ICMS Highlights

Edition 11
November 2018

MATHEMATICS FOR COMPLEXITY

Focus on Dynamics & Control and Network Theory

FROM THE MOLECULE TO THE DEVICE

OLED screens, surgical robots and Mars Rover dust removal

ICMS COURSE ON SCIENTIFIC SKILLS

ICMS
INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS
TU/e

10 YEARS ICMS

INTRODUCTION

ICMS Highlights

Interconnecting scientific strengths in the field of complex molecular systems is an exciting and at the same time challenging exercise. At ICMS we constantly strive to bring scientists and research organizations closer together and stimulate science unrestricted by barriers. The ICMS organization enables researchers to draw inspiration from our in-house pool of expertise, and from our expanding international network of research institutes.

In view of intertwining expertise, enthusiastic researchers at the ICMS focus area Grip on Complexity have taken the initiative to connect theory in the area of Networks and Dynamics & Control with experimental fields such as biological computing. This development is of great importance to increase our understanding of complexity. Moreover, it provides a theoretical basis for the design and synthesis of complex molecular systems. More details on this new initiative can be found in this edition of ICMS Highlights. Also noteworthy is that researchers at the ICMS focus area Molecular Devices actively pursue opportunities to integrate responsive material and/or molecular concepts into the field of robotics.

Executing science at the frontiers of knowledge requires excellent talent and the ability to convince others of the validity of your ideas. ICMS would like to congratulate Jurjen Tel, Sandra Loerakker, Yoeri van de Burgt and Bart Jansen, who have all received ERC starting grants for their daring and promising novel scientific approaches. Kees Storm and Patricia Dankers held their inaugural addresses as full professors and shared their thoughts about their research plans for the coming years.

These are exciting times for research on complex molecular systems, and ICMS is dedicated to creating the optimal environment for these researchers and all its other members to realize their scientific ideas.

We hope you enjoy reading this edition of our ICMS Highlights!

Jan van Hest
Scientific director

Monique Bruining
Managing director

Calendar

March 11 & 12, 2019
ICMS OUTREACH SYMPOSIUM
De Filmzaal & Blauwe Zaal at TU/e

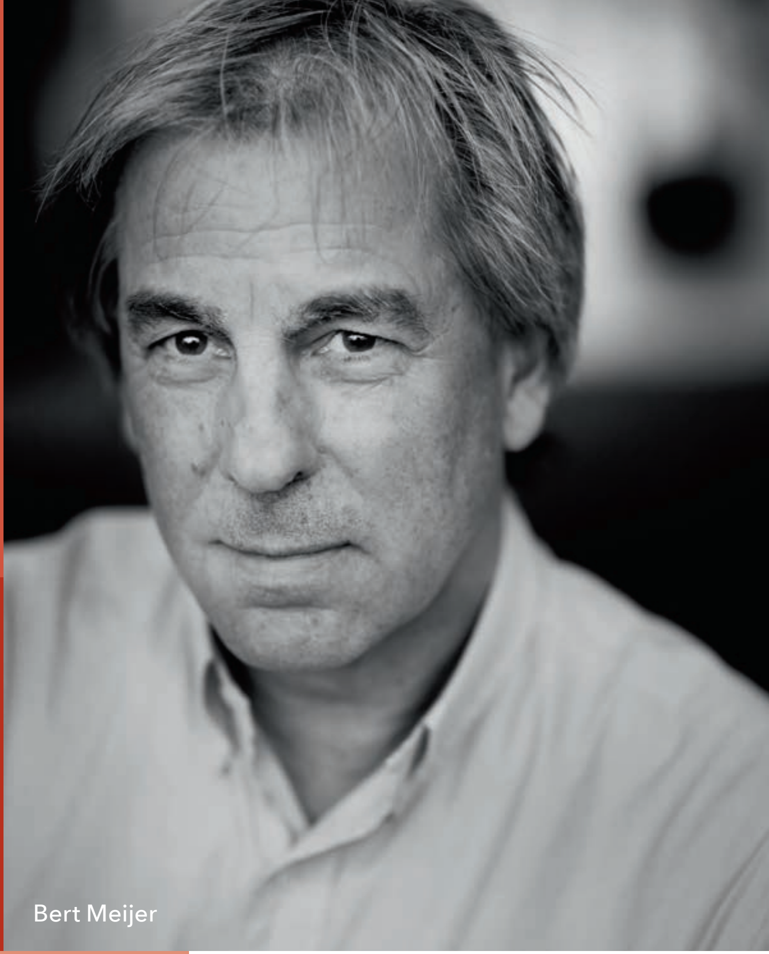
For more details on our events please visit our website **www.tue.nl/icms**

Content

COVER Artist impression of soft robotics. The covers depicts how light with different colors influences the physical properties of soft matter.

FUNCTIONAL SUPRA-
MOLECULAR SYSTEMS

Functional Supramolecular Systems



Bert Meijer

SELF-ASSEMBLY IS DECEPTIVE

We need to thoroughly reconsider our views on the formation of supramolecular structures, says Bert Meijer. “Supramolecular structures are the result of a series of reaction steps, just like complex molecules are. That is why we should start thinking in terms of non-covalent synthesis, which implies that we need to develop synthetic methods, just like we do in classic organic synthesis.” But how? That is what the focus area on Functional Supramolecular Systems aims to find out.

Fortunately, there are two sources of inspiration that offer guidance, says Meijer. “The first is the immense body of knowledge that chemists have built over the past 150 years on how to make molecules. We know a lot about covalent organic synthesis and that allows us to create the most complex molecules we can imagine. But all these techniques and approaches are also very valuable to supramolecular chemistry. We can use those insights to develop methods for what I like to call non-covalent synthesis.”
The second source of inspiration, says Meijer, is Nature itself.
Living organisms are very skilled in constructing supramolecular structures that exhibit a desired functionality. “These structures contain all kinds of polymers and although we know a lot about covalent polymer synthesis, we don’t yet understand how Nature creates these highly functional polymer-based structures. Biological examples will offer clues on how we can apply the concepts used by Nature to develop synthetic analogues.”

For Bert Meijer, there is no question when it comes to defining the key challenge in supramolecular chemistry. "We are all convinced that supramolecular systems are essential to realize new applications in important areas such as materials, energy and health care, but we lack a fundamental understanding of how such systems are formed. How do the various molecules in a system come together and how can we control and direct that process? Both questions are still unanswered. It is completely unchartered territory that we need to explore." This immediately brings new questions to the table, because how and where do you start exploring the unknown?

"CHEMISTS NEED TO TAKE CONTROL AND NOT SIMPLY LET THE SYSTEM RUN ITS COURSE AND ACCEPT WHATEVER IT DELIVERS"

A LITTLE SHAKE

Which brings us to self-assembly, Nature's way of making what it needs. It is by now also the preferred approach of supramolecular chemists around the world. When asked why we actually need new methods, Meijer sighs and throws up his arms. "I know, everyone talks about self-assembly and self-organization and I understand that, because it sounds really attractive. But self-assembly is a deceptive term. It implies that everything just happens by itself and the only thing you need to do is put all the compounds together, give it a little shake and then sit back and wait until it's done. But this means you completely rely on thermodynamics to deliver the final structure. The problem is that in this approach you will always end up with the outcome that is most favorable under those particular conditions. And that is not necessarily the structure you want."

Listening to Meijer, one gets the impression that chemists need to take back control and not simply let the system run its course and accept whatever it delivers. But what can chemists do to influence and steer a self-assembling system in the right direction? "It starts by studying the fundamental mechanisms of the various reaction steps that together make up the assembly process. Each assembly step is a reaction step, just like we have in multistep covalent synthesis. I consciously use these terms, because I want to convince the field that self-assembly is a synthetic process. And if you understand the mechanisms that underlie the various steps, you can look for ways to promote or inhibit certain steps." Although Meijer immediately admits that he doesn't have a ready-made solution, he has a number of ideas on where to start. "So far, all the focus has been on thermodynamics, but the kinetics of these self-assembly processes have been largely ignored. Studying the kinetics is a must, because we all know that the kinetics determine the route towards a certain end product. And if a system has multiple routes available, you have to make sure that your desired route is, or becomes, the most favorable one. Otherwise your system will get stuck in a kinetic trap. The only way to do this is to study the kinetics of all the potential pathways and then devise a strategy to push the system towards the pathway of your choice. For covalent synthesis, these questions were already asked in the 1890s, but now we need to address them for non-covalent synthesis as well."

CHAPERONES

This is just one illustration of the overall shift in thinking that Meijer advocates. The current view is that chemists actively make molecules, but they don't 'make' supramolecular structures. These somehow just emerge from a completely autonomous process that is beyond our reach. "Of course, it would be great if we could just throw all the ingredients together and be done with it. That would also be very attractive for classic organic synthesis. Think about the very complex synthesis of vitamin B12. Wouldn't it be wonderful if you only had to put all the required atoms in a flask, shake it and that's it. The strange thing is that nobody would even consider this to be possible for vitamin B12 or any other molecule. But somehow, when it we talk about supramolecular structures, the general feeling is completely different."

Interestingly, Meijer adds, Nature - the field's premier source of inspiration - is not taking the 'throw it together and lean back'-approach at all. "A perfect example are chaperones, which are needed to fold proteins into the right conformation. This is the only task of chaperones, these compounds serve a synthetic purpose. Another example is collagen. In the cell, the collagen filaments are formed with a little extra structure on the ends. Once the filaments exit the cell, these little structures are removed and then the filaments can start to assemble into larger fibrils. To me, those little structures are the equivalent of a protective group that we use in organic synthesis. They serve the same purpose and that is to control a reaction step in a larger synthetic process."

In spite of all the fundamental knowledge we still need to gain, Meijer is optimistic that we will make substantial progress over the coming years. Moreover, it is imperative that we do, he concludes. "Because if we don't, we will just keep on running into the same wall over and over again."

MATERIALS AND REGENERATIVE MEDICINE

Unravelling the secrets of human elasticity

AMAZING TROPOELASTIN

In July this year, Tony Weiss from the University of Sydney presented an ICMS lecture on "Interplay of human protein biomaterials and accelerated wound repair". The Weiss Lab focuses on the assembly of human elastic tissue, its damage and its repair. He is very interested in the amazing, self-assembling elastic protein tropoelastin, and in the use of synthetic elastin to repair elastic tissues in skin, artery, bladder and lung.

WHY IS ELASTIN SO IMPORTANT IN THE FIELD OF TISSUE ENGINEERING AND REGENERATIVE MEDICINE?

Elastin is an essential part of the human body. Wherever you find elasticity in the body, you find elastin. For example, elastin enables the expansion and contraction of blood vessels with every heartbeat, and gives skin its flexibility. It is the fundamental protein building material for elasticity. So if we want to make appropriate materials that will work well in soft elastic environments, we have to look at elastin and find ways to build elastin in the laboratory.

WHAT IS YOUR WAY TO ACHIEVE THAT?

