ICMS Highlights

Edition 3
September 2014

Four PhD students, four molecular quests

INTERVIEW
/ Samuel I. Stupp

THE STATIC SURFACE IS HISTORY

INTERVIEW
/ Carlijn Bouten & Cecilia Sahlgren

& more...

Institute for Complex Molecular Systems

Technische Universiteit
Eindhoven
University of Technology

Where innovation starts

ICMS Highlights

Dear reader,

Every scientist dreams of pushing the frontiers of science and solving some of the most intriguing societal challenges at the same time. However, we are neither Pasteur nor do we live in his time. Despite this, Universities have always played an essential role to make important steps for society's bright future.

Whereas in the past, most of the groundbreaking steps were made by individuals, the complexity of today's challenges requires joined and multidisciplinary research programs. We are pleased that the TU/e hosts research groups in both basic sciences and the applied sciences creating engineering solutions for industry. Within ICMS, we try to bring these two together. This makes it an ideal place for performing use-inspired fundamental research to bridge the gap between disciplines.

We like to challenge our members and those attracted to today's challenges to see how they can contribute, and we welcome all suggestions in this area. It is our full belief that, by collaborating between disciplines, the outcome will be more than the sum of the parts. Even when the outcome is different than hoped for, it brings a lot of fun. This magazine will give you a glimpse of the many examples of use-inspired research within our Institute. As they will shape the future and will provide tomorrow's answers, we also introduce some of our young members to you.

We hope you enjoy reading,

Sagitta Peters
Managing director

Bert Meijer
Scientific director

Calendar

September 30, 2014, 10.30 hr
Heineken Award Lecture by prof. C.M. Dobson
Location: Blauwe Zaal

September 30, 2014, 14.00 hr
Scientific lecture by prof. C.M. Dobson
Location: Ceres

October 9 & 10, 2014
NextGenChem@NL 2014
Location: Ceres

October 16, 2014, 17.00 hr
Nobel Prize meeting
Location: Zwarte Doos

October 24, 2014, 15.00 hr
ICMS Discussion meeting with Andreas Walther
Location: Ceres

November 4, 2014, 09.00 hr
Workshop Advanced Fluorescence Techniques
Location: Ceres

November 7, 2014
Eindhoven Multiscale Institute Symposium
Location: Ceres

November 17 & 18, 2014
CHAINS 2014
Location: Koningshof Veldhoven

January 22 & 23, 2015
ICMS Outreach Symposium
Location: Zwarte Doos

The complete calendar can be found on our website.

Content

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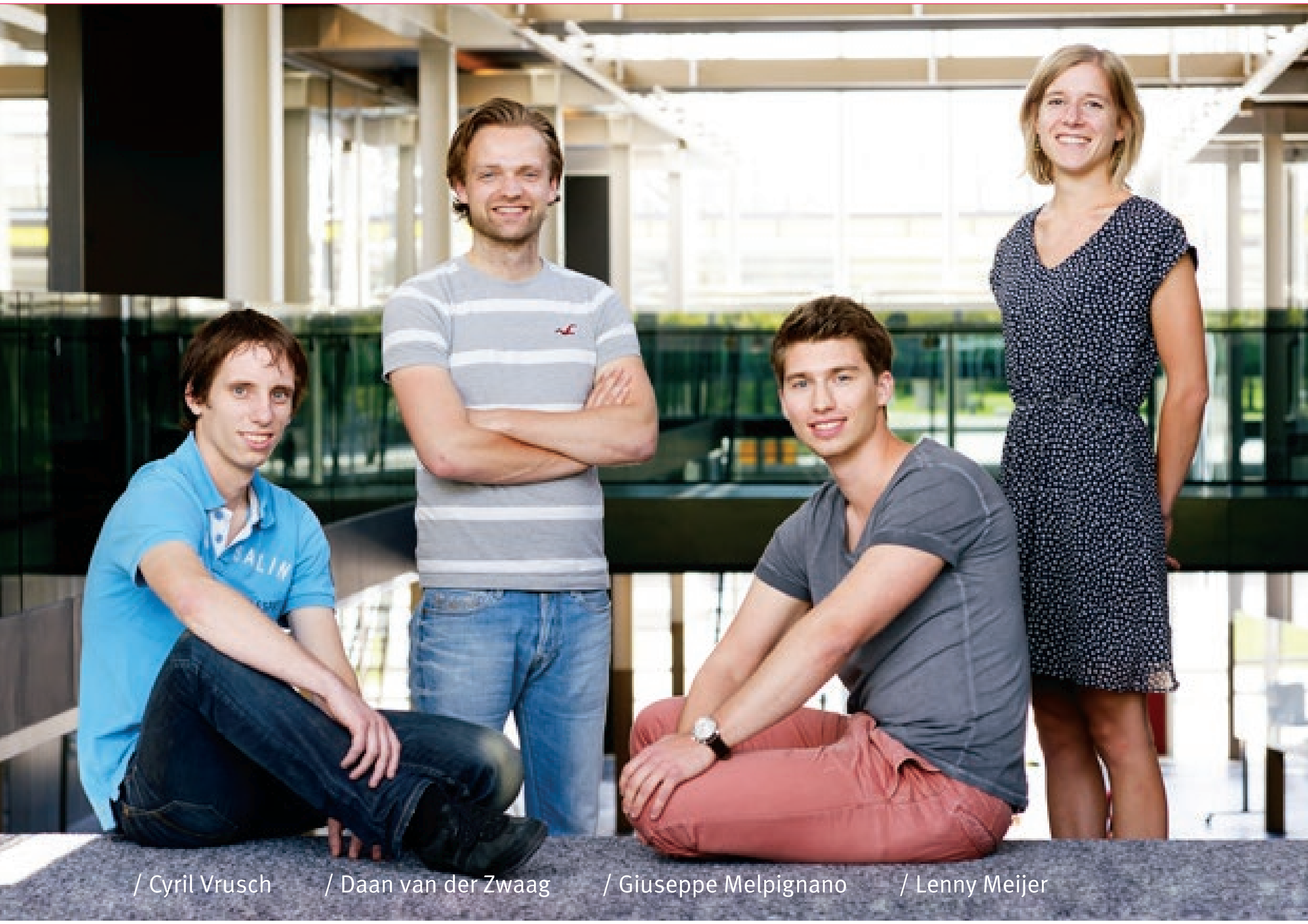


Four PhD students, four molecular quests

On its mission to master the complexity of supramolecular assembly, ICMS brings together mathematicians, physicists, biologists, chemists and engineers to build up knowledge and boost scientific progress. Simultaneously, the institute accommodates the education and development of young talent. ICMS Highlights spoke to four of its PhD students. Read the excerpt from an interesting conversation with our next gen molecular system engineers below.

What is going on in your research today?

Cyril: "When I rounded off my Bachelor, I didn't think that I had enough theoretical background. I decided to do a Master's, and during my internship at DSM, I did a lot of research on the forces of polymers. The behaviour, the different time scales, translating findings into computer simulation, it immediately fascinated me. Diving deeper in polymer networks here at the ICMS came as a logical next step."

Lenny: "It's very challenging work. I think that goes for all of us: we are the first researchers on our specific topics. So it requires perseverance. Next to my research, I am also bridging between the modellers and the lab workers. There can be quite a gap between the two approaches."

"THAT'S WHAT I FIND HARDEST IN THIS WORK: GETTING TO THE RIGHT QUESTION

Daan: "As you can see in all of our work, computer simulation is a valuable way to get a lot of information. Simulations help to understand your system, because a model will only work if you've correctly analysed the molecular behaviour. For an accurate model, the key is to combine simulations and experiments in an appropriate way. That's what I find hardest in this work: getting to the right question."

Giuseppe: "To a mechanical engineer like me, the world of microsystems is relatively new. Somehow, everything I learned comes together here and yet, due to the smaller length scale, everything changes. I am challenged to change my thinking."

To what extent does an affiliation with the ICMS help?

Giuseppe: "The main reason why the ICMS works so well is the short communication lines. As mechanical engineers, we are used to approaching things from a broader perspective by applying multiple disciplines. Since I am working on dynamic surfaces, which change their surface chemistry, I also have to think in specialized chemical processes like chemical surface modifications. At ICMS,

/ Daan van der Zwaag

Department: Department of Chemical Engineering and Chemistry
Section: Macromolecular and Organic Chemistry
ICMS promotor: Bert Meijer
PhD Status: 2 years

Project:
So far, molecular system assembly has been counting heavily on the self-organization effects of the molecules. However, coincidence plays an important part in getting the results you desire, and that is precisely what we want to counter. I am studying the mechanisms by which we can consciously give direction to the construction of supramolecular systems. I use a combination of computer simulation and microscopy to watch and clarify the behaviour of the molecules.

/ Cyril Vrusch

Department: Department of Applied Physics
Section: Theory of Polymers and Soft matter
ICMS promotor: Kees Storm
PhD status: 4 months

Project:
I study the behaviour of polymer networks on curved surfaces and cylindrical shapes, that resemble the shapes of biomedical fibers, such as intervertebral discs and walls of blood vessels. The behaviour of the polymers can be mechanically described and translated into computer simulations. With these models and simulations, I am building up knowledge on the behaviour and the creation of order in polymer networks and fibers.

I can connect to chemists easily. What is a simple question for them is a very long search for me. That's efficiency!"

Lenny: "It gets you outside your box as well. There are a lot of meetings and Friday afternoon discussions in which you meet new people and new ideas. Looking outside your field can really help."

HERE, EVERY DAY IS DIFFERENT

Daan: "It actually works better than I imagined. Today, almost all projects are multidisciplinary. You cannot solve the current complex challenges from one perspective, or even from one department. Furthermore, there is increasing attention to application. If you want to run things in practice, you need all sorts of different disciplines. That's what ICMS has to offer: direct connection to a wide variety of scientists."

What will your future look like?

Lenny: "I do not have a very clear idea yet. There's one thing I found out: I do not like routine. Here, every day is different, and I really like the atmosphere at the University. However, I haven't explored the business side yet. Working at a smaller R&D company might be nice. My main motive is to develop myself."

