EUROPEAN SOFT MATTER INFRASTRUCTURE

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Free Access for European Soft Matter Scientists to World-Class Instruments

Newsletter

Editorial

Welcome to the first issue of the European Soft Matter Infrastructure (ESMI) Newsletter! ESMI is an Infrastructure Project supported by the European Union's Seventh RTD Framework Programme, designed to provide access to the most advanced research infrastructure for users in the European soft matter community.

Earlier this year, we introduced ESMI by launching the ESMI web portal and by mailing flyers and posters containing basic ESMI-related information. The Newsletter has now been set up as a further important information channel intended to reach, in addition to ESMI partners and users, a broader, more general audience. To serve this purpose, the ESMI Newsletter will appear regularly twice a year. In the early publications, the ESMI partner laboratories will be introduced in detail along with the infrastructure they provide. In this first issue we offer a choice of articles displaying the complete breadth of the available infrastructure, comprising of highly specialized synthesis expertise, cutting edge experimental instrumentation and front end supercomputer facilities.

For those of you not yet familiar with the infrastructure project ESMI, this issue of the Newsletter also features an article that summarizes the most important information about ESMI as a whole. In future, the Newsletter is intended to become a forum where ESMI users may announce scientific achievements, which result from access to the infrastructure granted by ESMI. As a service to the reader, the Newsletter will communicate information which is crucial for the soft matter community, through columns such as Personalia, Coming Up and Openings.

Complementary to the Newsletter, continuously updated information on ESMI is available through the web portal: ***www.esmi-fp7.net***

Jan Dhont and Peter Lang

About the author

Prof. Jan K.G. Dhont *(Scientific Coordinator of ESMI) is Head of the Soft Matter Division ICS-3 in the Institute of Complex Systems at Forschungszentrum Jülich, Germany. In his group, chemical synthesis, physical experiments, theoretical physics and computer simulations are employed to gain a microscopic understanding of colloidal systems. His scientific focus is on the dynamics of colloids in external fields and non-equilibrium phenomena.*

ESMI – Top Level Infrastructure for the European Soft Matter Community

The FP-7 infrastructures project ESMI was founded with the aim of bundling top-level scientific infrastructure, and making it available free of charge to the community of European soft matter scientists.

22 research groups in 17 partner institutions from 10 different countries, among them four industrial partners, have pooled their equipment on three platforms. The experimental platform will allow scientists to use experimental techniques which are not available in their home laboratories, the synthesis platform provides expertise for the development of new soft matter systems, and the supercomputing platform supports access to the most powerful European computer facilities for the modelling of soft matter systems. Users of the ESMI infrastructure will receive support from ESMI scientists in conducting their research.

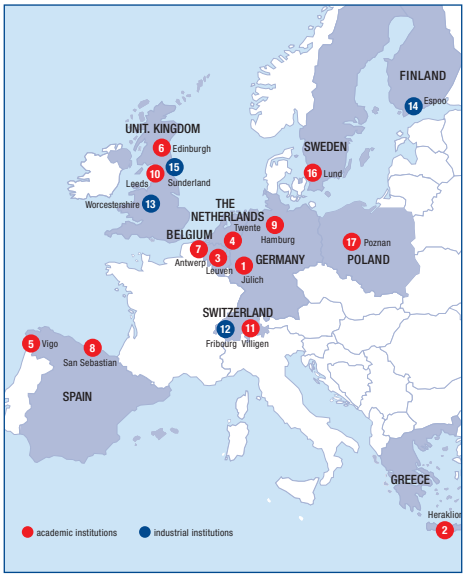
The experimental platform pools commercial apparatus together with unique, highly specialized equipment for soft matter research. The assembly of scattering (neutrons, X-rays and light) and microscopy (light and electron) facilities, spectroscopic (dielectric and NMR) methods and mechanical (rheology) techniques represents a comprehensive toolbox for the experimental investigation of soft matter systems.