We have developed tropoelastin which is a precise copy of the natural elastic protein present in the human body. Nature has been working on

Tony Weiss is the McCaughey chair in Biochemistry, professor of Biochemistry & Molecular Biotechnology, with co-appointments in the Charles Perkins Centre and the Bosch Institute at the University of Sydney. The Weiss Laboratory is the leading research site for tropoelastin & synthetic elastin biomaterials. Tony Weiss was recently awarded the 2018 Johnson & Johnson Eureka Prize for Innovation in Medical Research and the 2018 Premier's Prize for Science & Engineering Leadership in Innovation, rewarding excellence in the fields of research & innovation, leadership, science engagement and school science.

The lecture of Tony Weiss marked the kick-off in the ICMS 'Great Debate Series' on the Synthetic Extracellular Matrix. Through a series of lectures in 2018/2019, the ICMS focus area Materials for Regenerative Medicine encourages young scientists to discuss potential new strategies to drive this field forward. Coming lectures will be held by Patricia Dankers (TU/e) and Michael Raghunath (Zurich University of Applied Sciences).

"TROPOELASTIN IS A LONG TERM RESEARCH PROJECT OF NATURE, WHICH WE HAVE JOINED RECENTLY."

tropoelastin for many millions of years, which we view as a long term research project of Nature. We have joined that project relatively recently, by making tropoelastin ourselves and by utilizing it. We are working with a very sophisticated molecule, and by continuing with the recombinant form of the protein, which mimics the precise properties of the natural molecule, we are able to leverage the extraordinary properties of this molecule that nature has already developed. As a result of that, we are getting very interesting results.

THE HUMAN BODY IS PROBABLY THE MOST COMPLEX STRUCTURE ON EARTH. HOW DO YOU SEE A SCIENTIFIC APPROACH THAT TACKLES A VERY SPECIFIC PART OF IT, ESPECIALLY WHEN YOU THINK OF THE FINAL AND SO COMPLEX "APPLICATION"?

With current technologies, we cannot recreate the overall complexity of human tissue - we can only approximate it. And the way to do that is to understand each of the building components. Our mission is to understand the contributions of all these components towards elasticity within the body. In addition, even though we deal with less complex systems than the entire body, in our laboratory we try to use materials that approximate their biological counterparts as much as possible. Our expectation is that, when implanted, the human body will recognize these materials as "natural" and surrounding cells and tissue will gradually modify, convert and improve the implanted materials. So our belief is that nature will at a certain point take over and do the rest of the healing job for us. And while our focus is on understanding elasticity, there are other scientists who work on completely different aspects of the structural and the interactive components of the human body. Collectively, as a research community, we are all contributing towards the building of much more complex structures.

HOW DO YOU ENVISION THE COMING FUTURE? HAS THIS TECHNOLOGY MADE IT TO CLINICAL TRIALS YET?

We finished four clinical trials. Also, I founded a start-up company that became a clinical stage company and was recently sold in to a major pharma company. It was actually one of the largest healthcare transactions in the history of our nation, which is a wonderful achievement in the field of tissue engineering. I am eternally optimistic by nature, and I am happy to commit to long-term strategies. We have shown that clinical trials work and I am optimistic about the near future too.

YOUR LAB HAS ALSO DEVELOPED METHACRYLATED TROPOELASTIN, OR THE SO CALLED "METRO TECHNOLOGY". IT IS PRESENTED AS A SURGICAL GLUE WHICH PROMISES TO ELIMINATE THE NEED FOR SUTURES AND STAPLES DURING SURGICAL PROCEDURES, WHILE PROMOTING TISSUE HEALING. WHAT IS THE RANGE OF APPLICATIONS YOU HAVE IN MIND AND HAS THIS TECHNOLOGY ALREADY BEEN TESTED IN HUMAN TRIALS?

We have been testing the MeTro technology in a pre-clinical environment and we want to move to human studies very soon. We have consistently shown that our material is comparable or superior to existing sealants. Deep inside the body, in wet environments, you need to have a powerful elastic sealant, and sealants that are currently in use do not meet all the needs. Our technology does, and I expect significant applications both in emergency treatments, for example when it might be necessary to save a life by quickly stopping blood flow, and in surgical settings, that would benefit from the fact that the MeTro technology is biologically compatible.

GRIP ON COMPLEXITY

Mathematics for complexity

"THROUGHOUT TU/E THE THEME OF COMPLEXITY HAS A RATHER STRONG PRESENCE."

Remco van der Hofstad (right) is a full professor and chair of probability in the Department of Mathematics and Computer Science, Eindhoven University of Technology (TU/e).

Henk Nijmeijer (left) is a full professor at Eindhoven University of Technology (TU/e) and chair of the Dynamics and Control group.

FOCUS ON DYNAMICS & CONTROL AND NETWORK THEORY

Remco van der Hofstad and Henk Nijmeijer present new plans for the ICMS focus area Grip on Complexity. At the heart will be a mathematics inspired approach that combines Network Theory with expertise from the field of Dynamics and Control. And it's not only about gaining understanding; the design and synthesis of new complex systems will be an integral part. The first such system is in the exciting new field of Biological Computing.

What is to be expected when complex molecular systems are studied from the proposed viewpoint? Remco van der Hofstad, the younger and more outspoken of the two mathematicians, explains: “The essence of complex systems is the large number of components that are all connected to each other. Although these mutual interactions can in themselves be simple and predictable, on the scale of the entire system they can lead to emergent and unpredictable behavior. By applying mathematics we want to discover how to deal with such phenomena. Not just to understand them, but also to use the knowledge for the sensible design of novel complex systems”.

SYSTEM OF SYSTEMS

Van der Hofstad contributes with his expertise in stochastic Network analysis, his elder and more cautiously speaking colleague Henk Nijmeijer has extensive experience in the field of Dynamics and Control. Working at the department of Mechanical Engineering, Nijmeijer approaches complexity from a ‘systems of systems’ perspective where mathematics complements experiments and systems design. “We are for instance concerned with developments in vehicle automation, such as cooperative driving. There you create a new driving entity, a new system consisting of individual systems – the cars. Each has its own characteristics in vehicle dynamics, but you want them to synchronize their driving and operate as a new, composed entity. We think that knowledge developed in the field of Dynamics and Control will benefit multiple other systems, for instance human tissue consisting of individual cells.”

Van der Hofstad is excited about cooperating with Nijmeijer: “Put bluntly, in Henk’s field you have complex dynamic entities in a relatively simple network, in my field the network is complex and the dynamics are fairly simple. It is exciting to bring these two approaches together to investigate complex networks consisting of complex dynamic entities. We want to explore what can still be modelled then, and how.”

BEYOND MOLECULAR SYSTEMS

The question of course is what these mathematical explorations of complexity might bring the field of complex molecular systems. Van der Hofstad: “At the celebration of the 10th anniversary of ICMS I have sort of jokingly said that we might consider the future use of the abbreviation ‘ICMS’ for ‘Institute of Complex and Molecular Systems’. But jokes aside, at the ICMS focus area Grip on Complexity we explicitly expand our scope beyond molecular systems. We set out to further develop this focus area from a broad fundamental perspective, which after all is the forte of ICMS.” Nijmeijer adds: “Complex systems are all around us: large ones, such as the climate, the Internet and the global economy, and smaller ones, such as a platoon of cooperative vehicles, drones or mobile robots. We think that by combining the strength of TU/e both in Dynamics and Control and in Network analysis we will be able to contribute to the broader field of complexity. This will, in the end, also be of relevance to molecular systems, of course. For instance, if complexity research helps to understand how thousands of biomolecules in our bodies react to each other in networks, we will be able to develop new drugs for serious diseases such as cancer. And we will learn to design biochemical molecules that assemble themselves into new, smarter materials that would otherwise not be produced.”

THE LANGUAGE OF ENGINEERS

Approaching complexity from a thorough mathematical viewpoint perfectly fits the TU/e, the professors argue. Being a University of Technology, mathematics is widely supported and appreciated. After all, it is the language of engineers, and of engineering sciences. Nijmeijer: >>

"As mathematicians, or rather as researchers having a mathematics background, at TU/e we are comfortable being in touch with other disciplines. Which perfectly fits another main aspect of ICMS, that of interdisciplinarity. We live in an era where the developments will really take place in multidisciplinary fields. We do not have to abandon disciplinary approaches, certainly not, as these form our core competencies. But I think that many disciplines will see the need to work in a multidisciplinary way."
Van der Hofstad adds: "In fact, throughout TU/e the theme of complexity has a rather strong presence, even though it is not always very visible as such. Whether you develop molecular systems, photonic systems, software systems and so forth, very often there is a complexity aspect to it."
On the other hand, cooperating with researchers from other disciplines is not always easy. Nijmeijer:
"Every expertise area is full of jargon, so it might take quite some time before you really understand each other. I have run projects with IT specialists, with mechanical engineers, with electrical engineers. It could take a year before it was perfectly clear what exactly was meant by the term 'system' or 'model'. But there is always a strong feeling that mathematical language has a connecting role."

COMPLEXITY SYNTHESIS

An explicit goal of the focus area Grip on Complexity is to not only increase the understanding of complexity itself, but also to design and synthesize complex systems based on the findings. A concrete example of this aspect of 'engineering complexity' is the research of ICMS scientist, Tom de Greef, towards biological computing. This rapidly growing research field includes biological programs that store data in (and retrieve data from) living cells, or memory devices that can record molecular events directly onto DNA. Exciting applications of biological computing devices are emerging in the area of cancer immunotherapy and biosensing, but can also be expected in other areas such as tissue engineering or chemical biology. The investigation of biological computing from a complexity perspective is a quite promising approach, since complexity research worldwide is predominantly aimed at acquiring understanding. Van der Hofstad: "Most complexity research does little work regarding synthesis: building systems, generating data and trying to understand the system through mathematical modeling. I expect ICMS to really stand out in this perspective."

"WE WANT TO USE THE KNOWLEDGE FOR THE SENSIBLE DESIGN OF NOVEL COMPLEX SYSTEMS."

BUILDING BRIDGES

Van der Hofstad and Nijmeijer expect to build future bridges reaching out from the Grip on Complexity focus area towards other ICMS focus areas. All ICMS researchers will at one time or another experience issues that touch the theme of complexity, whether their research is about molecular devices, regenerative materials, novel polymers or artificial cells. Van der Hofstad: "We are more than willing to help by complementing their efforts with our theoretical framework. As a matter of fact that does not have to be limited to theories of Networks or Dynamics and Control, but can be much broader. We can help formulate the right model for what people are building or observing. I would not go so far as to call our focus area a 'help desk', but we will for certain make an inventory of the complexity issues within ICMS by means of seminars and workshop. We really think this will be very exciting."

A flock of birds is a perfect example of complexity at work. The interaction between neighboring birds can be very simple, yet in the emergent behavior of the flock very complex phenomena can be observed. Network analysis of the interactions between the birds can yield insight in the system as a whole. An approach from a Dynamics & Control point of view can enhance this understanding by obtaining insight in the sensory systems of the birds that enable them to fly together and follow each other's rapid moves. Another example from the world of birds is that of migratory birds flying in a V-shape. When more birds join, at a certain point such a V falls apart and two separate V's arise. It seems that the emergent behavior is fairly sensitive to a certain threshold. Complexity analysis can help understand these phenomena. Image: Wikimedia Commons.