Giuseppe: "With an application-oriented PhD, working in industry is a logical next step. Getting to know another way of thinking will be great. However, the career path of my supervisors Jaap den Toonder and Dick Broer (returning to the university after years at Philips) seems an attractive route for me as well."

Cyril: "I stepped into this PhD because the subject really fascinates me. I am just curious to explore it further, and I'd like to conduct research. I've been working on this PhD for four months now, and I think there will be opportunities enough after this."

Daan: "I would also like to experience the industry. Working at a large chemical company seems very interesting to me. I think large companies can create opportunities because of their excellent facilities and large(r) budgets. It is also a chance to really contribute to society with the realisation of products that people need everyday."

/ Lenny Meijer

Department: Department of Biomedical Engineering
Section: Computational Biology
ICMS Promotor: Peter Hilbers, Luc Brunsveld
PhD Status: 3 months

Project:
I study DNA networks and focus on DNA parts that can perform specific biomedical functions. We have found, for instance, that small pieces of DNA can work like a tiny biotechnical computer; you can give them input, and after a processing step, they give a certain output. It is like Lego, but with biomaterial. I use modelling to find the desired design (protocols) and predictability.

/ Giuseppe Melpignano

Department: Department of Mechanical Engineering
Section: Microsystems
ICMS Promotor: Jaap den Toonder, Dick Broer
PhD Status: 12 months

Project:
My project is called "DynaClean: Dynamic self-cleaning surfaces". Using an intelligent material that responds to both water and light, a hydrogel, the surface chemistry and structure change upon application of both. Water causes autonomous swelling of the surface, whilst the application of light causes the switching between aforementioned effects. The surface autonomously enables self-cleaning effects when in contact with water and exposure to light. Ultimately, DynaClean will find application in solar panels and windows.

NEWS, AWARDS & GRANTS

ECHO-STIP funding for

CHRISTIAN OTTMANN

Christian Ottmann received an ECHO-STIP grant of 260.000 euros. This grant is awarded by NWO Chemical Sciences and is meant for excellent researchers in chemistry. The ECHO-STIP program stimulates newly appointed researchers. Christian Ottmann aims at developing new drugs to treat diseases like diabetes and obesity.

Second ICMS Fellow

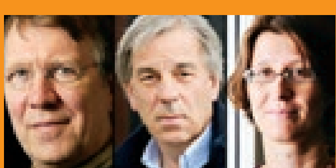
LOUIS PITET

Because of his excellent scientific track record, dr. Louis Pitet has been awarded an ICMS Fellowship. The ICMS Fellowship will support him during his final year in Eindhoven as a set up to an independent academic career. Louis Pitet works in the field of advanced polymer materials, in general, and for nanolithography, in particular. ICMS aims at the start of another three ICMS Fellows in the next two years. Dr. Lorenzo Albertazzi was awarded the first ICMS Fellowship.

NSF CAREER Awardee @ ICMS

YAO LIN

Dr. Yao Lin has received an NSF CAREER grant 'Research Opportunities in Europe' for visiting the group of Bert Meijer. Yao Lin is an assistant professor of the Polymer Program in the Institute of Materials Science, Department of Chemistry University of Connecticut (USA). He will visit ICMS during the period February-July 2015.



TOP-PUNT grant for

DICK BROER, BERT MEIJER AND ANJA PALMANS

NWO Chemical Sciences has awarded the ICMS team of Bert Meijer, Dick Broer and Anja Palmans a TOP-PUNT grant. The researchers will receive 2 million euros funding for their research proposal 'Polymers in Motion'.
The amplification of collective molecular motions from the nanoscopic to the macroscopic scale is probably one of the most intriguing challenges in materials science and remains to be fully discovered in the decades to come. Two approaches can be distinguished: artificial molecular machines and stimuli-responsive materials. In their 'Polymers in Motion' research project, the team is aiming at closing the gap between both approaches by making use of their knowledge in liquid-crystalline polymer networks, the hierarchical self-assembly of supramolecular polymers and adaptive materials.

Jan Rajchman prize for

DICK BROER

The Society for Information Display (SID) is comprised of the top scientists, engineers, corporate researchers and business people of the display industry. SID awards the Jan Rajchman Prize annually since 1993 to scientists which have an outstanding scientific or technical achievement in, or contribution to, research on flat panel displays.

This year, the Jan Rajchman prize has been awarded to Dick Broer.
He received this recognition for his pioneering discovery and development of UV-polymerizable liquid-crystalline polymers and his outstanding contributions to their applications in flat panel displays. The award has been presented in a ceremony on June 2, 2014 in San Diego, CA.

ELLEN SCHMITZ

second prize in KNCV Golden Master Award

Ellen Schmitz has received the second prize in the KNCV Golden Master Award competition for her master thesis. Her master thesis work was largely performed in the clinical lab of the Catharina Hospital Eindhoven. Ellen Schmitz is now a PhD student in the group of Luc Brunsveld.

3 HIGHLY CITED RESEARCHERS

in ICMS

René Janssen, Martijn Wienk and Bert Meijer have been identified as 2014 Thomson Reuters Highly Cited Researchers.

The Highly Cited Researcher process identifies influential researchers as those who have contributed to a significant number of the most highly cited publications in a field. Only few institutes have multiple Highly Cited Researchers among their members.

Vidi grant for

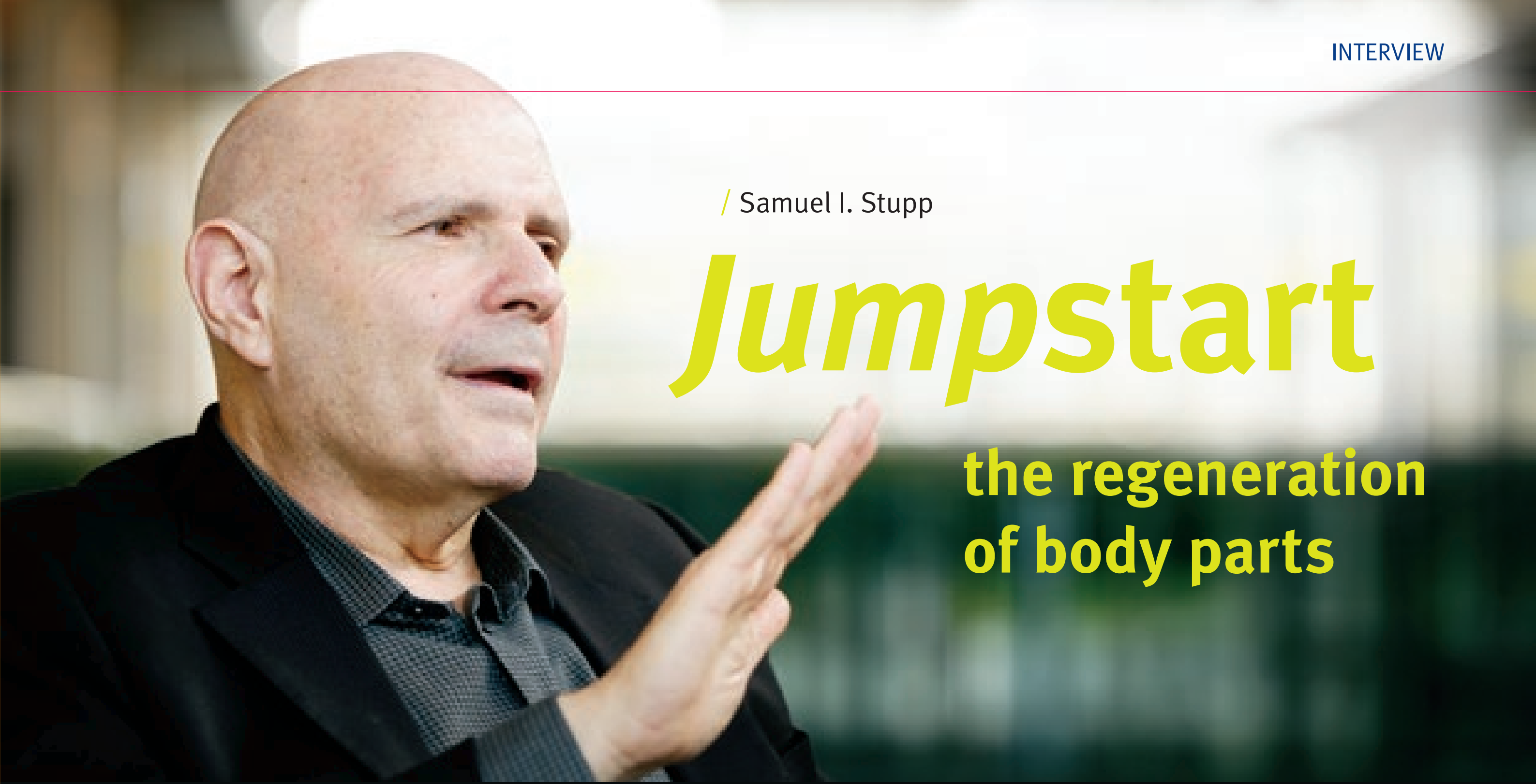
PETER ZIJLSTRA

Dr. Peter Zijlstra of the group Molecular Biosensors for Medical Diagnostics has received a Vidi grant of NWO worth 800.000 euros to start his own research line. Peter is going to use gold nanoparticles to study single enzymes in a living cell.

MINISTER BUSSEMAKER

visited ICMS

Dr. Jet Bussemaker, Minister of Education, Culture and Science of the Netherlands, has visited ICMS on June 16, 2014. Her visit aimed at getting to know better the four running Gravitation programs in which the Eindhoven University of Technology is involved. The first program of these four that received a Gravitation grant is the Research Center Functional Molecular Systems in which ICMS is one of the partners.



