ studies utilizing a multitude of dedicated sample environments and auxiliary techniques. However, ESS will not only provide exciting opportunities for traditional soft matter areas such as colloids and polymers. It will also have enormous implications for SoftComp activities devoted to biological matter. When attempting to decipher the intricate cellular machinery and the biological function of complex multi-component structures, modern life sciences have to seek structural

its unprecedented neutron flux combined with the exciting possibilities offered by the planned deuteration laboratory and computer modelling activities will have the potential to revolutionize many areas in the life sciences. This will include key experiments that utilize, for example, small-angle neutron scattering to understand what makes individual proteins aggregate at the onset of a condensation disease, neutron spin echo to characterize the motions of proteins in the crowded environment of a cell, and neutron tomographic imaging to study the three-dimensional organization of biological tissues and organisms.

A number of SoftComp groups are not only eagerly waiting for ESS to become



and dynamic information that ranges from atomic and molecular details all the way to the structure and functioning of an entire organism. This is where neutrons in combination with selective isotope labelling excel with their ability to discern separate components and subunits and characterize their structure and their motions. However, current requirements for sample volume, the limited neutron flux and the present state of the art of preparing partially deuterated biological macromolecules at concentrations comparable to those in native biological systems make many important experiments unfeasible today. ESS with operational, but are already actively involved in design and development tasks. Several of SoftComps educational and outreach activities are helping to create the next generation of expert users who can fully profit from ESS's unique capabilities from day one, thus further strengthening Europe's leading role in soft matter research. However, given the difficult financial situation that many European countries face we can't take things for granted, and as a community we need to become actively involved to make sure that this unique opportunity for our research activities will not remain a dream.



The European Spallation Source - the Next Generation Facility for Soft Matter, Materials Research and Life Sciences (continued)

ESS Project Overview

The need for an advanced, high-power neutron facility was articulated 20 years ago. Attempts to realize a 10MW, long- and short-pulse target station facility failed. In 2008, this concept was identified as the way forward by the European User Community and was acknowledged by the ESFI/ESS Site Review Group, In 2009, the European research authorities decided that ESS would be built in Lund, Sweden. During a design update phase from 2010 to 2013, the present concept of a 5MW single long-pulse source was developed and is documented in the ESS Technical Design Report. The European Spallation Source (ESS) will be a multi-disciplinary research laboratory based on the world's most powerful neutron source. ESS can be likened to a large microscope, where neutrons are used instead of light to study materials - ranging from polymers and pharmaceuticals to membranes and molecules - to gain knowledge about their structure and function. ESS will be around 30 times brighter than existing facilities, opening up new possibilities for researchers in, for example, health, chemistry, fundamental physics, environment, climate, energy, transport sciences and cultural heritage. ESS is an intergovernmental research infrastructure project. Currently 17 European countries are partners in the ESS project, and will

take part in the construction, financing and operation of the ESS. The partner countries are: Sweden, Denmark, the Czech Republic, Estonia, France, Germany, Hungary, Iceland, Italy, Latvia, Lithuania, the Netherlands, Norway, Poland, Spain, Switzerland and the United Kingdom. The European Spallation Source ESS AB is a state-owned limited liability company, today owned by the host countries Sweden and Denmark. ESS AB is currently working on finalizing the ESS technical design, planning future research at ESS, preparing for construction, and planning the future international ESS organization. This is done in collaboration with a large number of partner laboratories, research institutes, and universities around the world. The ground-breaking is planned for 2014, the first neutrons will be produced in 2019 and the facility will be fully operational mid 2023. ESS is expected to support a user community of at least 5000 European researchers and will have great strategic importance for the development of the European Research Area. MAX IV, a laboratory that will be one of the world's finest synchrotron radiation facilities is presently being built in the direct vicinity, see page 7. During the 65 years of operation two instrument suites of 22 instruments each are foreseen. The total yearly manpower is estimated at 500FTEs.

Life-Cycle Cost [at 2013 prices]

Construction Yearly Operation [during 65 years] Decommissioning













Topical Workshop: Proteins & nanoparticles @ membranes

Lipid and surfactant membranes are important building blocks for many applications of soft matter physics, and play an essential role for biological systems. A detailed understanding of protein, nanoparticle and virus interactions with membranes is important for a variety of processes - ranging from material transport within the cell and cellular uptake to viral infection and nanotoxicity. The relevant mechanisms can only be understood by considering simultaneously the physicochemical properties of membrane, nanoparticles, and proteins. Therefore, this workshop intends to bring together researchers who are interested in particles and proteins, as well as those interested in lipid membranes and surfactants.