Kahina Ouchaou
Research Chemist at Stahl

Stahl

INDUSTRIAL CONSORTIUM

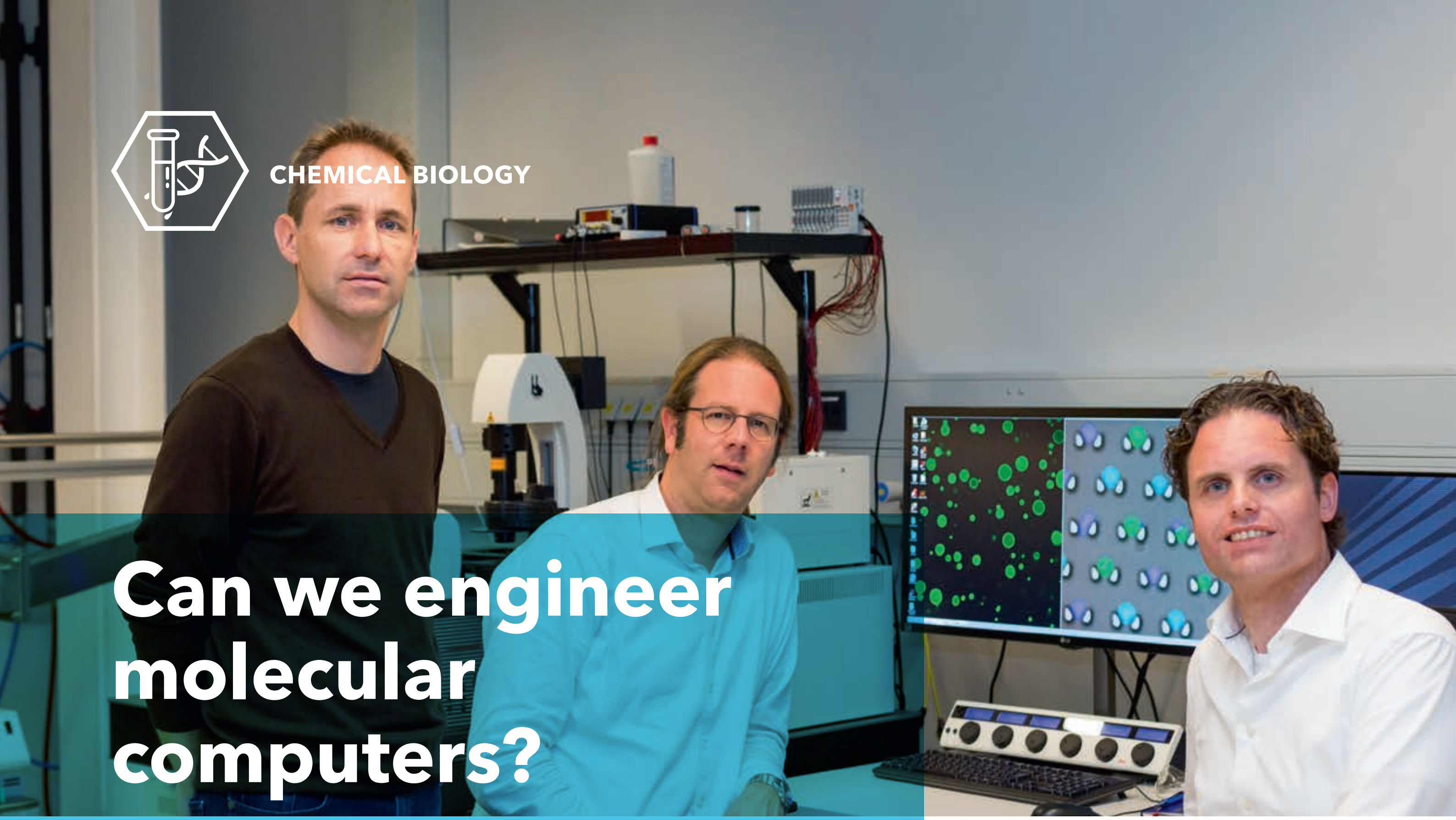
Although you may not realize it, Stahl products can be found almost anywhere in daily life, whether it is in your car or at home. Stahl, as market leader in coating solutions for leather and other flexible materials, helps to ensure the desired level of appeal, functionality, durability and comfort to the automotive, fashion, home interior and lifestyle industry. With more than 2,000 employees, at 13 manufacturing sites and 38 application labs in 24 countries, we offer a wide range of solutions to our customers all over the world.

facts

90 FTES OF RESEARCH & DEVELOPMENT DEALING WITH MORE THAN

300 PROJECTS THERE IS A CLEAR FOCUS ON INNOVATION AT STAHL.

Sustainability is one of the major topics within the company: improving the quality of our products while reducing the environmental impact. As a Research Chemist within Stahl, I help to develop innovative, waterborne polyurethane products. This includes PolyMatte®, the matt coating resin that provides a low gloss and luxurious feel to the finished article. Leather and synthetics like vinyl, polyurethane or polyolefin based materials can be given a long-lasting matt finish with superior aesthetic and technical value. The haptic characteristics of this material depend on the polymer backbone and the size of the polymer particles. PolyMatte requires a lot of analysis, and part of my job is to keep on developing unique PolyMatte varieties that fit our customers' needs. Stahl believes that by understanding the chemistry and physics of our products we can provide our customers with high quality products and support. We believe that via collaboration we can find solutions for the challenges we encounter every day. That is why we have joined the Industrial Consortium of ICMS. Working with ICMS helps us to obtain a better understanding of our material and opens up new research possibilities.



CHEMICAL BIOLOGY

Can we engineer molecular computers?

THE ANSWER OF TOM DE GREEF, LUC BRUNSVELD AND MAARTEN MERKX

Maarten Merkx (left), Luc Brunsveld (middle), Tom de Greef (right)

SEVEN PILLARS, ONE INSTITUTE

ICMS blew out ten candles and got itself a brand new look. Research within ICMS was recently reshaped into seven focus areas. The Chemical Biology focus area includes three familiar faces of the Biomedical Engineering Department of TU/e: Luc Brunsveld is full professor of Chemical Biology, Maarten Merkx is full professor of Protein Engineering, and Tom de Greef is associate professor of Synthetic Biology.
They reflect on their experience within ICMS, and their past and future collaborations in the field of DNA-based computers, protein engineering, and supramolecular architectures.

CAN WE ENGINEER BIOLOGY FROM SCRATCH?

That is the question for Tom de Greef. Living organisms such as the human body are based on living cells which are able to sense and adapt to their environment. In a very simplistic way, living cells are - in the words of De Greef – "nothing more than chemical computers with molecular software and predefined rules".

REVERSE AND FORWARD ENGINEERING

De Greef : "For many decades, biologists have studied cells via a reverse engineering approach deconstructing complex living systems into their constitutive elements, in order to extract knowledge on the molecular software". In the last 20 years, scientists started moving towards a 'forward engineering approach', building complex biological systems starting from lower-level details like molecular circuits and networks. "In our group, we use DNA as a programmable substrate to make those networks. We engineer biology from scratch", explains De Greef.

"IN BIOLOGICAL ENVIRONMENTS DNA-COMPUTERS STILL DEMONSTRATE THEIR FRAGILITY."

DNA-BASED COMPUTERS

DNA can spontaneously process molecular operations via hybridization, a phenomenon in which single stranded molecules pair together via hydrogen bonds. It's no surprise then that researchers worldwide have started looking at DNA as an appealing material for computing. DNA molecules have been used to create simple logic gates and circuits, the basic building blocks of computing. And, as DNA computers can naturally interface with biological signals, DNA-based computers opened the way for biological applications that, to date, conventional silicon based computers haven't been capable to address. In biological scenarios, DNA computers are "the most efficient machines to control molecular operations", says Brunsveld, and the perfect reflection of our modus operandi. De Greef: "Human beings compute using molecular signals. Our immune system, for example, can be seen as a neural network that learns from chemical patterns and, based on those, takes decisions."

INTELLIGENT PROTEIN-BASED SENSORS

Merkx: "In our group, we use protein engineering to make protein-based sensors. We would like those sensors to be intelligent or, in other words, capable of sensing and responding to different biological signals". That is how Merkx got interested in DNA computing. "The incorporation of all those functions in a single protein was simply too difficult. We practically reached the limits of what you can do with a single protein", explains Merkx. And that's when Merkx and his colleagues started looking at DNA and its "inherent advantage of being programmable". Combining protein engineering and DNA nanotechnology, Merkx and De Greef are currently busy with the development of intelligent biomolecular sensors for applications in intracellular imaging, diagnostics and, possibly, antibody-based therapies.

NO HUMAN INTERVENTION

Merkx: "To date, most of the research on DNA computing is DNA-based only, with DNA both as an input and as an output. Instead, we are very much interested in connecting DNA computing to the real world, the world of proteins. To do so, we use proteins, small molecules or antibodies as inputs. These inputs are used to control the release of drugs for specific therapies", says Merkx. His ultimate dream is an autonomous, closed-loop therapeutic system where "human intervention is no longer contemplated."

CONFINED, ORGANIZED, FASTER

Even though DNA-based computers are on the horizon, Merkx acknowledges their current limitations: "Current DNA computers are very slow. Also, they are usually tested in diluted solutions, in systems that are not confined. However, when it comes to complex diagnostic and therapeutic environments, you must confine these systems to some extent." In a recent publication, Merkx and colleagues demonstrated how to do so using supramolecular polymers. Merkx: "We developed DNA-functionalized supramolecular polymers, which could be used as dynamic scaffolds for DNA-based molecular computing." Organizing the DNA circuits within supramolecular architectures, Merkx and his colleagues were able to accelerate the kinetics of reactions a hundredfold, elevating supramolecular polymers to efficient autonomous systems for molecular sensing, computation, and actuation.

NEW FRONTIERS FOR DIAGNOSTICS?

De Greef: "Typically, a disease cannot be classified based on a single biomarker. Patterns, more than single biomarkers, are the real signatures of a disease state." In this respect, the potential of DNA computers is endless, especially when compared to current diagnostic methods. DNA-based computers could detect a disease state in its entireness and in one shot, by sensing patterns of biomarkers, and by processing and responding to this information in a fully autonomous way.

ARE WE THERE YET?

All the ingredients for the implementation of DNA-computers in clinical routine are undeniably there. But, the journey isn't over yet. In biological environments DNA-computers still demonstrate their fragility. De Greef: "Take for example blood, which contains nucleases: enzymes that are capable of destroying DNA computers. This poses a major limitation which current research is still trying to overcome."

MULTIDISCIPLINARITY

The 'fingerprint' of the research of Brunsveld, De Greef and Merkx is their multidisciplinary approach which matches perfectly with the ICMS vision. Brunsveld: "ICMS brings together scientists with different backgrounds that interact in a very open way. We ask each other critical questions, which can making our projects stronger or result, sometimes, in completely new lines of thought."