/ Samuel I. Stupp

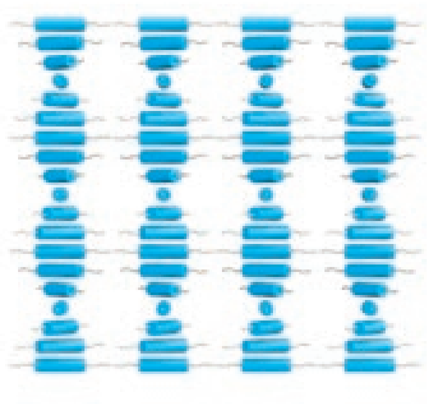
Jumpstart the regeneration of body parts

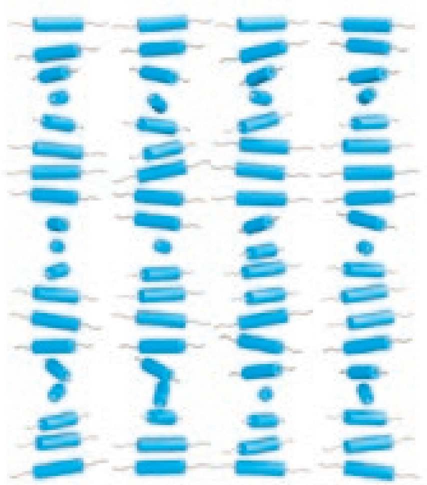
Professor Samuel I. Stupp is a pioneer in supramolecular self-assembly. Stupp, Director of the Simpson Querrey Institute for BioNanotechnology in Medicine at Northwestern University (Chicago) and international chair of ICMS, is recognized worldwide for his stunning work on bioactive materials that could revolutionize therapies in regenerative medicine. Among other achievements, he and his team created an extensive platform of self-assembling molecules that are able to promote regeneration of the spinal cord in paralyzed mice and of other tissues such as cartilage and bone.

Stupp in a YouTube interview: "I dream of a time where supramolecular nanotechnology will have a key impact in the field of regenerative medicine. Using bioinspired supramolecular materials one can jumpstart - in the adult body - the regeneration of a tissue that is missing or an organ not functioning properly anymore." In one example by designing self-assembling nanofibers (containing portions of natural proteins), Stupp and his team are able to create a so-called 'noodle gel' that has regeneration abilities after spinal cord injury by guiding the growth of axons in the proper direction. While on a brief visit to ICMS in July, Stupp gave two inspiring lectures on his work. In addition to biomaterials, the highly interdisciplinary Stupp group (integrating chemistry, materials science, and medicine) is utilizing self-assembly to create nanostructures and materials for solar photovoltaics, solar fuels and ferroelectrics for memories. Stupp at ICMS: "The common denominator of our diverse research portfolio is the exciting field of supramolecular chemistry in which discoveries are currently leading to many new ideas. On the bio-side our work on regenerative medicine is very promising and we are making progress toward the goal of testing our materials in clinical trials. As always, we are in need of capital, both human and financial. Recently, we received a generous endowment from the Querrey Simpson Foundation that will help enormously to take our research to the next level. I am very thankful for that and look forward to our future research."

Interested in Stupp's work?
See: **stupp.northwestern.edu**

The STATIC SURFACE is history; welcome to Dynamic Surface Topographies



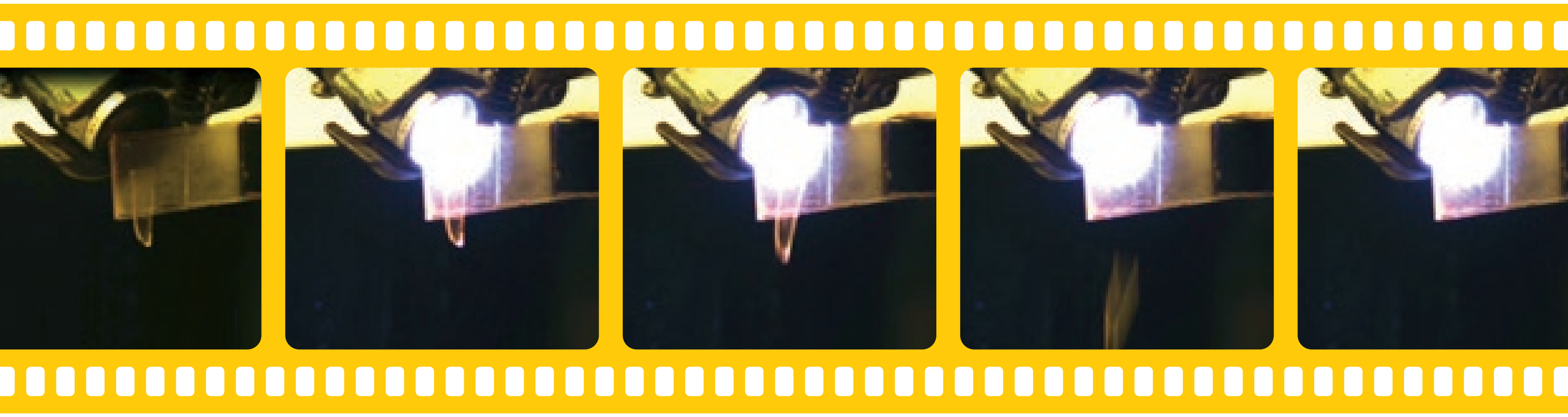


Intelligent surfaces, adding value by performing functions, that is in brief what prof.dr. Dick Broer and dr. Danqing Liu are working on at ICMS. With their research on the behaviour, organization and manipulation of polymerized liquid crystal networks, they are opening a new field in the area of functional organic materials: dynamic surface topography. This can lead to interesting applications, such as self-cleaning surfaces, sensitive robotic hands and more.

The study by Broer and Liu finds its roots in something Broer discovered in the eighties. Chemically modifying liquid crystals makes it possible to change the way the molecules organize and let through light, broadening the view angle.
This technology is now used in every LCD screen. Broer and Liu are taking the manipulation of molecules a step further. Broer: “We have built a demonstrator with a surface that we can switch from flat into static position to a predefined corrugated state when triggered by light.” Broer and Liu thereby created a dynamic surface with all kinds of possibilities. Liu adds: “We can design different structures. We started off with a regular structure, but now we are also exploring the possibilities of an irregular or random structure like a fingerprint, every single one unique. This last one is a lot easier to make - using the molecules’ self-organization abilities - and offers advantages for mass production.”

Triggers

Broer: “The nice thing about liquid crystal is that you can use several triggers for actuation; in addition to light, it can work with water (vapour), gasses, pH, temperature and electrical current. With that in mind, you can imagine surfaces that can change their characteristics autonomously.
We are looking into this interesting field from both a scientific and application perspective. One application we think of is self-cleaning surfaces.” This kind of



application would be ideal for large solar parks in desolate dry areas. Here PV-panels are subjected to dry contamination such as sand, dust and particles. Liu: "By covering solar cells with a dynamic surface, the PV-panel - triggered by the absence of light - could remove the particles themselves and increase the yield." Broer continues: "We are looking towards a technology that uses mechanical energy to establish the self-cleaning effect. A breakthrough in our research will be if we get the dynamic surface oscillating. In that way, it can remove the particles more effectively. At this moment, our materials respond on a timescale of seconds, but we need to go to subseconds. However for a self-cleaning window that changes its wettability when it rains, such rapid response times are less important."

Constant change

Before applications based on dynamic surface topography arrive, there is a road ahead. Although the chemically modifying of a liquid crystal is a mature technology, there is still a lot to learn. Broer and Liu are building up knowledge around the molecular system, the mechanics of the polymers and the polymer network itself. This is where the connection with ICMS started. Together with prof.dr. Bert Meijer, the group received an NWO-grant for further research. Broer and Liu take the opportunity to look deeper into the basis of oscillating. Broer: "We want to use the molecular dynamics to get the surface oscillating." The most veritable approach to the solution seems to be to make use of a supramolecular system in a non-equilibrium state. As in the human body, the constant interplay of molecules causing macroscopic events is what drives actuation and motion.

Robots with fingerprints

While examining and experimenting with different kinds of dynamic surfaces, the range of possible applications expands. Based on the same principles, it must be possible to make applications such as a pumping or mixing micro fluidic device. By increasing or decreasing the volume of a surface, it could become a self-focusing lens, which can be beneficial for the further improvement of the yield in solar energy panels. Using the corrugated/flat characteristics, one can think of a smartphone screen for visually disabled people, or a sensitive robotic finger that can pick up both heavy and very delicate objects. Liu: "And since we are able to make random, irregular structures, the robot could even have a fingerprint!"

Dynamic surface technology, as explored by Broer and Liu, shows a promising future where objects go from static to adaptive. This fits a tendency towards the creation and use of more intelligent, autonomous environments that improve and enhance our daily (working) lives.

Dr. Danqing Liu

More about this topic:

T. Verho, J.T. Korhonen, L. Sainiemi, V. Jokinen, C. Bower, K. Franze, S. Franssila, P. Andrew, O. Ikkala, R.H.A. Ras (2012), Proc. Natl. Acad. Sci. U.S.A., 109, 26

D.P. Holmes, A.J. Crosby (2007), Adv. Mater. 19, 3589

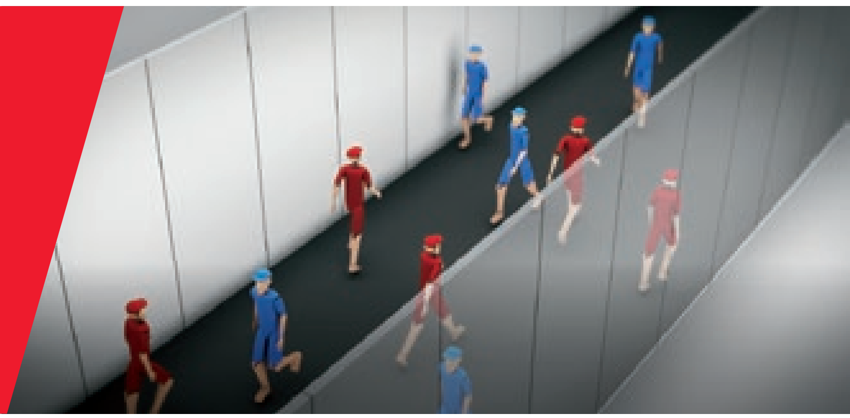
D. Liu, D.J. Broer (2014), Angew. Chem., Int. Ed. 53, 4542

See the ICMS animation at YouTube: youtu.be/RVqGqLTGj1c

Protecting a crowd

How can a gathering be dissolved without causing panic? How wide must the aisles of Ikea be to prevent congestion? These situations can be difficult to evaluate with human test subjects. However, computer models can mimic and predict the behavior of crowds. They tell us that you are sometimes more likely to survive if you leave the crowd.