The synthesis platform combines three laboratories with different specializations for the synthesis of soft materials. The systems offered span a wide range of specially-designed colloidal particles and sophisticated polymer architectures, as well as standard systems. Thus, this platform provides well-characterised soft matter systems tailored for the specific needs of the ESMI-user.

The supercomputing platform provides access to the JUROPA supercomputer located at Forschungszentrum Jülich.

All soft matter scientists within the EU are welcome to apply for access to the infrastructure offered by ESMI by submitting a proposal via the ESMI web portal. Proposals will be evaluated by the ESMI Review Panel. After a proposal has been accepted, all expenses associated with the use of the ESMI infrastructure, including travel, accommodation and subsistence costs will be covered by the ESMI project. This funding is possible thanks to financial support from the EU of € 7.8 million over the project period of 4 years.

Joint research activities among ESMI partners aim to continuously improve the available infrastructure, and the project is rounded off by a networking programme for disseminating knowledge and educating the next generation of soft matter scientists. ■



ESMI bundles infrastructure from 22 research groups in 17 partner institutions which are located in 10 different European countries.

About the author

***Dr. Jochen Arlt**. My research activities revolve around the development of optical instrumentation for life-sciences and soft matter studies, such as various optical micro-rheology techniques. Current scientific focus is on microscopic swimmers such as motile bacteria, from the details of their individual propulsion mechanisms to their collective behaviour.*

COSMIC – Optical Characterization and Manipulation of Complex Materials

The Collaborative Optical Spectroscopy, Micromanipulation and Imaging Centre (COSMIC) was established more than a decade ago as an inter-disciplinary research facility to serve the University of Edinburgh's soft matter and biosciences communities. The centre provides state-of-the-art facilities for optical characterisation of complex materials from single molecules to living biological cells and colloidal glasses.

Fast confocal rheo-imaging set-up

Fluorescence based microscopy techniques are instrumental in providing real-space data of complex material. In particular, confocal microscopy is an essential tool to study bulk samples such as colloidal crystals, gels and glasses in three dimensions. The centre offers several complementary instruments, e.g. capable of capturing high quality images of colloid stabilised bicontinous emulsions [1] or the fast dynamics of colloidal glasses under shear [2].

Microscope systems for single molecule imaging are also available within the centre. These are capable of optical super-resolution imaging, as used for example for lambda-DNA studies [3].

The centre has several systems to perform time domain fluorescence lifetime measurements. The fluorescence lifetime of a fluorophore depends in a measurable way upon its local environment (e.g. local viscosity, pH or refractive index). Fluorescence lifetime spectroscopy of bulk samples provides an extremely sensitive method of studying molecular interaction, such as DNA enzyme interactions [4]. Fluorescence lifetime can also be used to provide quantitative information through imaging [5].

A Raman microscope and a coherent anti-stokes Raman scattering (CARS) microscope provide options for label-free imaging of samples, relying on inherent molecular vibration to provide the image signals [6].

These imaging techniques are complemented by optical tweezers systems, from user-friendly 'click and trap' systems to force measurement setups for passive and active micro-rheology, as demonstrated for example on dense colloidal suspensions [7].

However, the main strength of the centre is arguably its capability to combine these various techniques with each other and with a variety of novel sample environments. The prime example is the rheo-imaging setup developed within COSMIC, where the combination of a fast scanning confocal system with a commercial rheometer and software developments enable high resolution imaging of dense colloidal suspensions under shear [2]. ■

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[4] R. Neely et al, Nucleic Acids Research **33**, 6953 (2005)

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[6] Iain Robinson et al., Journal of Biophotonics **3**, 138 (2010)

[7] L.G. Wilson et al., EPL, **93** 58007 (2011)

About the author

***Dr. Godehard Sutmann** is a member of staff at the Jülich Supercomputing Centre, Head of the Simulation Laboratory Molecular Systems and Director of the Jülich CECAM Node. His scientific interests are parallel computing, molecular dynamics and fast methods for long range interactions.*

High Performance Computing in ESMI – JuRoPA

The Jülich Supercomputing Centre (JSC) at Forschungszentrum Jülich (FZJ) in Germany operates various high performance computing systems, each with a different application focus. Since 2004, JSC has adopted a dual system in supercomputing, where two different high end systems are operated and CPU time is offered to the scientific community. One line of installation addresses the demand for capability computing and has the potential to run large scale, parallel jobs on thousands of processors. The other line of installation caters to the large demand of the community to run jobs in parallel on a smaller

number of processors. Not only are the scaling of programs but also memory demands characteristic for the two different lines.