News, awards & grants

BEN FERINGA TO STUDENTS:

"You can change the future"

Long lines assembled in the TU/e Auditorium on the afternoon of Tuesday 8 May, where students, employees and other interested individuals were waiting for the lecture of 2016 chemistry Nobel laureate Ben Feringa. As part of its tenth birthday celebrations, the Institute for Complex Molecular Systems (ICMS) had invited 'The man behind the nanocar' to treat his audience to an afternoon full of 'The Joy of Discovery'.

As a takeaway message Feringa showed the students that a world of discovery awaits them. "Follow your dreams, don't give up too easily, and let yourself be seduced by the questions that make science so fascinating. Because it are not the answers, but the ever-changing questions that lead to groundbreaking research."

ICMS Fellowship for Ghislaine Vantomme

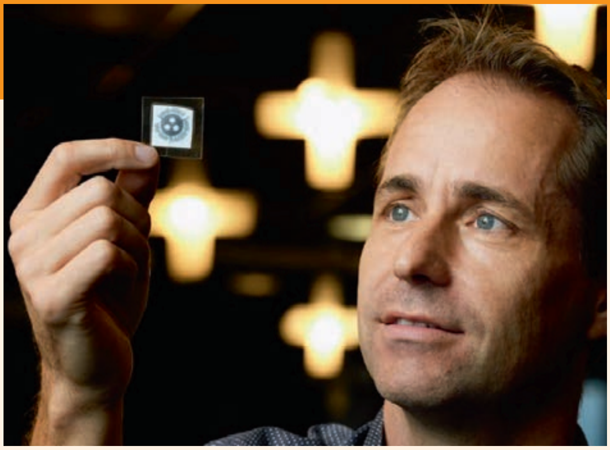
We are very excited to announce that Ghislaine Vantomme has been awarded an ICMS Fellowship. Her enthusiasm for science in general and her research resulted in a prestigious VENI grant in 2017 and co-authorship of a Nature paper on making waves in a photoactive polymer film. Last but not least she won the innovation and the public award at the first ICMS Industrial Challenge 2017 together with José Berrocal and Jody Lugger. This fellowship enables Ghislaine to work in all freedom on her research projects while being fully supported by the departmental TU/e group and by ICMS for a maximum of three years. Dr. Lorenzo Albertazzi, the first ICMS Fellow, dr. Louis Pitet, and dr. Danqing Liu have preceded Ghislaine in this program. We are looking forward to more science from the hands of Ghislaine.

Four ERC Starting Grants

FOR YOUNG TU/E RESEARCHERS

Clockwise: Sandra Loerakker, Bart Jansen, Yoeri van de Burgt, and Jurjen Tel.

Four talented assistant professors of TU/e were awarded individual Starting Grants by the European Research Council (ERC). They received up to € 1.8 million each for their projects on predicting the performance of cardiovascular implants, exploiting the immune system for superior cellular vaccines, pre-processing techniques to accelerate time-consuming algorithms, and brain-inspired lab-on-chip devices for cancer screening.



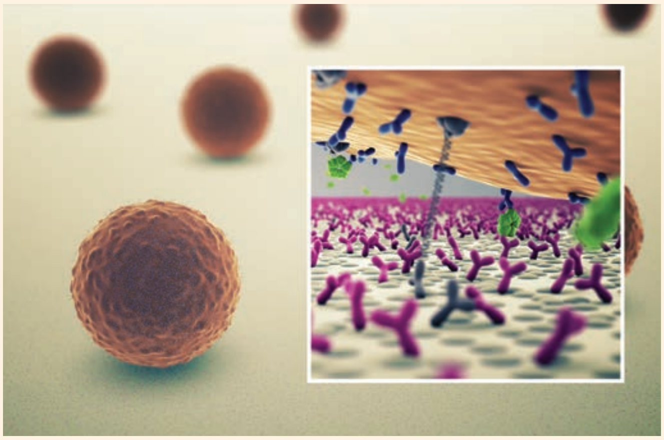
Research leader Maarten Merkx with one copy of the 'glow-in-the-dark' test. Photo: Bart van Overbeeke

Glow-in-the-dark paper

AS A RAPID TEST FOR INFECTIOUS DISEASES

Researchers from Eindhoven University of Technology (TU/e) and Keio University (Japan) presented a practicable and reliable way to test for infectious diseases. As they wrote in the scientific journal Angewandte Chemie, all you need is a special strip of glow-in-the-dark paper, a drop of blood, and a digital camera. Not only does this make the technology very cheap and fast – after just twenty minutes it becomes clear whether there is an infection – it also makes expensive and time-consuming laboratory measurements in the hospital unnecessary.
The test has a lot of potential for the easy testing of tropical diseases in developing countries.

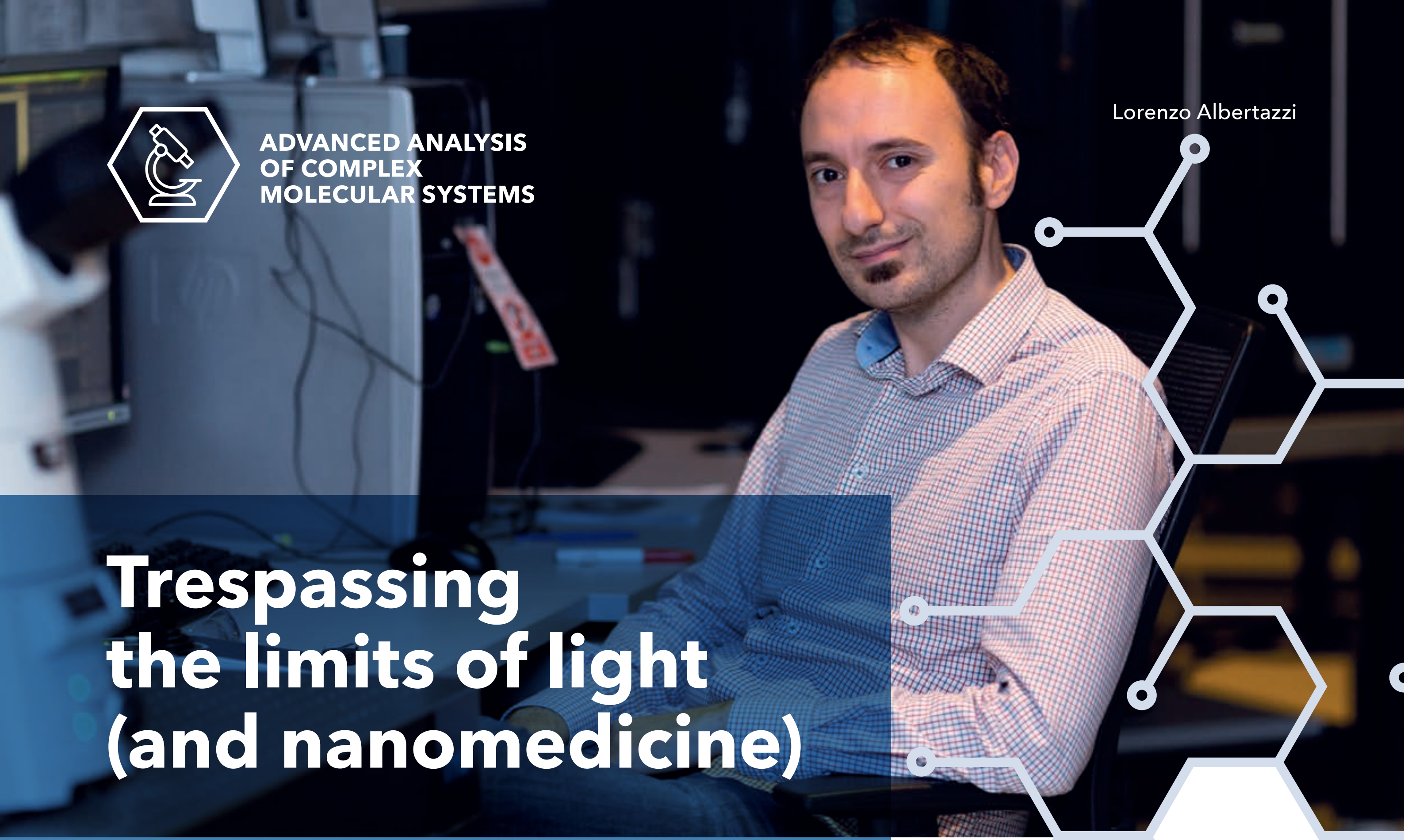
New sensor technology



A still from the video which explains the concept.
Image: ICMS Animation Studio

FOR SUPER-SENSITIVE LIVE MONITORING OF HUMAN BIOMOLECULES

The human body is an extremely complex molecular machine, of which the working can be followed by means of so-called biomarkers. Unfortunately, it is not yet possible to monitor biomarkers present in minuscule concentrations in live patients. Researchers at Eindhoven University of Technology have developed a new technique as a plain and simple method for the live and super-sensitive monitoring of biomarkers. They presented their technique in June in Nature Communications.



Lorenzo Albertazzi

ADVANCED ANALYSIS OF COMPLEX MOLECULAR SYSTEMS

Trespassing the limits of light (and nanomedicine)

Lorenzo Albertazzi is associate professor in the research group of Molecular Biosensing for Medical Diagnostics, at the Biomedical Engineering department at TU/e. Albertazzi is also junior group leader at the Institute of Bioengineering of Catalonia (IBEC) in Barcelona, where he leads the Nanoscopy for Nanomedicine group. In his research, Albertazzi aims to achieve a molecular understanding of synthetic materials in the biological environment, using both optical microscopy and nanoscopy. The ultimate goal of his research is to design nanomaterials for the next generation of targeted, super-efficient cancer treatments.

Over the last decades, the engineering of materials to the nanometer scale has opened up for novel and promising medical therapies, such as the design of nanoparticle-based drugs for cancer treatments. As in the case of the research performed by Lorenzo Albertazzi within the Biomedical Engineering Department and ICMS at TU/e. Albertazzi: "Within the nanomedicine field, we are trying to develop nanoparticles for targeted drug delivery, with prostate and breast cancer as main applications."

Do you want to know more about the work of Lorenzo Albertazzi?
Visit his personal page at: https://www.tue.nl/en/research/researchers/lorenzo-albertazzi/

A SPECIAL PLACE IN A CROWDED FIELD

"The field of nanomedicine is as big as it is crowded", says Albertazzi, "yet, we try to tackle it via our own, original angle: the use of advanced microscopy. This is also our main technical expertise, with super resolution microscopy being one of our favorite techniques."

SUPER RESOLUTION MICROSCOPY: BY-PASSING THE LIMITS OF LIGHT

Albertazzi: "Optical microscopy is one of the most used type of imaging, since hundreds of years. However, the resolution of optical microscopy is limited by the intrinsic nature of light, which makes it impossible to visualize objects smaller than 200-300 nm." Held back for a long time by this assumption, optical microscopy found a new twist in the last decade of the 20th century, when the 2014 Nobel Laureates in Chemistry circumvented this limitation, bringing optical microscopy into the nano-scale. Albertazzi: "Super resolution microscopy is an optical technique which by-passes the limits of conventional optical microscopy. The name itself is very explicative. It is an optical technique with better resolution, meaning that you can resolve much smaller objects, even at the nanometer scale."