> "When people are ***in the dark***, their intuition fails. So do our models of **CROWD DYNAMICS**."
>
> Adrian Muntean, researcher at ICMS



Busy streets

The way we walk in busy streets is full of unspoken conventions. We do not touch each other, keeping a certain distance from strangers. Furthermore, we tend to follow friends, and we have a destination in mind. A pedestrian follows very predictable behavioral rules. These rules can be programmed into a computer, in much the same way that a scientist can model the behavior of atoms in a cloud, with their mutual attraction and repulsion. These few simple rules for attraction and repulsion between people suffice to make a realistic simulation of crowds. For instance, in a crowded corridor where people are walking in opposite directions, lanes will form with people walking behind each other. When the number of people increases, people get stuck and cannot move anymore. When a place is so crowded that nobody can move, people can easily panic and be trampled. So it is important for engineers to know beforehand whether a place can cope with the onrush. Computer simulation may help them.

In the dark

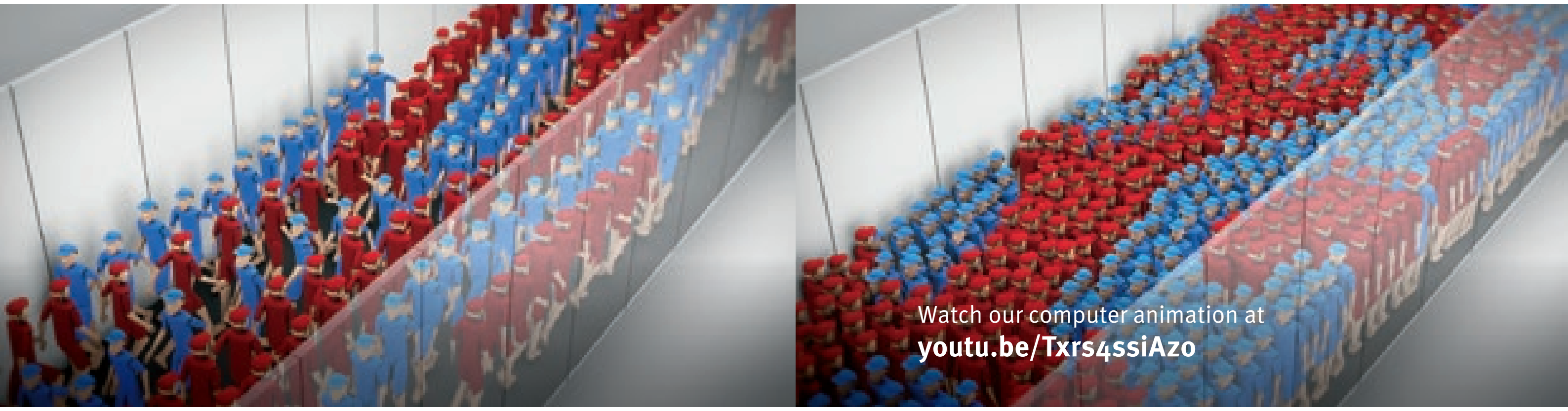
Yet, these simple models fail when we cannot see each other. When the lights go out, we do not have the behavior of other people to hold on to and our intuition fails. We use visual information to spot an exit and find people to help us. That is why it is so difficult to evacuate people from a dark subway station full of smoke. The simple rules for attraction and repulsion between people are no longer valid. Neither are the insights from group psychology about leadership or cooperation. In disaster training, we learn to stay together, to give each other a hand, and to cooperate in finding an exit. However, this has never been tested. Is buddying really the best strategy? “To learn about escaping these situations, we studied how atoms in a gas move through a hole”, says Adrian Muntean, assistant professor at the department of Mathematics and Computer Science in Eindhoven, and associated with ICMS. “We used a computer model for the random trajectories of atoms, assuming that people without sight have no other choice than to try to walk in an arbitrary direction.” Only when people meet in the dark do they behave differently from atoms, Muntean explains. “In our model, they then stick together, precisely the kind of cooperation firefighter manuals prescribe.” To examine whether cooperation is always the best strategy, Muntean set limits to the group size. When the bunch of people became too large, he let newcomers go their own way. In the computer simulations he played with the critical group size and the number of people wandering around. It turned out that cooperation is not always the best strategy. Especially when the space is crowded, more people escape when groups remain small and many go their own way. But this result depends on the circumstances. This simple model is probably not precise enough to decide when selfishness is more advantageous than cooperation. “Quite probably, we’ll have to include more sophisticated deliberations than only group size. Already this simple model shows that it is useless to give general advice to cooperate or to be selfish. Reason enough to revise calamity trainings”, Muntean remarks.

People and polymers

Muntean also tried a different approach, inspired by polymer dynamics, involving monomers grouping together. Mathematically, this gives a continuous description, as opposed to the discrete atoms and lattice-inspired approach. “We got similar results. Also in this model, it is not advantageous to join large groups. In fact, it is not favorable at all to join a group, as it takes time to associate, and you need to dissociate in order to go through the exit—especially when the door is small. It suggests that some major disasters in the past would have been smaller if only people had not helped each other.”

Real world

Muntean is now measuring the movements of students taking the stairs entering the cantina at the university and of people walking through a railway station. He tries to capture accelerations due to interactions between people who know each other. This would add some inertia to the models, because of people clogging together. Another extension would be to include anisotropy in the models. The simple models do not take into account that we have eyes only in our face, which makes it easy to avoid people who approach us in front, but less so from the side. The same is true for our perceptions of hearing, touching and smelling. Muntean is presently examining how this anisotropy influences the outcome of model simulations.



Watch our computer animation at
youtu.be/Txrs4ssiAzo

More about this research:

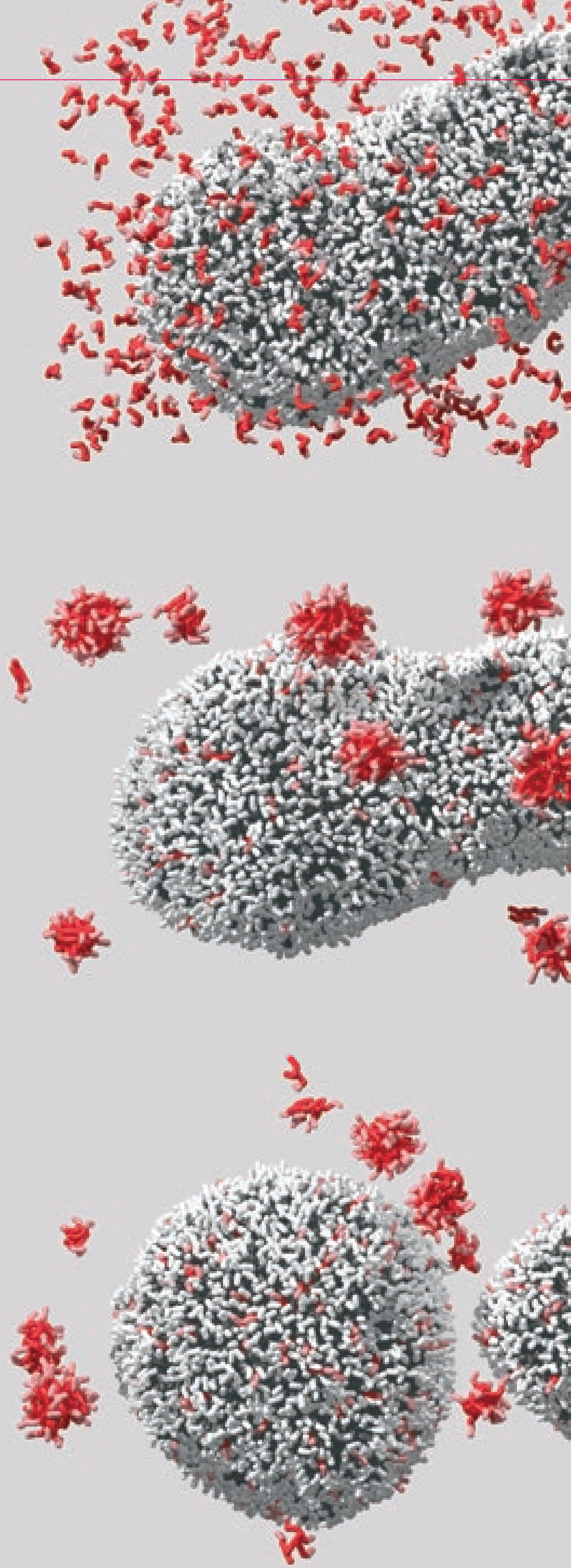
E.N.M. Cirillo, A. Muntean (2013) Physica A, 392, 3578–3588

L. Gulikers, J.H.M. Evers, A. Muntean, A.V. Lyulin (2013) J. Stat. Mech., 04025

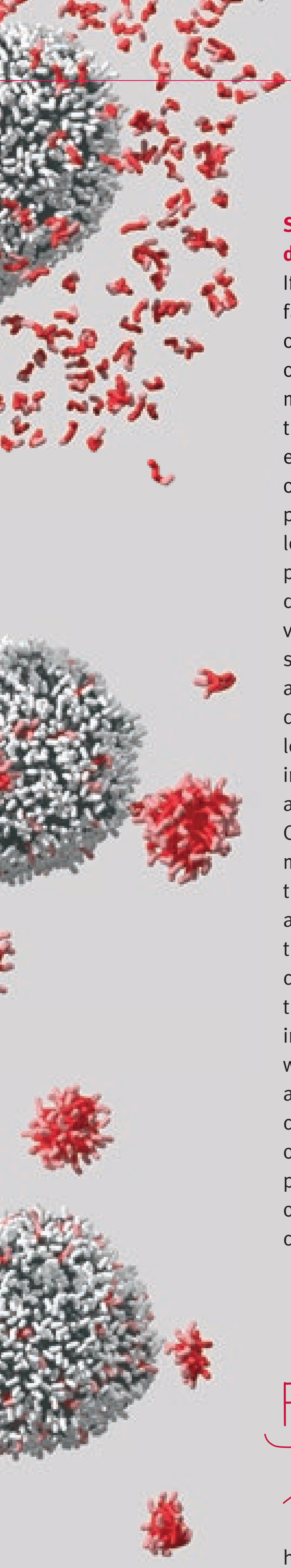
A. Muntean, E.N.M. Cirillo, O. Krehel, M. Böhm (2014). ‘Pedestrians moving in the dark: Balancing measures and playing games on lattices’, in: A. Muntean, F. Toschi (eds.), Collective Dynamics from Bacteria to Crowds, Springer

Computer simulation

Observing hidden worlds



Simulation is the computational study of the spatial and temporal evolution of real-world systems. Simulations can provide unobstructed access to structural and dynamical features at all relevant length scales, and are increasingly deployed to aid in the analysis and design of complex molecular systems. ICMS-affiliated computational groups are developing and implementing a range of state-of-the art techniques to push the boundaries of *in silico* science.