While a large number of computer nodes operate in line with a smaller memory on the nodes (currently 0.5 GB/core), the general-purpose machine offers a larger memory and also a larger number of cores on each node, making it possible to also run memory-intensive applications.

At present, the dual hardware line is provided on the one hand by Jugene, an IBM Blue Gene /P, with 73728 nodes, feeding 294912 computer cores, which is currently

still the largest number of processors worldwide, making this machine very attractive for scaling benchmarks and large scale parallel applications, attracting national and international research groups. On the other hand, the general-purpose computer at Jülich is the JuRoPA (Jülich Research on Petaflop Architectures) system, which is a co-development of Bull, Sun, ParTec, Intel, Mellanox, Novell and Forschungszentrum Jülich. It is made up of 2208 computer nodes consisting of two Intel Nehalem-EP quad-core processors (Xeon X5570) with a clock rate of 2.93 Ghz, giving a total of 17664 computer cores. Each node is equipped with a 24 GB memory, so enabling the running of applications with large memory demands. Peak performance of the system is 207 Tflop/s. In combination with its twin system HPC-FF, a performance of 274.8 TFlop/s was reached in Linpack benchmark runs, which brought the system in June 2009 to No.10 in the Top500(1) list of the fastest supercomputers in the world. It is not only jobs with a moderate parallelism thatare able to run on this general-purpose platform, a fact impressively demonstrated by the cosmological Millennium Simulation(2) last year, which ran for several weeks on 12288 cores.

Within ESMI, high performance computing is offered via JuRoPA, where the soft matter community can run simulations on a larger scale or perform efficient interpretation of numerical data. For applications, a large number of software packages is on offer. Besides standard numerical libraries, simulation software is available for classical molecular dynamics (e.g. AMBER, Gromacs, LAMMPS, NAMD, Tremolo), ab initio molecular dynamics (CPMD, CP2K) or DFT and ab initio calculations (e.g. ADF, Columbus, GPAW, Molpro, NWChem).

Applications for computer time may be submitted using the ESMI web pages. A total of 148000 Tflop-hours for the ESMI project is allocated over a project period of 4 years, which corresponds to about 2% of total machine capacity. Currently there is no deadline foreseen for new projects and users are invited to submit their proposals via the interface at any time. Users not yet familiar with parallel computing or who need to optimize their parallel applications, may profit from the support of the Simulation Laboratory Molecular Systems(3), a support unit of JSC. The unit works in cooperation with user groups in order to parallelize or improve the performance of applications, or to co-develop methods for parallel molecular applications. ■

References:
www.top500.org
www.par-tec.com/news
www.fz-juelich.de/ias/jsc/EN/AboutUs/