FROM CELLULAR TO SUBCELLULAR LEVEL

Albertazzi: "We make objects that are small and very challenging to characterize." For Albertazzi and his team, advanced optical microscopy is the enabling technology to solve this challenge. "Besides being extremely helpful for the characterization of our nanoparticles in the laboratory", explains Albertazzi, "optical microscopy can be used in cells, human tissues and organs." Highly complex cellular environments where details matter. Albertazzi: "With super resolution microscopy, we can target subcellular organelles and even single proteins. For example, in the case of nanoparticles and their interactions with cells, we can see to which and how many cellular receptors the nanoparticles bind to."

SCIENCE PUBLICATION

Albertazzi: "Super resolution microscopy is a quite recent technique. The first papers were published approximately 10 years ago. When we bought our first microscope for STORM - Stochastic Optical Reconstruction Microscopy - there were only few other comparable microscopes in Europe. Also, back then, super resolution microscopy was mainly intended for biologists and no one had ever performed measurements on synthetic objects. Thus, the first big step for us has been to measure a man-made object, which was not obvious because of the substantial differences in sample preparation and imaging procedures we had to deal with." A huge effort for Albertazzi and, amongst others, Bert Meijer and Remco van der Hofstad, which was rewarded with a publication in Science in 2014.

CROSS-FERTILIZATION OF DISCIPLINES (AND MINDS)

Worldwide, research on nanomedicine is now driven by innovators across disciplines such as engineering, biology, medicine, and chemistry. Albertazzi: "Our work implies a multidisciplinary approach, which requires a joined effort from all the different scientific communities involved. Very often biophysicists don't know about chemistry, and chemists don't know about optical microscopy. Yet, to answer specific questions, you need to master biology, chemistry and microscopy. The magic happens when you combine these fields. In this sense, ICMS was the perfect place to do so."

NANOPARTICLES AND CLINICAL TRANSLATION: ARE WE THERE YET?

Albertazzi: "Nanomedicine for cancer treatment is out since many years, to the point that it can almost be considered as an old research field. The amount of publications within this field is enormous. Yet, if you look at what's brought in the clinic, there is almost nothing out there. After the first drug was approved for clinical use, in 1997, only a few drugs have been approved, which are all very similar to each other and not very sophisticated."

So, why the big promise of nanomedicine has not delivered yet? Possibly due to "knowledge gaps" - as Albertazzi defines them - between the behavior of drug-eluting nanoparticles in vitro (in the laboratory) and their interactions with cells in vivo (in the human body). Albertazzi: "Nowadays we are capable of characterizing nanoparticles in the laboratory in a pretty adequate way. However, once these nanoparticles are injected in the human body, their behavior and their side-effects in such a black box remain very difficult to understand."

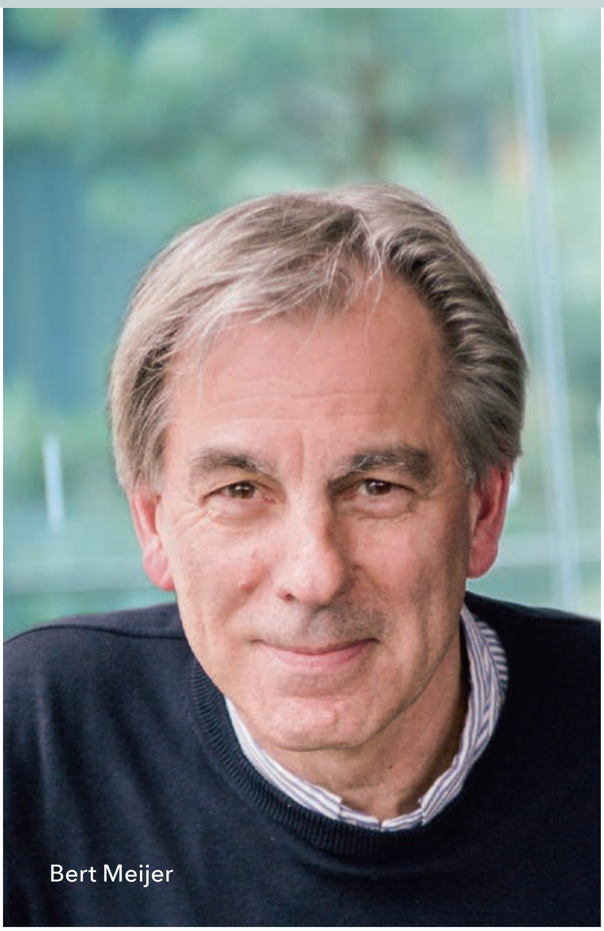
And that is where the challenge for Albertazzi and colleagues starts: "We want to understand and characterize the behavior of nanoparticles from the moment of their injection in the patient to the very end-phase. Rather than going for lucky shots, we want to decompose the problem and answer fundamental questions first." The answers to those questions provide Albertazzi and his colleagues the key information that will allow the design of the next generation of nanoparticles: precise, effective and safe therapeutic tools for clinical use.

ALLIANCES

MAINZ - EINDHOVEN AND VICE VERSA

New insights come from unexpected angles

Tanja Weil



Bert Meijer

ICMS and the Max Planck Institute for Polymer Research in Mainz (MPI-P) are strengthening their collaboration in the field of functional biomaterials. Researchers of both institutes share a strong belief in the supramolecular approach and agree that there are fundamental questions that still need to be tackled. “We each have our own expertise and approaches, but we understand each other immediately”, says Tanja Weil, director of MPI-P. “The beauty of such a complementary collaboration is that we all learn so much more.”

Despite years of large-scale research efforts in the fields of nanomedicine and functional biomaterials, the number of successful clinical applications in these areas is astoundingly low. “Thousands of groups are active in this field, but the development of useful functional biomaterials for the clinic still remains an enormous challenge”, says Bert Meijer, who heads the Functional Supramolecular Systems program within ICMS. “Only a small part of this massive effort focuses on supramolecular chemistry, but we are convinced that the supramolecular approach will deliver new systems that are stable and dynamic at the same time. And that combination of stability and dynamics is what we need to really make progress in this area.”

Both MPI-P and ICMS are already strong players in supramolecular chemistry. What is there to gain by joining forces? “We are very complementary in terms of expertise, technologies, equipment and the types of materials we study”, explains Tanja Weil, director of MPI-P. But doesn’t that lead to just a bigger group of people working along the same lines? Weil: “No, we are not doing the same, we each have our own methods and approaches. But we are all moving in the same direction. We can apply our methods and techniques to materials developed in Eindhoven and vice versa. Because we work on different systems composed of different materials, exchange of knowledge and ideas can lead to the discovery of similarities between different compounds. We can all learn more if we include each other’s methods or materials in our own work. That is the beauty of being complementary. It is very inspiring to discuss our research with ICMS groups, like that of Patricia Dankers and hear from them how they approach certain issues.”

DYNAMICS

The fundamental questions all boil down to the same topic: the interactions between the synthetic biomaterials and the cell. Meijer: “We need to understand what happens there, but so far the number of studies focusing on these interactions is very limited.” And the few studies that are being done often lack reproducibility, says Weil. “There is no standard in the field, which makes it very hard to compare findings. Each group has its own specific material, which is often not easily available to others. And then there is the difference in cell types. We all talk about ‘the cell’, but we work on brain cells, or liver cells, or bone cells. These all have very different characteristics.” By combining cell types and materials, ICMS and MPI-P groups together can take a step forward towards a more uniform way of performing studies, which will enable results to be compared.

But a lack of standards is not an exclusive problem for the supramolecular chemistry field. What is the reason that we still lack fundamental insights into the material-cell interactions? Why is it so difficult? “It’s all about the dynamics”, says Meijer. “First we need to understand how the dynamics of our materials relate to their structure and their function. And then there is the dynamic character of the cell, which makes cell biology difficult. Cells are continuously moving and changing. It often happens that you make a material, a cell biologists applies it, and the response is that ‘it doesn’t work’. And then that’s where it ends. But we need to study why it doesn’t work. For that we need to understand the dynamics of the material-cell interactions.”

BIOACTIVE FIBRILS

A major obstacle are the limitations of the current imaging techniques. It is extremely difficult to study something that moves. If the movements are slow, there are some possibilities, but in highly dynamic systems, we need new methods to be able to picture what is really going on.

So the conclusion is quite frustrating: the fundamental issue that needs to be addressed is known, but there is no method to really get to the core of the problem. On the other hand, scientists are an optimistic species and Meijer and Weil are convinced that the MPI-P / ICMS collaboration will push the field in the right direction. Weil gives an example from her own work. “We work on peptide assemblies that form nanostructures such as fibrils. These exhibit interactions with cells and with lentiviruses. We found that spiking the fibrils with functional peptides results in a pattern along the fibrils that can stimulate for example neuronal growth by interaction with cellular structures, which are still unknown. The individual peptides don’t exhibit that effect, nor do the unspiked fibrils. But when you combine them, you obtain a bioactive material. You need a compound that forms the structural component and a compound that generates the bioactive function. The peptide fibrils apparently have a role in guiding interactions with different cells and viruses. This could be an interesting concept for other materials and cell types.”

She is already thinking ahead. “The peptide fibrils interact with lentiviruses, and viruses are the transporter of choice in applications like gene delivery. But guidance is a problem there. Perhaps a biomaterial based on our peptide fibrils can guide the virus to deliver its cargo to the desired location. And if you can stimulate virus uptake at certain sites, you might also get ideas on how to inhibit virus uptake in relation to infectious diseases.” For Weil, there is no doubt that this way of thinking will lead to more generic insights that can be relevant for different tissues or different applications. “Over and over again we see that new insights come from unexpected angles. The broader relevance is always there.”