Strength of simulations: detail, scaling, access

If the approximate numbers in the facts tell you anything, it is that in order to understand the behavior of individual actors (atoms/ molecules, cells or humans), their interactions (for instance, entropic, electrostatic, steric or social) and their emergent properties at an aggregated level (a cell, a body, or the global population), we must learn to deal with huge numbers and vastly different length and time scales. Often, those properties are prohibitively extreme for direct experimental access at all length scales, and only statistical information may be obtained about the behavior of the system. Computer simulations provide a means to study the behavior of those systems with unobstructed access at all relevant length and time scales. As such, simulations can act as a digital microscope that can observe the system of interest with infinite resolution, without interfering with it, and with precise control over conditions. The combination of a rapid increase in computer power with the development of increasingly sophisticated computer algorithms has led computer simulations to evolve from a purely descriptive tool to one that may be employed for predictive purposes: in silico numerical experimentation – properly coupled and validated with in vitro and in vivo efforts – is advancing our understanding of the fundamental processes in complex molecular systems, but also supporting and in some cases even replacing traditional trial-and-error screening and formulation procedures in industry.

The right tool for the job: multiscale methodology

Despite the exponential increase in computational power, even the most advanced supercomputers are insufficient to capture the molecular complexity of even the simplest cell. For this reason, researchers within the ICMS are developing multiscale procedures, where many individual actors are coarse grained into effective entities, for which the numbers and properties must be carefully chosen to prevent loss of essential information in the coarse grained system. Likewise, one must consider the type of question one seeks to address in simulation: for some systems, we are interested in predicting equilibrium structures, whereas for others the dynamics – a system's evolution over time – may be more relevant. Traditionally, Monte Carlo techniques are used for equilibrium computations, and Molecular Dynamics for time-resolved numerical experiments but today, at TU/e, many additional and even hybrid algorithms are developed and implemented to tailor the computational approach to the scientific question at hand.

Simulations and ICMS

ICMS groups across all participating TU/e departments perform computer simulations of a broad range of interacting actor systems, ranging from all atom studies (e.g. in studies of protein-ligand binding), polymers (in studies of soft matter and tissue mechanics) to individual humans (in studies of pedestrian traffic). Our ambition is to supplement the ICMS's experimental multi-scale characterization facilities with purpose-built simulational capacities, investigate into the fundamental processes of complex molecular structures, dynamics and performance.

FACTS

10^{9}
humans in the world

10^{13}
cells in the human body

10^{14}
atoms in one human cell

Watch the YouTube animations about coarse-graining:
youtu.be/ZuekF_fyqcU

and about collagen:
youtu.be/uXdOSUnCKtk

NEWS, AWARDS & GRANTS

NWO Rubicon for

PETER KOREVAAR

NWO has awarded dr.ir. Peter Korevaar a Rubicon grant. Peter will use this grant to fund a two-year post-doctoral period in the Biomineralization and Biomimetics Lab led by Prof. Joanna Aizenberg at Harvard University. He will work on materials that can convert a fuel in continuous movement at macroscale.

BERT MEIJER

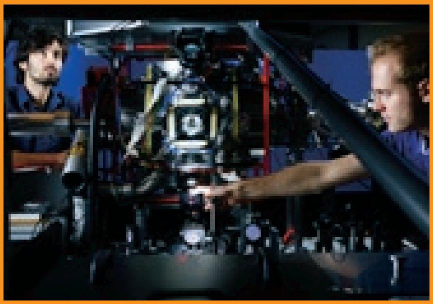
appointed Akademiehoogleraar KNAW

The Royal Netherlands Academy of Arts and Sciences (KNAW) awarded this year's "Prijs Akademiehoogleraren" to ICMS scientific director Bert Meijer and to biological psychologist Dorret Boomsma of the VU. The award honors the work of scientists who belong to the best of the world. The two scientists receive a million euros, to be spend on a scientific purpose of their own choice.

Research

JOM LUITEN & COLLEAGUES

in Physics Today



This summer, Physics Today has highlighted the work of Jom Luiten and colleagues with an honourable mention and an article. It draws the attention to their research on ultrafast electron diffraction. Physics Today is the news magazine of the American Institute of Physics and the American Physical Society.

NOORTJE BAX

Junior Postdoc Dutch Heart Association

Dr. Noortje Bax is appointed Junior Postdoc by the Dutch Heart Association. The goal of this personal grant within the dr. E. Dekker-program is, to let postdocs who recently received their PhD become an independent researcher. In her research, Bax will look at the regeneration of the heart muscle by using a combination of treatment methods. The grant received by Bax is for 280.000 euros, which will provide financial support for four years.

/ Carlijn Bouten / Cecilia Sahlgren

The beat of regenerative therapy

Professor Carlijn Bouten and assistant professor Cecilia Sahlgren are determined to bring the field of regenerative medicine steps ahead. Their research concentrates on cell behaviour, cell communication and in-situ tissue engineering. So far they have achieved promising results in studies of the heart valve, heart muscle and blood vessels.

“Our challenge is: can we ***steer*** and **control** cellular function well enough in **VARIOUS TYPES** of situations?”

Carlijn Bouten

Especially the living heart valve the Bouten group is working on in collaboration with colleague material scientists and mechanobiologists, is drawing a lot of attention in academic and medical circles. And the concept is impressive. In the future, a biodegradable implant will be an option for a patient suffering from heart valve malfunction. Implant valves are being designed to attract cells from the bloodstream and surrounding tissue, which develop into a regenerated living heart valve. The synthetic scaffold, being unnecessary for additional function, degrades into benign byproducts that are eventually expelled from the body. After the process, the patient is the happy owner of a new and healthy heart valve, probably lasting a lifetime. The research is in an advanced stage, and the first clinical trials are expected in a few years.

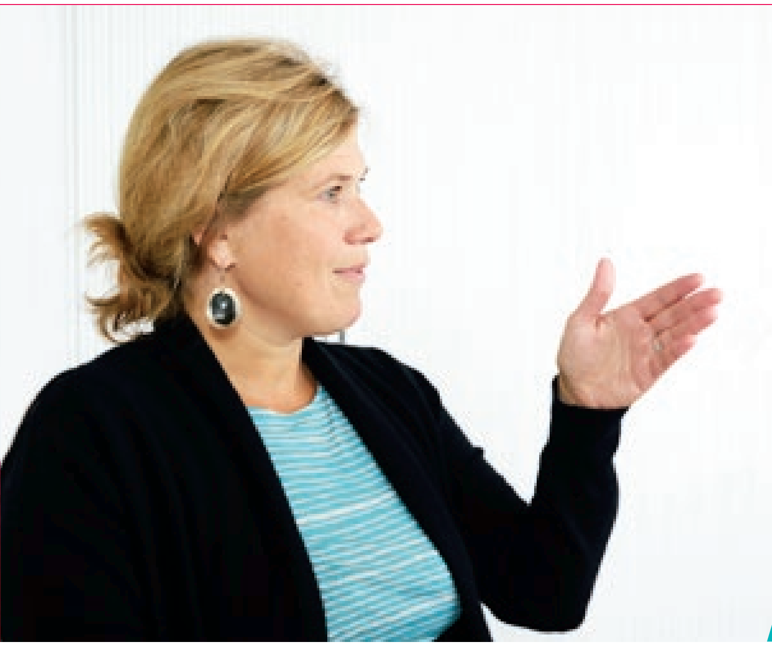
Watch the ICMS animations on YouTube:
youtu.be/HU_pgHlWsdc
youtu.be/oe_dmCbk7OY

Translate to diseased

Bouten: “We now have the extracellular environment, the synthetic heart valve that we can implant, that is strong enough, that degrades over time and in the mean time attracts cells and develops new tissue. Although we have progressed, there is still a lot of work to be done. Our heart valve works in the lab and in animals, but we have so far tested only under “healthy” conditions. Our challenge is: can we steer and control cellular function and tissue formation well enough in various circumstances? Can we develop a tissue that will remain stable for a lifetime? Does this valve behave well for young and older subjects? Can we make it work for people with a congenital heart defect: will tissue generation work well enough for the diseased?”

Unpredictable

Sahlgren: “The fundamental part of our research is very complex. It comes down to profound knowledge and understanding of cellular molecular biology to be able to get targeted control over tissue formation. How do the cells communicate? How is the correct tissue architecture found by communication between the cells? Can we guide tissue formation by synthetic materials? How does the synthetic scaffold influence the cell contact and behaviour? We work with a highly dynamic system, combining synthetic and biological material, and make use of molecular and cellular self-assembly. Working in this complex environment and under constant non-equilibrium is extremely difficult, but it also resembles what makes us function as human beings, and is therefore extremely interesting!” Bouten adds: “At times it can be frustrating for students. Engineers preferably think in terms of problem-solving or at least in predictable outcomes. In our field, prediction is possible but only within a certain bandwidth. In some cases the implanted scaffold functions correctly and we get great results. But there can also be complications.