About the author

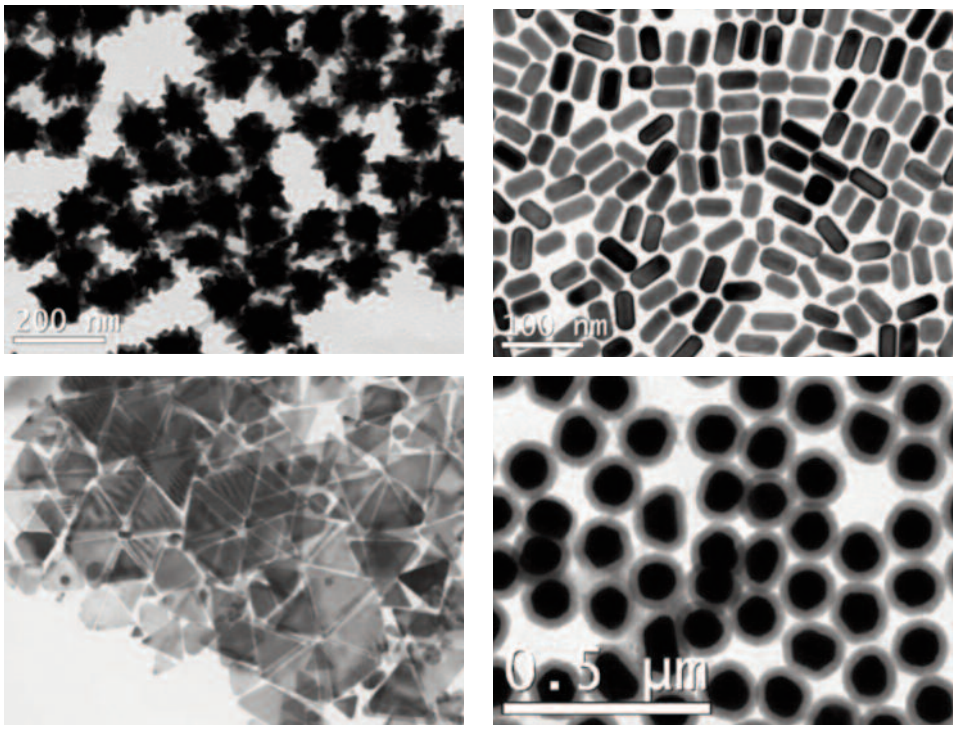
Prof. Luis M. Liz-Marzán *is a Professor of Physical Chemistry at the University of Vigo, Spain. His current interests include nanoparticle synthesis, directed self-assembly, nanoplasmonics, surface-enhanced spectroscopies, nanocomposites, and the development of nanoparticle-based sensing and diagnostic tools.*

Golden Stars and Other Tailor Made Colloids

The Colloid Chemistry Group (University of Vigo) is an interdisciplinary team with expertise in the various aspects of Nanomaterials and Colloid Science, from the chemical design of various types of nanoparticles and their surface modification, to their physical characterization and theoretical modelling using microscopic and spectroscopic techniques and numerical methods, to their processing into organized assemblies and complex nanostructures, and, finally, to the development of applications, mainly related to sensing for detection and diagnostics. The main persons involved in ESMI are the group leader (Prof. Luis M. Liz-Marzán) and three senior researchers (Isabel Pastoriza-Santos, Miguel Correa-Duarte, and Jorge Pérez-Juste) who are in charge of different types of materials. We thus offer extensive know-how on a number of competitive strategies for synthesis and characterization of complex nanoparticle colloids, mainly comprising noble metals, silica and carbon nanotube composites. Morphologies available include spherical, rod-shaped, triangular, polygonal, and star-shaped, in a proper volume range, all of which holding the potential of useful optical response.

We offer both synthesis and on-site training to interested users. Regarding surface functionalization, we offer expertise toward the attachment of different capping agents according to the needs of users, as well as homogeneous coatings with different metals or with silica. Representative images of available samples are shown in the figure below.

The synthesized nanoparticles can be characterized by different techniques including electron microscopy (HR-TEM, SEM) optical spectroscopy (transmitance, diffuse and specular reflectance), dark field microscopy (for single particle optical spectroscopy), spectroscopic ellipsometry, dynamic light scattering, electrophoretic mobility (for zeta potential determination), fluorometry, AFM, XPS, and confocal Raman spectroscopy. ■



Representative TEM images of metal nanoparticles readily available at University of Vigo. Upper panel: Au nanostars and nanorods. Lower panel: Ag nanoprisms and Au@SiO_2 spheres.

Job Offers

Postdoctoral and/or PhD position in Experimental Soft Matter at FORTH, Heraklion (Greece)

"Rheology and Slow dynamics in Soft Matter"

The Polymer & Colloid group of the Foundation for Research and Technology Hellas, (FORTH, Heraklion, Greece), is offering a 1+1 year post-doctoral position and/or a 3-year PhD position. The PhD position will be offered in collaboration with the Materials Science and Technology Department of the University of Crete.