Organizers: Thorsten Auth, Patricia Bassereau and Gerhard Gompper Date: 19 - 22 Oct. 2014 Location: Forschungszentrum Jülich **Registration & information:** www.fz-juelich.de/ics/pam-softcomp

Topical Workshop: Fracture of Soft Materials: from soft solids to complex fluids

This workshop will focus on the fracture behaviour of soft materials, such as synthetic and biological gels, foams, emulsions and colloidal suspensions. The aim is to discuss the microscopic mechanisms which make soft materials fail and to offer a new understanding of phenomena previously studied in a phenomenological way, such as yielding, stress localization, extreme shear thinning and slip. For these soft materials, in which weak interactions, heterogeneous microstructures and Brownian fluctuations play a governing role, ideas from classical fracture mechanics have only limited validity and new conceptual approaches need to be developed. In this workshop, leading experimentalists and theoreticians from various fields - soft condensed matter physics, rheology, solid mechanics and material science - will meet to explore new frontiers in soft failure mechanics and to stimulate the coming of age of this growing field. Organizers: Prof. Christian Ligoure,

Prof. Tristan Baumberger,

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Prof. Jasper van der Gucht, Dr. Joris Sprakel Date: 2014, exact date see weblink below Location: 'Centre des Congrès du Phare de la Méditerranée' in Palavas-les-Flots, near Montpellier

Registration & information: Exact date can be found soon at: www.eu-softcomp.net/news/cal

Coming Up ...

Conferences & SoftComp Topical Workshops

19 - 21 February 2014 NIBB 2014 'Neutrons in **Biology and Biotechnology'** Grenoble, France · Prof. T. Nylander

14 - 16 April 2014 The Physics of Soft and Biological Matter Homerton College, Cambridge, UK http://softbio.iopconfs.org

10 - 23 May 2014 5th Laboratory Course on Broad-band Dielectric Spectroscopy. http://www.sc.ehu.es/sqwpolim/PSMG/ **BDSLC**

16 - 23 May 2014 12th European Summer School on 'Scattering Methods Applied to Soft Condensed Matter Les Bruyères, Carcans-Maubuisson, Gironde, France · Dr. Peter Lindner http://www.ill.eu/fr/infos-evenements/ events/bombannes-2014/

18 - 23 May 2014 NaNaX6 Nanoscience with Nanocrystals Bad Hofgastein, Austria May 2014 http://www.nanax6.com/

26 - 30 May 2014 SoftComp Annual Meeting 2014 Heraklion, Crete, Greece Dr. Flavio Carsughi

22 - 28 June 2014 AMPERE NMR SCHOOL ZAKOPANE, Poland · S.Jurga www.staff.amu.edu.pl/-school

29 June - 3 July 2014 EUROMAR 2014 Zurich, Switzerland http://www.euromar2014.org/

21 - 25 July 2014 9th Liquid Matter Conference University of Lisbon, Portugal. www.fc.ul.pt/en/conferencia/ liquids-2014/general-information

1 - 6 September 2014 **ECIS Conference** Conference of the European Colloid and Interface Society Haifa, Israel. http://www.ecis-web.eu/

1 - 12 September 2014 17th JCNS Laboratory **Course Neutron Scattering** Jülich & Garching, Germany R. Zorn · reiner.zorn@gmail.com 12 - 16 September 2016 International Soft Matter Conference Grenoble, France · Dr. Peter Lindner lindner@ill eu

19 - 22 October 2014 **Topical Workshop:**

Proteins & nanoparticles @ membranes Organizers: Thorsten Auth, Patricia Bassereau, and Gerhard Gompper Location: Forschungszentrum Jülich Registration & information: http://www. fz-juelich.de/ics/softcomp-pam

Spring and Autumn 2014 **Basic Polymer Science and** Technology Training Courses, The University of Sheffield, UK www.polymercentre.org.uk/training

Autumn 2014 Topical Workshop: Fracture of Soft Materials: from soft solids to complex fluids Organizers: C. Ligoure, T. Baumberger, J. van der Gucht, J. Sprakel Centre des Congrès du Phare de la Méditerranée Palavas-les-Flots, near Montpellier http://www.eu-softcomp.net/news/cal

Autumn 2014

ICR Courses in Polymer Science and Technology' The University of Sheffield, UK www.polymercentre.org.uk/training

12 - 14 November 2014 Jülich Soft Matter Davs Seminaris Hotel. Alexander-von-Humboldt-Str. 20, 53604 Bad Honnef, Germany J. Dhont, D. Richter, G. Gompper

Personalia

Prof. P. Olmsted

Prof. P. Olmsted has accepted the position as Ives Professor of Physics at Georgetown University http://physics.georgetown.edu/ in Washington DC from January 2014.

New contact data:

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

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