"How do the cells **COMMUNICATE?** How is the *correct architecture* found by communication between the cells?"

Cecilia Sahlgren

As we do not yet fully understand the interactions between cells, materials and new tissue formation, we cannot fine-tune them or predict the outcomes."

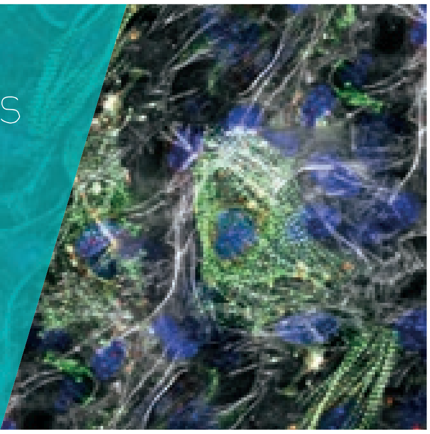
Closer

Sahlgren: "To come to better and reliable predictions we are building up knowledge. My main need is a laboratory model that mimics the in-situ situation. You cannot do this research in the body; it is very difficult to image dynamic cellular and molecular processes in the body. We are starting to combine existing models and build new, more complex model systems, both numerical and live. This need for development of new tools I find a very interesting part of my work. However, I am also glad to have the opportunity to work in an environment that is closer to an actual application. Classical molecular biology works quite far from application. And since it is our aim to boost regenerative medicine and improve the life of patients; it can't be better!"

Put it in an envelope

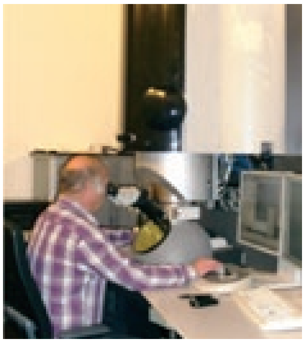
It is clear that Bouten and Sahlgren work in a challenging environment and that their research and findings do have the potential to provide effective regenerative therapies in the future. Bouten: "It is great working on therapies that will possibly set new standards. What keeps our pace up is the consciousness that we are developing a therapy that will help more people. For starters, material-based tissue regeneration will be much cheaper than the existing therapies. Furthermore, the material has off-the-shelf availability. In the case of heart valves a young patient with a defect heart valve currently needs to be operated 2-3 times during life. Our heart valve grows with the patient, and the patient thus faces surgery only once in a lifetime. This cuts the costs by 60% and increases quality of life enormously. It is possible to do the implant minimally invasive via the groin so you do not need open-heart surgery. And you can put a synthetic valve in an envelope, send it to Indonesia and a local surgeon can use it. So it serves a worldwide market and can therefore become available to a lot of patients."

THE INTERNAL CELL STRUCTURES OF CARDIO-MYOCYTES AND FIBROBLASTS COMPOSING CARDIAC TISSUE



CryoTEM

Cryogenic transmission electron microscopy (cryoTEM) allows the visualization of soft matter in its native hydrated state, in three dimensions and with (sub)nanometer resolution. In the Soft Matter CryoTEM Research Unit (www.cryotem.com) high resolution and time-resolved cryoTEM is combined with diffraction and spectroscopic techniques to study simultaneously the development of morphology, structure and chemistry in soft-matter and hybrids materials.



The TU/e CryoTitan, a one-of-a-kind electron microscope tailor made for the cryoTEM analysis of synthetic soft matter.

FACTS

CryoTEM samples are thin films with a thickness of

30-300 nm

prepared by plunge freezing into melting ethane with a temperature of

-183 °C

Radiation damage is prevented by using electron doses

< 100 electrons/Å²

CryoTEM of Soft Matter

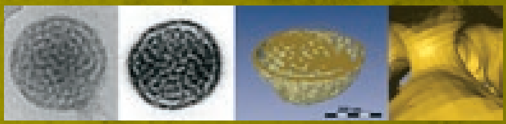
The analysis of nano- and mesostructured soft matter requires detailed imaging, often with (sub)nanometer resolution. Where scanning-probe techniques, such as STM and AFM, are the most important tools for imaging surface-associated structures, cryoTEM is the technique of choice to study self-assembled and nanoscopic structures in solution. In recent years, it has become an important tool to study physical and (bio)chemical processes that control the organization of matter in solution and at interfaces.

Where conventional TEM imaging of inorganic structures uses the contrast of the elemental distributions within these materials, such contrast is not provided by the organic components in self-assembled structures and biological materials. Moreover, as TEM samples must be inserted into the high vacuum of the microscope column, solution samples and hydrated specimens must be dried before they can be studied. Both staining and drying may affect the structure and morphology of the sample, e.g. through complexation reactions, concentration of components, or structural collapse. CryoTEM avoids these issues through the rapid fixation of samples by plunge freeze vitrification and by using phase contrast imaging.

The specimen: fixation and protection

During the plunge freeze vitrification high cooling rates are used (10^4 – 10^5 K/s) such that the sample becomes embedded in an amorphous film that is transparent for the electron beam. This rapid fixation makes cryoTEM an ideal technique for the time resolved study of nanostructures, as the vitrified samples can be studied for as long as one likes, and with different techniques as long as they are kept at cryogenic temperatures.

To avoid damage to the sample by exposure the high energy (mostly 200-300 kV) electron beam of the microscope, “low dose” procedures are used that limit the exposure of the sample to a total dose of less than 100 electrons/Å². Although for a long time this has limited the resolution of cryoTEM, the development of advanced CCD cameras and energy filters now allows sub-nanometer structures to be resolved and even lattice imaging has been achieved.



CryoTEM analysis of a bicontinuous polymer nanosphere. From left to right: a 2D cryoTEM image, a cross section through a tomographic reconstruction, computer rendering of the reconstructed volume and visualization of the internal pore structure. Adapted from A.L. Parry et al, Angew Chem. Int Ed. 47 (2008) 8859-8862.

A versatile technique

Although projection images obtained by cryoTEM imaging in principle only provide two dimensional information, three dimensional information can be obtained by tilting the sample and recording a series of images under different tilt angels, typically between -65 °C and +65 °C. From this series a volume can be reconstructed to obtain three dimensional information, which can be further visualized using computer aided segmentation.

The versatility of cryoTEM is illustrated by the variety of systems that have been studied. These range from self-assembling block copolymer structures, protein-tagged vesicles, dendrimer-based networks, supramolecular hydrogels, mineralizing collagen, Langmuir monolayers, and nucleating mineral solutions. Also detailed 3D imaging in organic solutions was recently demonstrated for the nanostructure of semiconducting poly-3-hexyl thiophene nanowires.

The CryoTEM Unit continually aims at further development of methods, techniques and infrastructure to expand the limits of soft matter imaging, and to "visualize the invisible".

ICMS TOP PUBLICATIONS

February 2014 – August 2014

1. *M.M.C. Bastings, S. Koudstaal, R.E. Kieltyka, Y. Nakano, A.C.H. Pape, D.A.M. Feyen, F.J. van Slochteren, P.A. Doevendans, J.P.G. Sluijter, E.W. Meijer, S.A. Chamuleau, P.Y.W. Dankers*
A fast pH-switchable and self-healing supramolecular hydrogel carrier for guided, local catheter injection in the infarcted myocardium
Adv. Healthc. Mater. 3, 70-78 (2014)

2. *E. Ducrot, Y.L. Chen, M. Bulters, R.P. Sijbesma, C. Creton*
Toughening elastomers with sacrificial bonds and watching them break
Science 344, 186-189 (2014)

3. *L. Albertazzi, D. van der Zwaag, C.M.A. Leenders, R. Fitzner, R.W. van der Hofstad, E.W. Meijer*
Probing exchange pathways in one-dimensional aggregates with super-resolution microscopy
Science 344, 491-495 (2014)

4. *D. Florea, S. Musa, J.M.R. Huyghe, H.M. Wyss*
Long-range repulsion of colloids driven by ion exchange and diffusiophoresis
Proc. Natl. Acad. Sci. U.S.A. 111, 6554-6559 (2014)

5. *M.Y. Guo, L.M. Pitet, H.M. Wyss, M. Vos, P.Y.W. Dankers, E.W. Meijer*
Tough stimuli-responsive supramolecular hydrogels with hydrogen-bonding network junctions
J. Am. Chem. Soc. 136, 6969-6977 (2014)

6. *V. Ballotta, A. Driessen-Mol, C.V.C. Bouten, F.P.T. Baaijens*
Strain-dependent modulation of macrophage polarization within scaffolds
Biomaterials 35, 4919-4928 (2014)

7. *M. Scheepstra, L. Nieto, A.K.H. Hirsch, S. Fuchs, S. Leysen, C.V. Lam, L. in het Panhuis, C.A.A. van Boeckel, H. Wienk, R. Boelens, C. Ottmann, L.-G. Milroy, L. Brunsveld*
A natural-product switch for a dynamic protein interface
Angew. Chem., Int. Ed. 53, 6443-6448 (2014)

8. *P.A. Korevaar, C.J Newcomb, E.W. Meijer, S.I. Stupp*
Pathway selection in peptide amphiphile assembly
J. Am. Chem. Soc. 136, 8540-8543 (2014)

9. *A. Mirsaidi, K. Genelin, J.R. Vetsch, S. Stanger, F. Theiss, R.A. Lindtner, B. von Rechenberg, M. Blauth, R. Müller, G.A. Kuhn, S. Hofmann Boss, H.L. Ebner, P.J. Richards*
Therapeutic potential of adipose-derived stromal cells in age-related osteoporosis
Biomaterials 35, 7326-7335 (2014)