The applicant should have a PhD (for the post-doctoral position) or a Masters degree in related areas such as Soft Matter physics or physical chemistry. Experience in scattering techniques and rheology is most welcome, but not mandatory.

For a detailed description of the research project please visit the ESMI web portal at: **www.esmi-fp7.net/news/Jobs**

Contact: George Petekidis
e-mail: *georgp@iesl.forth.gr*
www.iesl.forth.gr/
http://www.materials.uoc.gr

PhD position in Experimental Soft Matter at Forschungszentrum Jülich, ICS-3

"Interactions, Structure Formation and Dynamics of Biomimetic particles Near Solid Interfaces"

The Soft Matter group at the Institute of Complex Systems (ICS-3), Forschungszentrum Jülich is offering a 3-year position for a PhD student.

The applicant should have a Masters degree or a diploma in physics, physical chemistry or biophysics. Preferably they will have some experience with scattering and/or microscopy techniques.

Forschungszentrum Jülich offers a highly interdisciplinary research environment, excellent infrastructure and a PhD program for ca. 350 students. The successful applicant will have the opportunity for complementary training within the framework of the International Helmholtz Research School "BioSoft".

For a detailed description of the research project please visit the ESMI web portal at: **www.esmi-fp7.net/news/Jobs**

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www.fz-juelich.de/ics/ics-3/EN

Coming Up …

Conferences and Schools

15. - 18. Nov. 2011

Jülich Soft Matter Days 2011
The meeting taking place at Gustav Stresemann Institut in Bonn, Germany will focus on biosystems, colloids, polymers and self-assembly.
Further information is available at: *http://www2.fz-juelich.de/iff/jsmd2011*

19. - 20. Dec. 2011

British Society of Rheology Midwinter Meeting 2011
This meeting, to be held at University College London, aims to provide an overview of current research across the whole spectrum of complex fluids in complex flow situations - encompassing theory, simulations and experiments.
conferences.bsr.org.uk/conference.php?conf=39

5. - 7. Mar. 2012

8th Zsigmondy Colloquium of the German Colloid Society
Zsigmondy Colloquia have the scope of bringing together PhD students, PostDocs and young researchers to exchange ideas and results in the fields of colloid, surface and interface science. The focus of the 8th Zsigmondy Colloquium will be on the latest advancement in the area of wetting of complex fluids, both from an experimental and from a modeling point of view. But, like it is tradition, all topics of colloid and interface science will be covered.
Registration via internet at:
www.csi.tu-darmstadt.de/news/events/zsigmondy_kolloquium/home_19.de.jsp

5. - 16. Mar. 2012

43rd IFF Spring School 2012
The school entitled "Scattering Methods for Condensed Matter Research: Towards Novel Applications at Future Sources" will provide a solid introduction to the basics of scattering methods, an overview of the current understanding of the structure and dynamics of various condensed matter systems and examples of topical applications in various fields of science.
Registration via internet at: *www.iff-springschool.de* before December 09, 2011

20. - 23. Mar. 2012

CODEF III
The scientific focus of the conference, to be held at Gustav Stresemann Institut in Bonn, Germany, is on the physics of colloids in confining geometries, under shear, as well as in electric, laser-optical and magnetic fields. Self-organization phenomena in equilibrium and non-equilibrium, where colloidal dispersions play a pivotal role as model systems, will be discussed. Particular emphasis will be put on the combined use of complementary methods, such as experiment, computer simulation and theory.
Registration before 6. January 2012 at: *www.codef.de/p_reg.php*

Personalia

Dr. Flavio Carsughi
has left ESMI as a project manager and has accepted the position of the head of the JCNS user office. He will continue supporting ESMI as a member of the project executive committee.

Imprint

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This newsletter does not represent the views of the European Community.
ESMI is not responsible for any use that may be made of the information contained in the Newsletter.

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