Theses

NOVEMBER 2017 – SEPTEMBER 2018

Exploring the process-structure-property relationship of organic solar cells by high performance computer simulations
VIKAS NEGI
September 26, 2018
PhD advisors:
prof.dr. P.A. Bobbert,
prof.dr.ir. R.A.J. Janssen,
dr. A.V. Lyulin

Emergent magnetism in intercalated epitaxial graphene by hydrogen and tungsten
AMENEH NAJAFI
September 25, 2018
PhD advisors:
dr.ir. C.F.J. Flipse,
prof.dr.ir. R.A.J. Janssen

Moving beads and drops in magnetic microfluidic chips
STIJN VAN PELT
September 25, 2018
PhD advisors:
prof.dr.ir. J.M.J. den Toonder,
dr.ir. A.J.H. Frijns

Modelling interfaces in fluids with applications to foams and blends
CHRISTOS MITRIAS
September 20, 2018
PhD advisors:
prof.dr.ir. P.D. Anderson,
dr.ir. M.A. Hulsen

Design and application of hydrophobic deep eutectic solvents
DANNIE VAN OSCH
September 18, 2018
PhD advisors:
prof.dr.ir. R. Tuinier,
dr. A.C.C. Esteves

Conjugated polymers for organic solar cells with reduced photon energy loss
RUURD HEUVEL
September 12, 2018
PhD advisors:
prof.dr.ir. R.A.J. Janssen,
dr.ir. M.M. Wienk

Protein sensing and actuation using DNA-based molecular systems
WOUTER ENGELEN
September 5, 2018
PhD advisors:
prof.dr. M. Merkx,
dr.ir. T.F.A. de Greef

Immunomodulatory materials for in situ cardiovascular tissue engineering
VALENTINA BONITO
September 13, 2018
PhD advisors:
prof.dr. C.V.C. Bouten,
dr. A.I.P.M. Smits

Critical Percolation on Random Networks with Prescribed Degrees
SOUVIK DHARA
August 28, 2018
PhD advisors:
prof.dr. R.W. van der Hofstad,
prof.dr. J.S.H. van Leeuwaarden

Lead halide perovskite solar cells
BARDO BRUIJNAERS
June 28, 2018
PhD advisors:
prof.dr.ir. R.A.J. Janssen,
dr.ir. M.M. Wienk

Engineering signaling circuits using a cell-free synthetic biology approach
LENNY MEIJER
June 11, 2018
PhD advisors:
prof.dr. P.A.J. Hilbers,
prof.dr. M. Merkx,
dr.ir. T.F.A. de Greef

A novel microfluidic platform to study cancer cell invasion: self-standing matrices integrated in microfluidic chips
HOSSEIN ESLAMI AMIRABADI
June 11, 2018
Prof.dr.ir. J.M.J. den Toonder,
dr. R. Luttge

Dimer fatty acid micellar hydrogels: synthesis, structure and properties
MARKO MIHAJLOVIC
May 31, 2018
PhD advisors:
prof.dr. R.P. Sijbesma,
prof.dr.dr. P.Y.W. Dankers

Orientation of transition dipole moments in solution processed small molecular emitters
ALESSIA SENES
May 24, 2018
PhD advisors:
prof.dr.ir. R.A.J. Janssen,
dr. S.C.J. Meskers

The interplay between cardiac progenitor cells and their microenvironment
ARIANNA MAURETTI
May 22, 2018
PhD advisors:
prof.dr. C.V.C. Bouten,
prof.dr. C.M. Sahlgren,
dr. N.A.M. Bax

Stimuli responsive photonic polymers
MONALI MOIRANGTHEM
May 16, 2018
PhD advisors:
prof.dr. A.P.H.J. Schenning,
prof.dr. D.J. Broer

Introducing bioactivity into electrospun scaffolds for in situ cardiovascular tissue engineering
SHRADDHA (TINA) THAKKAR
May 14, 2018
PhD advisors:
prof.dr. C.V.C. Bouten,
prof.dr.dr. P.Y.W. Dankers

Bio-inspired design strategies for semi-flexible polymer networks
CYRIL VRUSCH
May 7, 2018
PhD advisors:
prof.dr. C. Storm,
prof.dr. C.V.C. Bouten

Light responsive polymers: from molecule to device
JEROEN TER SCHIPHORST
April 18, 2018
PhD advisors:
prof.dr. A.P.H.J. Schenning,
prof.dr. D.J. Broer

Development and evaluation of protein quantitation assays for use in health care
ELLEN SCHMITZ
April 4, 2018
PhD advisors:
prof.dr. V. Scharnhorst,
prof.dr.ir. L. Brunsveld

Development of a micro-optofluidic sensor for in-line electrolyte monitoring: towards individualized dialysis treatment
MANOJ SHARMA
March 29, 2018
PhD advisors:
prof.dr.ir. D.M.J. Smeulders,
prof.dr. J.P. Kooman,
dr.ir. A.J.H. Frijns

Biomimetic strain-stiffening hydrogels
MARCOS FERNÁNDEZ-CASTAÑO ROMERA
March 28, 2018
PhD advisors:
prof.dr. R.P. Sijbesma,
prof.dr. C. Storm

Deep eutectic solvents: a new generation of designer solvents
ADRIAAN VAN DEN BRUINHORST
March 22, 2018
PhD advisors:
prof.dr.ir. M.C. Kroon,
prof.dr. J. Meuldijk,
dr. A.C.C. de Esteves

Self-organization of polyelectrolytes as mediated by surfactants, dyes and ions
LEO VLEUGELS
March 19, 2018
PhD advisors:
prof.dr.ir. R. Tuinier,
dr.ir. I.K. Voets

Nanoporous films from discotic liquid crystals
JODY LUGGER
March 15, 2018
PhD advisors:
prof.dr. R.P. Sijbesma,
prof.dr. A.P.H.J. Schenning

In pursuit of mathematical principles in systems biology
SAEED MASROOR
March 13, 2018
PhD advisors:
prof.dr. M.A. Peletier,
dr.ir. T.F.A. de Greef

Towards structure-performance relations of well-defined model systems in (photo) electrocatalysis
ANDREY GORYACHEV
March 12, 2018
PhD advisors:
prof.dr.ir. E.J.M. Hensen,
dr. J.P. Hofmann

The art of perfection: on the self-assembly of discrete block co-oligomers
BAS VAN GENABEEK
March 6, 2018
PhD advisors:
prof.dr. E.W. Meijer,
dr.ir. A.R.A. Palmans

Computational analysis of cell-mediated remodeling of collagenous tissues
TOMMASO RISTORI
March 5, 2018
PhD advisors:
prof.dr.ir. F.P.T. Baaijens,
prof.dr. V.S. Deshpande

Supramolecular drug delivery systems: molecular engineering of carrier affinity
MAARTEN BAKKER
January 30, 2018
PhD advisors:
prof.dr.dr. P.Y.W. Dankers,
prof.dr. E.W. Meijer

Quantifying the effect of structural manipulations on cellular stress generation
INGE VAN LOOSDREGT
January 23, 2018
PhD advisors:
prof.dr. C.V.C. Bouten,
prof.dr.ir. C.W.J. Oomens

Mechanics and dynamics of soft, sponge-like particles
FRANK AANGENENDT
January 18, 2018
PhD advisors:
prof.dr.ir. J.M.J. den Toonder,
prof.dr.ir. P.D. Anderson

High-performance poly(butylene terephthalate) vitrimers
YANWU ZHOU
December 18, 2017
PhD advisors:
prof.dr. R.P. Sijbesma,
prof.dr.ir. G.W.M. Peters

Modules for the synthetic supramolecular signalling toolbox
ANNIEK DEN HAMER
December 11, 2017
PhD advisors:
prof.dr.ir. L. Brunsveld,
prof.dr. M. Merkx

Measuring and modifying plasma density profiles to confine high power lasers
JOOST DANIËLS
December 4, 2017
PhD advisors:
prof.dr.ir. O.J. Luiten,
dr.ir. W.P. Leemans

On the edge: imaging soft interfaces by single-molecule localization microscopy
ANTONIO ALOI
November 30, 2017
PhD advisors:
prof.dr.ir. O.J. Luiten,
dr.ir. I.K. Voets

Ultracold Rb focused ion beam
GIJS TEN HAAF
November 21, 2017
PhD advisors:
prof.dr.ir. O.J. Luiten,
dr.ir. E.J.D. Vredenbregt

Engineering sensor proteins for antibody detection by design and evolution
MARTIJN VAN ROSMALEN
November 20, 2017
PhD advisors:
prof.dr. M. Merkx,
prof.dr.ir. L. Brunsveld

Model-driven engineering in supramolecular systems
TIM PAFFEN
November 15, 2017
PhD advisors:
prof.dr. E.W. Meijer,
dr.ir. T.F.A. de Greef

Kinetics, structure and function of a supramolecular polymer in water
RENÉ LAFLEUR
November 14, 2017
PhD advisors:
prof.dr. E.W. Meijer,
prof.dr. M. Merkx

MOLECULAR DEVICES

From the molecule to the device

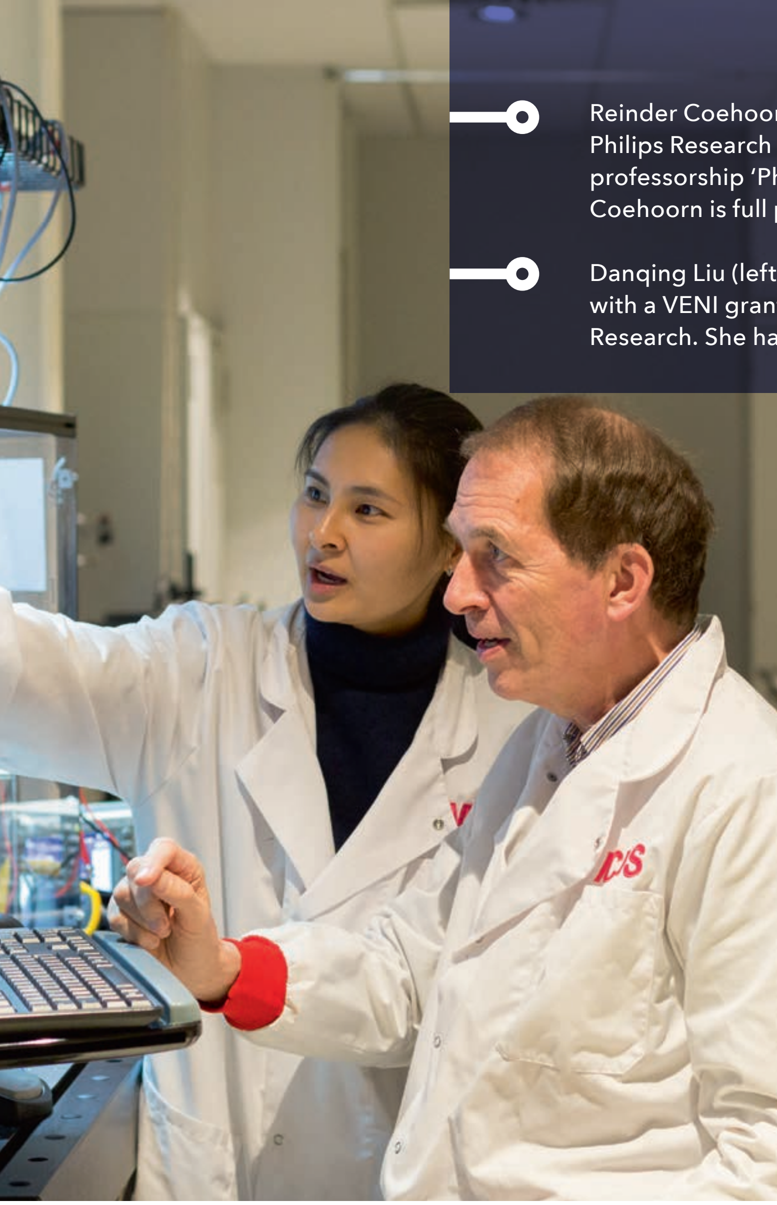
OLED SCREENS, SURGICAL ROBOTS AND MARS ROVER DUST REMOVAL

Functional organic materials have widespread technological application, ranging from protective coatings and liquid crystalline displays to polymer solar cells. Research in the ICMS focus area Molecular Devices establishes the foundations that enable further improvements and future innovati-ons. Meet Reinder Coehoorn, experienced professor in organic electronic materials and devices, and Danqing Liu, postdoc researcher and VENI laureate in soft responsive materials. "As materials scientists we need to know about chemistry, physics, electrical and mechanical characteristics, and when we go to application also about design. ICMS is a platform where all different disciplines meet at one place and we can really advance our research.