10. *M.J. Hollamby, M. Karny, P.H.H. Bomans, N.A.J.M. Sommerdijk, A. Saeki, S. Seki, H. Minamikawa, I. Grillo, B.R. Pauw, P. Brown, J. Eastoe, H. Möhwald, T. Nakanishi*
Directed assembly of optoelectronically active alkyl-pi-conjugated molecules by adding n-alkanes of pi-conjugated species
Nature Chem., published online (2014)

11. *S.N. Semenov, A.J. Markvoort, T.F.A. de Greef, W.T.S. Huck*
Treshold sensing through a synthetic enzymatic reaction – diffusion network
Angew. Chem., Int. Ed. 53, 8066-8069 (2014)

12. *A.P.H.J. Schenning, S.J. George*
Phases full of fullerenes
Nature Chem. 6, 658-659 (2014)

13. *L.T. de Haan, J.M.N. Verjans, D.J. Broer, C.W.M. Bastiaansen, A.P.H.J. Schenning*
Humidity-responsive liquid crystalline polymer actuators with an asymmetry in the molecular trigger that bend, fold, and curl
J. Am. Chem. Soc. 136, 10585-10588 (2014)

14. *V. Ballotta, A.I.P.M. Smits, A. Driessen-Mol, C.V.C. Bouten, F.P.T. Baaijens*
Synergistic protein secretion by mesenchymal stromal cells seeded in 3D scaffolds and circulating leucocytes in physiological flow
Biomaterials, published online (2014)

15. *D.J. Broer*
A new view on displays
Nature 511, 159-160 (2014)

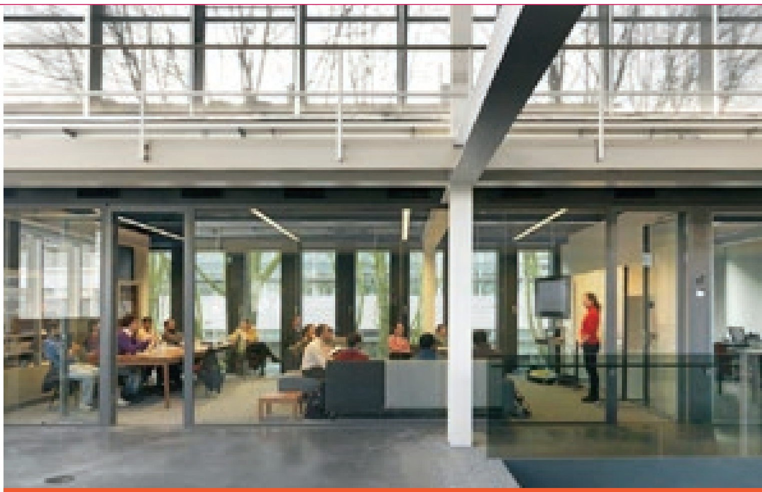
16. *D. Liu, D.J. Broer*
Self-assembled dynamic 3D fingerprints in liquid-crystal coatings towards controllable friction and adhesion
Angew. Chem., Int. Ed. 53, 4542-4546 (2014)

17. *Z.S. Kean, J.L. Hawk, S. Lin, X. Zhao, R.P. Sijbesma, S.L. Craig*
Increasing the maximum achievable strain of a covalent polymer gel through the addition of mechanically invisible cross-links
Adv. Mater., published online (2014)

18. *A. van Reenen, A.M. de Jong, J.M.J. den Toonder, M.W.J. Prins*
Integrated lab-on-chip biosensing systems based on magnetic particle actuation – a comprehensive review
Lab Chip, published online (2014)

19. *A. Hernandez-Garcia, D.J. Kraft, A.F.J. Janssen, P.H.H. Bomans, N.A.J.M. Sommerdijk, D.M.E. Thies-Weesie, M.E. Favretto, R. Brock, F.A. de Wolf, M.W.T. Werten, P. van der Schoot, M. Cohen Stuart, R. de Vries*
Design and self-assembly of simple coat proteins for artificial viruses
Nat. Nanotechnol, published online (2014)

Scientific progress through discussion



Scientific progress is not possible without intense and passionate discussions. The past has shown that world-changing ideas have never been accepted without these critical ingredients. For strengthening less controversial hypotheses the exchange of thoughts with peers is required as well, in a surrounding where helpful criticism and open questions are continuously encouraged. The ICMS Advanced Study Center has been designed and established exactly for this capacity.

Although ICMS' main topic is molecular complexity, the Advanced Study Center has a university-wide scope, far beyond the institute's own fields of research. It serves as a place to discuss topics in science and engineering for all who are working on the boundaries of knowledge. It was founded to stimulate cross fertilization between disciplines and developing a scientific vision for the coming years.

The ASC is located in the Ceres building on the TU/e campus and is part of the Institute for Complex Molecular Systems (ICMS). It consists of a colloquium hall, the common room and several meetings rooms.
We provide facilities, support and expertise for organizing interdisciplinary scientific activities, like workshops and lectures. External participants are welcome to participate in the Advanced Study Center activities.

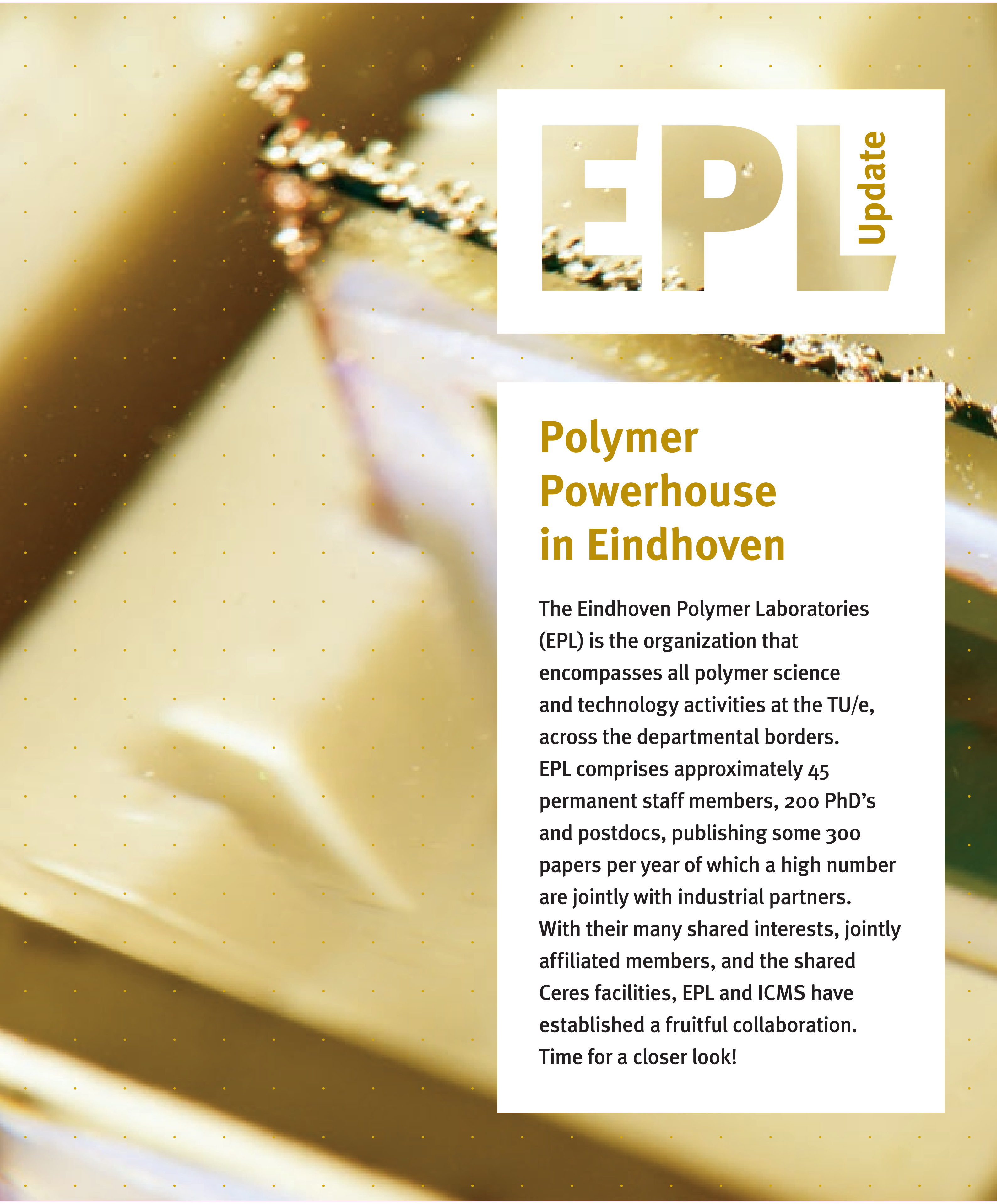
Honors students organized scientific debates

During the academic year 2013-2014, ICMS offered one of the six tracks in the TU/e Honors Academy. The ICMS track "The scientific debate" aimed at bringing back the scientific debate at the campus.

As final activity within the track, the participating bachelor students Bart Hendriks, Rick Jongen, Stijn van Leuken, Reanne Rust, Ali Saadun and Camiel Steffanie organized three debates with speakers from within and outside our university. They discussed topics around sustainable energy, ranging from solar cells and biofuels to the relation between politics and science. Speakers were among others drs. Stientje van Veldhoven (D66, Dutch Lower Chamber), ir. Simon Rozendaal (journalist Elsevier magazine), and prof.dr. Niek Lopez Cardozo (TU/e Applied Physics).

> "The ICMS Advanced Study Center serves as an ***intellectual home*** for original thinkers and scientists..."

Sagitta Peters, managing director



EPL Update

Polymer Powerhouse in Eindhoven

The Eindhoven Polymer Laboratories (EPL) is the organization that encompasses all polymer science and technology activities at the TU/e, across the departmental borders. EPL comprises approximately 45 permanent staff members, 200 PhD's and postdocs, publishing some 300 papers per year of which a high number are jointly with industrial partners. With their many shared interests, jointly affiliated members, and the shared Ceres facilities, EPL and ICMS have established a fruitful collaboration. Time for a closer look!