"As a postdoc at the research group Stimuli-responsive Functional Materials & Devices, Danqing Liu is happy to be part of ICMS. Two years ago she received a VENI grant from NWO, the Netherlands Organisation for Scientific Research, as part of its Innovational Research Incentives Scheme. At the department of Chemical Engineering and Chemistry she is now working on future soft robotic materials with sensory and actuating functions that enable active self-cleaning, haptic feedback and other features. "I build on the technology for liquid crystal displays in which TU/e has world class knowledge. My challenge is to develop this into soft robotic materials and explore the future of soft robotics."

SOLAR CELLS AND OLEDS

The research team of Reinder Coehoorn also harbors world class knowledge, in particular in the field of the photophysics of organic light emitting diodes (OLEDs). At the interdepartemental research group Molecular Materials and Nanophysics he heads the team at the department of Applied Physics. "The motto of our group



Reinder Coehoorn (right) has worked the major part of his career at Philips Research laboratories, since 1998 in combination with a part-time professorship 'Physics and Application of Nanosystems' at TU/e. Since 2015, Coehoorn is full professor at TU/e.

Danqing Liu (left) obtained her PhD at TU/e and is now a postdoc researcher with a VENI grant from NWO, the Netherlands Organisation for Scientific Research. She has been awarded an ICMS Fellowship.

is 'From the molecule to the device'. The part of our group that resides at the department of Chemical Engineering and Chemistry is focusing mainly on the design and synthesis of molecules for organic solar cells, and on the fabrication and characterization of devices. Here on the physics side we put a lot of effort in understanding the physics of the organic electronic materials and devices, both at the microscopic level and the device level."
Coehoorn's own field of expertise is in the device physics of OLEDs for displays, which is in a global perspective at present a far more important and bigger field than organic solar cells: the OLED market is already a billion dollar market and it is growing rapidly. Production is very much dominated by industries in Asian countries such as South-Korea, Japan and Taiwan. "China is also rapidly gaining momentum in this field", Coehoorn adds. "There are however quite a few European companies, and therefore also universities, supporting the technology chain by means of components and materials, or in our case by providing an understanding of the basic device physics and software."

VIRTUAL OLED

Coehoorn's group has acquired a thorough understanding of working OLEDs, applying fundamental insights, zooming in until the molecular scale and even incorporating quantum-chemical aspects. "The essence is in the transfer of electrons or excitons from one molecule to the next, and the next, and so on. This is very difficult to fully comprehend since when you remove or add an electron, a molecule immediately deforms. We take that in account in a quantum-mechanically correct way - correct in a sense that the theory becomes predictive - and combine the result with theories modelling other aspects of the materials behaviour. We thus arrive at a 'virtual OLED' so to speak, an overall simulation that is so complex that the human brain can't even try to oversee it. But it is perfectly manageable in a high volume computing environment."
Coehoorn is now looking at new research directions beyond OLEDs, inspired by ICMS. He is expanding the modelling efforts toward high-energy excitations, resulting for example by extreme UV illumination, and toward ions (moving charged atoms or molecules). "Moving ions are crucial in living cells, in plants, and in our bodies, as well as in systems supporting the energy transition, such as batteries. However, to achieve practically meaningful simulations, we hope to learn from other ICMS researchers providing us with their knowledge of ionic processes."

SPIN-OFF COMPANY

Coehoorn says his group is very open to explaining what we do to leading companies and help them answer their questions based on the fundamental insights.
"For instance if there's a new OLED principle that is more efficient, has a higher lifetime, and solves color problems, then we want to apply our models as quickly as possible to that new OLED." To service industry, Coehoorn and several other co-founders have established a spinoff company called Simbeyond that markets the state-of-the-art simulation code for molecular-scale simulations of opto-electronic processes. "This is very stimulating for us at the scientific side. It is very inspiring to receive questions from the real world. These can be as deep as the fundamental questions, but they are often quite different. In the end, the goal is to have something that works.
To me that is a very good criterium for good research: a working device or a predictive simulation methodology is as much a measure for success as high-impact papers in respected journals."

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Although for Danqing Liu real working devices with soft robotic functions are somewhat farther away, she is working hard to make them become reality. “Now that the application of robots is expanding to a real human environment we would like to develop an alternative for these ‘hard’ robots” she explains the background of her research. “These ‘soft robots’ require new, softer materials. The responsive materials we develop at our group are perfectly suited for this and they have the added advantage of sensory and actuating functionalities. This simplifies design of the robot since no separate sensors, actuators and connective wiring are needed.”

The materials Liu is working on are based on organic liquid crystal display (LCD) technology invented by group leader Dick Broer. It is an established class of materials with well-known parameters such as durability. “Since the technology was developed for displays, the focus has predominantly been on optical properties. But it is in fact an almost infinite class of materials with endless possibilities”, Liu says. “There’s a lot to be discovered.”

LCD technology offers great opportunities for the development of responsive materials. It has for instance been shown that is possible to activate one single LCD layer into complex origami-type bending and folding behaviour, Liu explains. She is now focusing on LCDs capable of two-dimensional surface deformation. One of the concepts under development concerns a surface changing from smooth to corrugated, thus introducing friction. “This can imply an enormous advantage for the robotics industry since it can modulate grip. You often see rubber being used to improve the grip. But since rubber has the tendency to stick to the surface, releasing an object from the robot’s grip is not always straightforward. By using materials that can adjust the friction between the robot and the object, you can assist the robot in releasing the object.”

“A WORKING DEVICE IS AS MUCH A MEASURE FOR SUCCESS AS HIGH-IMPACT PAPERS IN RESPECTED JOURNALS.”

“RESEARCHERS IN THE ICMS FOCUS AREA MOLECULAR DEVICES ARE CONCERNED WITH OLEDS, SOLAR CELLS, ORGANIC SEMICONDUCTORS, SENSORS, SOFT ROBOTICS, SMART WINDOWS AND DISPLAY TECHNOLOGIES.”

MARS ROVER

Another benefit of an active surface is that it can clean itself. As an example, Danqing mentions the Mars Exploration Rover that suffers from Martian sandstorms, covering the Rover’s solar cells with red dust. “All you can do is wait for the dust to come off, you can’t send an astronaut to wipe it clean. If NASA were to apply an active material as a surface coating, it could mechanically get rid of the dust, by means of a vibrating movement.” Liu shows a proof of concept video from a small sample produced in the Eindhoven laboratories. “This is more or less as far as we go at the university. I really want to scale up the process and be able to demonstrate this at a scale that is relevant for real application.” The concept could also be used at solar farms in desert environments, for instance. “Of course”, Liu says, “for that to become reality the material should be low-cost. In this early stage of development that’s not feasible, so we first focus on an application in space technology.”

Liu also plans to develop interactive materials that can generate a local change of friction activated by the touch of a finger. This would for instance make it possible to really feel a button on a touch screen, which would be an advantage for vision impaired users. “It would even enable the development of e-readers for blind people”, Liu adds. Also surgical robots could benefit from such responsivity. The operating surgeon now must exclusively rely on visual feedback provided by a camera. Applying responsive materials at the control sticks would enable haptic feedback to the surgeon’s fingers and hands, further improving the intuitivity of the robotic system. “That’s what we mean by communicative materials: materials that can transmit information to the user”.

Key publications

APRIL 2017 - AUGUST 2018

01. A NON-VOLATILE ORGANIC ELECTROCHEMICAL DEVICE AS A LOW-VOLTAGE ARTIFICIAL SYNAPSE FOR NEUROMORPHIC COMPUTING
Y. van de Burgt, E. Lubberman, E.J. Fuller, S.T. Keene, G.C. Faria, S. Agarwal, M.J. Marinella, A.A. Talin, A. Salleo
Nat. Mater. 16, 414-418 (2017)

02. AMPLIFYING (IM)PERFECTION: THE IMPACT OF CRYSTALLINITY IN DISCRETE AND DISPERSE BLOCK CO-OLIGOMERS
B. van Genabeek, B.A.G. Lamers, B.F.M. de Waal, M.H.C. van Son, A.R.A. Palmans, E.W. Meijer
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POLYMER SCIENCE AND TECHNOLOGY

EPL update

Remarkable insight in vitrimer dynamics

PUBLICATION IN PHYSICS REVIEW LETTERS

Wouter Ellenbroek is one of five principal investigators at the research group Theory of Polymers and Soft Matter, part of the department of Applied Physics. He leads the team for Responsive Soft Matter with four PhD students and contributes to the ICMS focus area Polymer Science and Technology, where he cooperates with chemists of the Eindhoven Polymer Laboratories.

The Responsive Soft Matter research team of Wouter Ellenbroek developed a new model for simulating the dynamics of vitrimers, a new class of smart, tuneable polymers with remarkable characteristics. The model is both elegant and functional: it has yielded new insight in how molecular details determine macroscopic behaviour. New materials are on the horizon.


Wouter Ellenbroek

At the end of July, all members of the research group Theory of Polymers and Soft Matter enjoyed a piece of 'vlaai', the traditional pie from the southern part of the Netherlands. The treat was presented by Wouter Ellenbroek on the occasion of a brand-new publication in Physics Review Letters (PRL). "It has become somewhat of a tradition in our group", Ellenbroek says. "PRL is where we want to be, so an accepted paper calls for a celebration".

With his team for Responsive Soft Matter, Ellenbroek focuses on the physical foundations of novel high-tech materials that respond to mechanical stimuli or other changes in their environment. Taking inspiration from natural materials and processes, he unravels molecular mechanisms and develops proofs of concept in order to create new materials. To achieve this goal, he and his team are continuously developing advanced computer simulations as well as novel methods to analyse the results of those simulations. The group currently focuses on a number of recent advances in polymeric materials, including toughening mechanisms in

"IN VITRIMERS A DYNAMIC CROSS-LINKING CONCEPT IS EXPLOITED BASED ON THE 'SWAPPING' OF CHEMICAL BONDS."

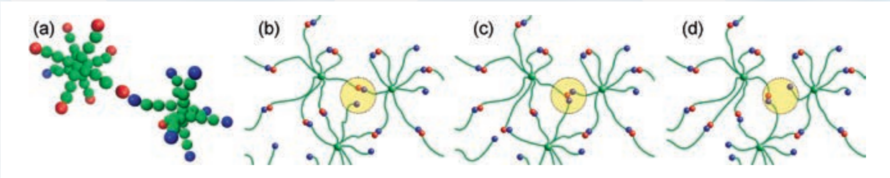
elastomers and gels, stress relaxation in vitrimers, and structure-function relations in biocompatible hydrogels. The research now published in PRL is in the field of vitrimers. It is part of the PhD research of Simone Ciarella and was financed through ICMS and Eindhoven Polymer Laboratories.

SMART MATERIALS

Vitrimers are class of exciting 'smart' future materials resulting from new chemical concepts in polymer science. Their characteristics can be tuned to vary between the two conventional classes of polymer, thermoplastics and thermosets. The first can be reshaped at will, while the latter are not deformable as a result of permanent molecular cross-linking. In vitrimers a dynamic cross-linking concept is exploited based on the 'swapping' of chemical bonds. At high swapping rates, the polymer is malleable just like a thermoplast, while at low swapping rates it performs as a thermoset.
"Although vitrimers are already entering commercial application, there's still a lot to be understood about these materials" says Wouter Ellenbroek. "Our paper in Physics Reviews Letters contributes to this understanding. We present a new way of modelling vitrimers that enables linking their macroscopic properties, especially stress relaxation, to the molecular details."

BEADS AND SPRINGS

In the modelling of polymer systems usually approximations are made to obtain results on interesting time scales. As an example, a popular technique is the representation of polymer chains as a sequence of beads connected by springs. This allows to include specific interactions at the molecular scale. However, the existing implementations of this popular model do not include the effects of molecular bond swapping – precisely where the particular vitrimer behaviour originates. Ciarella and Ellenbroek therefore developed a 'tailor made' coarse grained model for vitrimers. On top of the bead-spring chains, they superpose two- and three-body potentials to reproduce the dynamics of the bond-swapping mechanism (see illustration).
By introducing a coefficient in the three-body potential, the bond-swapping dynamics of the model can be tuned. Ellenbroek: "We can thus represent aspects of real vitrimer systems such as the catalytic control of bond swapping, or the effect of temperature." He is quite pleased with the model: "Not only does it match the macroscopic behaviour of the real vitrimer materials, it is also more elegant than the hybrid Monte Carlo methods that are often used to represent dynamic bonds in simulations."



Vitrimer polymers in the model presented by Wouter Ellenbroek and co-workers in Physics Review Letters. The interaction between the red- and blue molecular moieties defines the bond swapping, as represented in the yellow circles. In (b) and (d) a two-body potential represents the highlighted bond. Bond swapping occurs through the state represented in (c). There two two-body potentials are countered by an equally strong but negative three-body potential, effectively flattening out the energy barrier and thus representing the bond-swapping ability. Image: ICMS/ PhysicsReviewLetters.

A HIGHWAY TO STRESS RELAXATION

The new model yielded a particularly important insight regarding the effect of the formation of intramolecular bonds (so-called loops) on vitrimer behaviour. As it turns out, vitrimer molecules with a tendency to form loops will speed up stress relaxation, which is an important macroscopic parameter characterizing vitrimers. The key is that the formation of loops provides a quick path to disconnecting two molecular units in the network, thus relieving stress. Units that do not allow loop formation often have multiple (redundant) connections to their neighbors. In the latter situation many more bond swap events are required before stress can relax.

"Our results reveal the important role played by network defects in mediating the bond swapping reaction and speeding up stress relaxation. It thus can help polymer chemists to tune the molecular design of vitrimers so that the desired macroscopic parameters are obtained. Not so much that the model can already accurately predict these parameters, but it does provide the insight that guides the material design." Ellenbroek and his team already have "a bin full of ideas", for developing new vitrimer materials: "We can't wait to explore the possibilities."

ICMS course on Scientific Skills

Over the last years, ICMS has developed and perfected a yearly course on Scientific Skills for master's, PDEng and PhD students. The course focuses on gaining practical skills and a deeper insight into a number of aspects related to performing research in an academic or industry environment. Eline van Haaften, PhD student at the department of Biomedical Engineering of TU/e, shares her experience as an attendee to the 2018 Edition.

HOW DID YOU FIND OUT ABOUT THIS COURSE?
Van Haaften: "Two years ago, ICMS was looking for a new format for the course, so the institute organized a discussion meeting to understand its members' needs. I joined the meeting and afterwards my promotor Carlijn Bouten proposed that I should follow the newly shaped course."

HOW WAS THE COURSE STRUCTURED?
Van Haaften: "The Scientific Skills course consisted of several parts, such as setting up a research plan, performing literature searches, understanding the writing and publishing process of scientific articles, giving presentations, and obtaining insights in scientific integrity issues. Also, the course included several sessions with representatives from industry. For example, in our edition, employers from Philips and Johnson & Johnson were invited to come over and share their work experiences."

Eline van Haaften is a PhD student in the group of Soft Tissue Engineering and Mechanobiology (STEM) of Carlijn Bouten, at the department of Biomedical Engineering of TU/e. She is involved in the European consortium InSiteVx, which aims at developing artificial vascular access grafts that can develop into living, self-healing grafts once implanted in the human body. Van Haaften's contribution focuses on the role of blood-imposed loads on de novo vascular tissue formation. In 2018, together with other TU/e Master and PhD students, Van Haaften followed the ICMS course on Scientific Skills.

HOW WAS THE ASPECT OF SCIENTIFIC INTEGRITY DEALT WITH IN THE COURSE?

The course is also designed as an interactive training to recognize ethical issues in the daily work of a researcher and to discuss opportunities to deal with those. "At the beginning of the course", Van Haaften explains, "we participated in a game where we discussed in a nice way the scientific integrity issues that we might face. We also heard of real stories from people working in industry, which is an opportunity that as a PhD student I do not have on a daily basis. We have the tendency to believe that we will never encounter problems related to scientific integrity, or that these are over exaggerated. However, during the course we encountered some very specific examples that we could really relate to."

ARE SCIENTIFIC MISCONDUCT AND PUBLICATION PRESSURE TWO FACES OF THE SAME COIN?

Van Haaften: "I do see a connection between scientific misconduct and the mounting pressure to publish. However, there are also many more innocent forms of scientific misconduct that we should be aware of. For example, when recording data from a device, it might happen that some measurements are off. Suppose you are almost convinced that those points are off due to device-related causes, for instance power fluctuations, and not due to your way of performing research. What should you do in those cases? Are those off points to be included or not? Those are scenarios that you can really encounter yourself. And to discuss those beforehand, as we did in this course, can really help you to prevent or face them."

DID YOU FIND THE COURSE RELEVANT?

Van Haaften: "I believe that this course can make you a better scientist. You get detailed feedback on scientific skills that you do not learn in a laboratory or in a standard university course. In fact, the supervisors of this course normally operate in the same research areas of the course attendees. Also, the course provides useful information about the submission of scientific papers. Lastly, I found this course very helpful in the search of what you want to become, and the path you want to pursue, industry or academia, by increasing your self-awareness as a scientist."

Are you a PDeng, PhD or Master student at TU/e? Are you interested in the Scientific Skills course organized by ICMS?
Please contact icms@tue.nl

News, awards & grants

Inspiring lecture

BY XIAOWEN ZHUANG

Xiaowen Zhuang, professor of Physics, Chemistry and Chemical Biology at Harvard University, gave an inspirational SG/ICMS lecture during her visit at TU/e on 25 September 2018. She was visiting the Netherlands as recipient of the 2018 Dr H.P. Heineken Prize for Biochemistry and Biophysics.

The photo depicts Xiaowen Zhuang accompanied by Mrs. Charlene L. de Carvalho-Heineken, who awarded the prestigious prize on 27 September 2018 in Amsterdam.

NWO Vidi grant

FOR SANDRA HOFMANN

Sandra Hofmann, assistant professor in the Orthopaedic Biomechanics research group, has been awarded a Vidi grant of 800,000 euros from the Dutch research council NWO. She intends to use this money for biomedical research, in particular regarding bone cells.

American Chemical Society honors

BAS VAN GENABEEK AND BERT MEIJER

PhD student Bas van Genabeek was selected to receive the inaugural Global Outstanding Graduate Student Award in Polymer Science and Engineering from the Americal Chemical Society. It will be awarded on behalf of the ACS Division of Polymeric Materials: Science & Engineering, and the Chemical Marketing & Economics Topical Group of the American Chemical Society's New York Section. Bas van Genabeek is a PhD student with Bert Meijer who will receive the inaugural ACS Global Outstanding Mentor Award in Polymer Science and Engineering to acknowledge his dedication and commitment in mentoring graduate students in this promising field. Bas van Genabeek and Bert Meijer will each receive a commemorative plaque. The Student Award carries an additional cash prize of $2000. It will be presented to Bas at the Student & Mentor Awards Session during the Third ACS NASA Symposium "Chemistry for Humanity's Next Giant Leap" to be held on April 1-2, 2019 in Orlando.

The Institute for Complex Molecular Systems (ICMS)

CREATING FUTURE TECHNOLOGIES BY MASTERING COMPLEXITY

Advancing the fundamental understanding of complex molecular systems in materials science, energy, mobility, health, and life is the main driver of the Institute for Complex Molecular Systems. It addresses research challenges and pushes the boundaries of science by unifying basic principles of chemistry, biomedical sciences, engineering, physics and mathematics.

Since 2008, ICMS creates and maintains a versatile and fruitful research environment to:

- Expand and diversify the ICMS expert network
- Identify the underlying academic research questions;
- Enrich the scientific toolbox and infrastructure;
- Educate talented researchers in an interdisciplinary environment; and
- Inspire researchers through industrial research challenges;

The relationship with industry is strengthened via the ICMS Industrial Consortium – where science meets innovation. Furthermore, ICMS hosts the Advanced Study Center that serves as an intellectual home to scientists from all over the world, hosting discussions on the theme of complexity.

The ICMS research highlights the research of TU/e scientists in seven focus areas:

- Polymer Science and Technology
  We connect the entire chain of knowledge from theoretical calculations to understanding structure-property relationships, to be able to design improved and novel polymers with desired material properties.
- Chemical Biology
  We follow a molecular systems approach to understand and modulate biomolecular networks for the design of new therapies and diagnostics.
- Grip on Complexity
  We push forward the foundations and applications of complexity science in its broadest sense.
- Advanced analysis of complex molecular systems
  We are building a national characterization centre for the 4D-analysis of complex molecular systems at different length and time scales.
- Molecular Devices.
  We adopt an integrative approach for the design and synthesis of hierarchically structured functional and responsive materials for functional electronic and adaptive devices.
- Materials and regenerative medicine.
  We are aiming to regenerate tissue and organ function with intelligent biocompatible materials, using a materials-driven approach.
- Functional Supramolecular Systems
  We investigate the construction of functional life-like supramolecular systems to push the frontiers of supramolecular chemistry.

More information can be found via www.tue.nl/icms.
Please contact us with specific questions or remarks via icms@tue.nl or +31 40 247 5074.

ICMS in PRESS


'Ballenbak' meet levenssappen

Wetenschap

Glimwormtest ziet virus erg snel

OPMERKELIJK TIJDSCHRIFT VOOR BELANGWEKKENDE BIJZAKEN

Eenzame watermoleculen zijn de baas

EDITORIAL
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