What is EPL?

Founded in 2002, the EPL has been established to advance multidisciplinary polymer science and technology at the TU/e. EPL does this in three ways: firstly, by fostering collaboration and coherence between Eindhoven polymer researchers (through prioritized research themes, seminars, discussion meetings, and symposia). Secondly, by acting as host to all guest polymer researchers at our university, providing them with a shared home in Ceres. Thirdly, and most importantly, EPL places great importance in education, ensuring that the next generation of polymer receives all the support they need to shape the interdisciplinary future of polymer science.

In all of its research, education and industrial collaborations, EPL has since its very beginning embraced the Chain of Knowledge philosophy: polymer science is a truely multidisciplinary and multiscale endeavour, and EPL strives to integrate world class efforts along the entire spectrum of relevant topics; from polymer synthesis all the way up to processing and design.

Research at EPL

Based on recent trends in modern polymer science and technology and building further on the strength and unique capabilities of the present scientific staff, EPL defined four research areas to focus on for polymer science and technology at the TU/e:

- Polymer chemistry and self-assembly of polymer architectures
- Polymer processing, structure formation during flow, rheology and characterization
- Structure-property relations, functional, mechanical, tribological, etc
- Developing the tools of quantification: theory and multi-scale modeling

Since 2013, EPL is a formal interdepartmental center of the TU/e. Other centers at the TU/e that have overlapping interests with those of the EPL, are ICMS and the Eindhoven Multiscale Institute (EMI). As polymers are one type of complex systems with multiple scales of interest, several researchers of EPL are at the same time also active in ICMS and/or EMI. With these centers of competence being located at the same university, the close interrelations between them will be of mutual benefit.

In 2011, the Intelligent Community Forum voted Brainport Region Eindhoven as the World's Smartest one. By promoting close collaboration between industry, research, and government, the Brainport Region Eindhoven generates a productive climate for businesses and researchers alike. In the same spirit, the majority of research efforts of EPL are in close collaboration with multiple industrial partners.

The research activities of the groups participating in EPL is mainly funded by the Dutch government, the Dutch Science Foundation NWO, European Research Council ERC, and industry via the Dutch Polymer Institute (DPI) and via bilateral contracts.

Education at EPL

The success of the 'chain of knowledge' idea hinges on the researchers' training that should combine specialization with interdisciplinary overview. Therefore, adequate education of students is of high priority. EPL is a key partner in the National Dutch Graduate Program in Polymer Science and Technology (PTN), and an organizer and major contributor to the course series that leads to the official RPK-title ('Register PolymeerKundige'). RPK is nationally organized, is given in Utrecht, the centre of our country, and includes the following state-of-the-art courses (each of them requiring ten full days of lecturing): Polymer Chemistry, Polymer Physics, Polymer Properties, Polymer Rheology and Processing, and Polymer Innovation. To date, more than 1250 PhD students and postdocs followed the RPK courses, while 112 successfully finished four or more courses, obtaining the official RPK-title, 74 of whom are from the TU/e. At the TU/e, EPL aims at offering coherent course packages to students, both on Bachelor and Master levels.

THESES ICMS

March 2014 – August 2014

1

Mechanics and dynamics in colloidal systems with complex interactions

Daniel Florea

March 17, 2014
PhD advisors:
prof.dr.ir. P.D. Anderson,
dr.ir. H.M. Wyss

2

Laser-assisted growth of carbon nanotubes

Youri B. van de Burgt

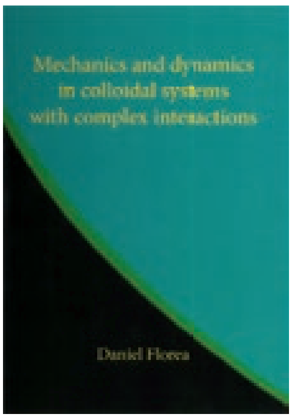
March 31, 2014
PhD advisors:
prof.dr.ir. J.M.J. den Toonder,
prof.dr. A.H. Dietzel

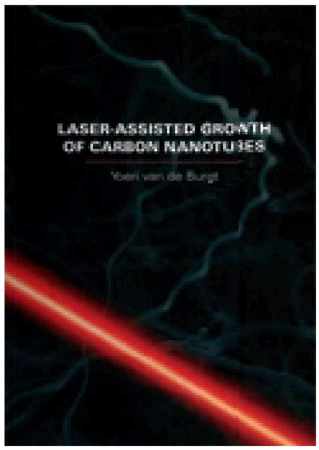
3

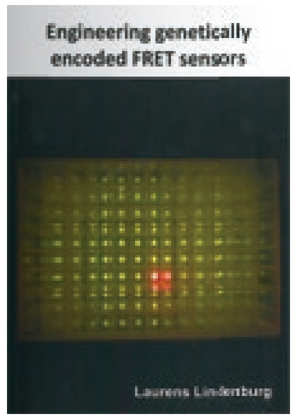
Engineering genetically encoded FRET sensors

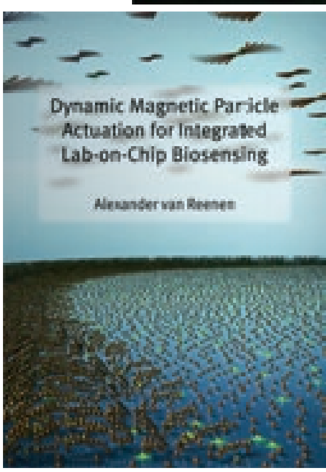
Laurens H. Lindenburg

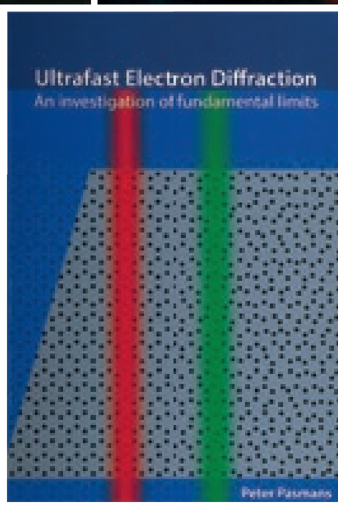
April 23, 2014
PhD advisors:
prof.dr.ir. L. Brunsveld,
dr. M. Merkx

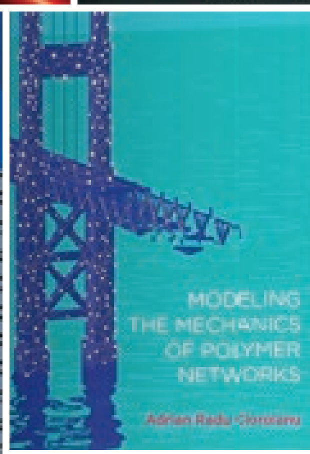












4

Dynamic magnetic particle actuation for integrated lab-on-chip biosensing

Alexander van Reenen

June 2, 2014
PhD advisors:
prof.dr.ir. M.W.J. Prins,
dr.ir. A.M. de Jong

5

Ultrafast electron diffraction – an investigation of fundamental limits

Peter L.E.M. Pasmans

June 19, 2014
PhD advisors:
prof.dr.ir. O.J. Luiten,
dr.ir. G.J.H. Brussaard

6

Modeling the mechanics of polymer networks

Adrian R. Cioroianu

June 30, 2014
PhD advisors:
prof.dr. M.A.J. Michels,
dr. C. Storm

Institute for Complex Molecular Systems

New technologies by mastering complexity

Mastering complexity requires a deep understanding on how matter – both natural and artificial – self-organizes into functional molecular systems. The Institute for Complex Molecular Systems (ICMS) of the Eindhoven University of Technology (TU/e) was established in 2008 and brings together mathematics, physics, biology, chemistry and engineering to stimulate education and research in this emerging field of science. Interdisciplinarity is the core of ICMS; with the specialized input from leading specialists in different branches of science and engineering, new avenues are explored, where mastering complexity is the leading theme. The scientific agenda of ICMS consists of three lines of research:

1. Functional molecular systems
   (program leader prof.dr. E.W. Meijer)
2. Bio inspired engineering
   (program leader prof.dr.ir. F.P.T. Baaijens)
3. Complexity Hub
   (program leaders prof.dr. Rutger van Santen and prof.dr. Mark Peletier)

ICMS hosts the Advanced Study Center, a breeding ground for new interdisciplinary research. It serves as an intellectual home to scientist from all over the world, hosting discussions on the theme of complexity. It is also the home of the Eindhoven Multiscale Institute (EMI) and the Eindhoven Polymer Laboratories (EPL).

ICMS aims at offering an ideal training environment for all young students and scientists to prepare themselves for a future career in science and engineering in a world of increased complexity. Therefore, we offer the Graduate Program in Complex Molecular Systems (MSc and PhD).

The relationship with industry is strengthened via the Industrial Consortium – where science meets innovation.

More general information can be found via our website **www.tue.nl/icms**. Please contact us via email icms@tue.nl or telephone +31 40 247 2482 with specific questions or remarks.

ICMS IN PRESS


KANKERONDERZOEK

Organen die op chip groeien

Het lijkt sciencefiction, maar het gebeurt op de TU/e: organen die groeien op een chip.

"Het duurt nu zeker tien jaar en een miljard dollar om een nieuw medicijn te maken"

'Wow, dat waterstof ging echt snel'

Editorial
ICMS Highlights is the half-yearly magazine of ICMS for ICMS members, colleagues, collaboration partners, policy makers and affiliated companies. ICMS Highlights is published in March and September.

Editorial staff
Sagitta Peters
(editor in chief)

Carla Bouwman
(editorial assistant)

Design and print
Zelv, Eindhoven

Illustrations and cover
ICMS Animation Studio

Article contributions
Moesasji & Bram Vermeer Journalistiek

Photography
Bart van Overbeeke Fotografie,
Ruud Strobbe Fotografie,
Ariane van Spreeuwel

Contact
P.O. Box 513, 5600 MB Eindhoven
The Netherlands
Telephone: +31 (0)40 247 2482
Email: icms@tue.nl

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