ICMS Highlights

Edition 4
May 2015

Making materials that make themselves

INTERVIEW
/ Mikko Karttunen

DREAMING OF A FIRST-IN-MAN STUDY

INTERVIEW
/ Frank Bates

& more...

Institute for Complex Molecular Systems

TU/e Technische Universiteit Eindhoven University of Technology

Where innovation starts

ICMS Highlights

Dear reader,

Being prepared for the unexpected is one of the key ingredients of discoveries in science. An intriguing view on scientific discoveries is given in the 2006 book chapter by Catherine Blake and Meredith Rendall from the University of North Carolina. “The nontrivial process of identifying valid, novel, potentially useful, and ultimately understandable patterns in data” is the definition of scientific discovery most often used and as described in the Knowledge Discovery Databases. These discoveries are all building on existing ideas, but are rare.

Most of us are following Kuhn’s normal science in our daily practice. We define a research question (hypothesis or targeted design) and perform experiments to verify the hypothesis or to make the targeted product or device. In order to increase the chances of finding the unexpected, it is important to use our creativity in defining the right research area to work in. This is one of the reasons we created the ICMS for bringing the different traditional disciplines together. It is now generally accepted that most of the discoveries are the result of multidisciplinary research with a strong basis in the traditional disciplines. We like to encourage our members to excel in bringing knowledge together and make intriguing discoveries.

We are an Institute of and for our members; this personal touch is our main reason of existence. Therefore we are very sad that our PhD student Giuseppe Melpignano passed away together with his girlfriend in a tragic car accident. He was so full of ideas and excited about his science as was highlighted in the previous Magazine. We will miss him.

Sagitta Peters
Managing director

Bert Meijer
Scientific director

Calendar

May 22 2015, 15.00 hr
ICMS Discussion meeting with Stephan Lotze
Location: Ceres

June 5, 2015 , 15.00 hr
ICMS Discussion meeting with prof. Martin van Hecke
Location: Ceres

June 19, 2015 , 15.00 hr
ICMS Discussion meeting with dr. Roman Koning
Location: Ceres

August 28, 2015 , 15.00 hr
ICMS Discussion meeting with prof.dr. Jacco van Rheenen
Location: Ceres

October 15, 2015, 16:30 hr
Nobel Prize meeting
Location: Zwarte Doos

December 14-18, 2015
ICMS/KNAW Complexity Science Winter School
Location: Ceres

January 21 & 22, 2016
ICMS Outreach Symposium
Location: Zwarte Doos

The complete calendar can be found on our website.

Content

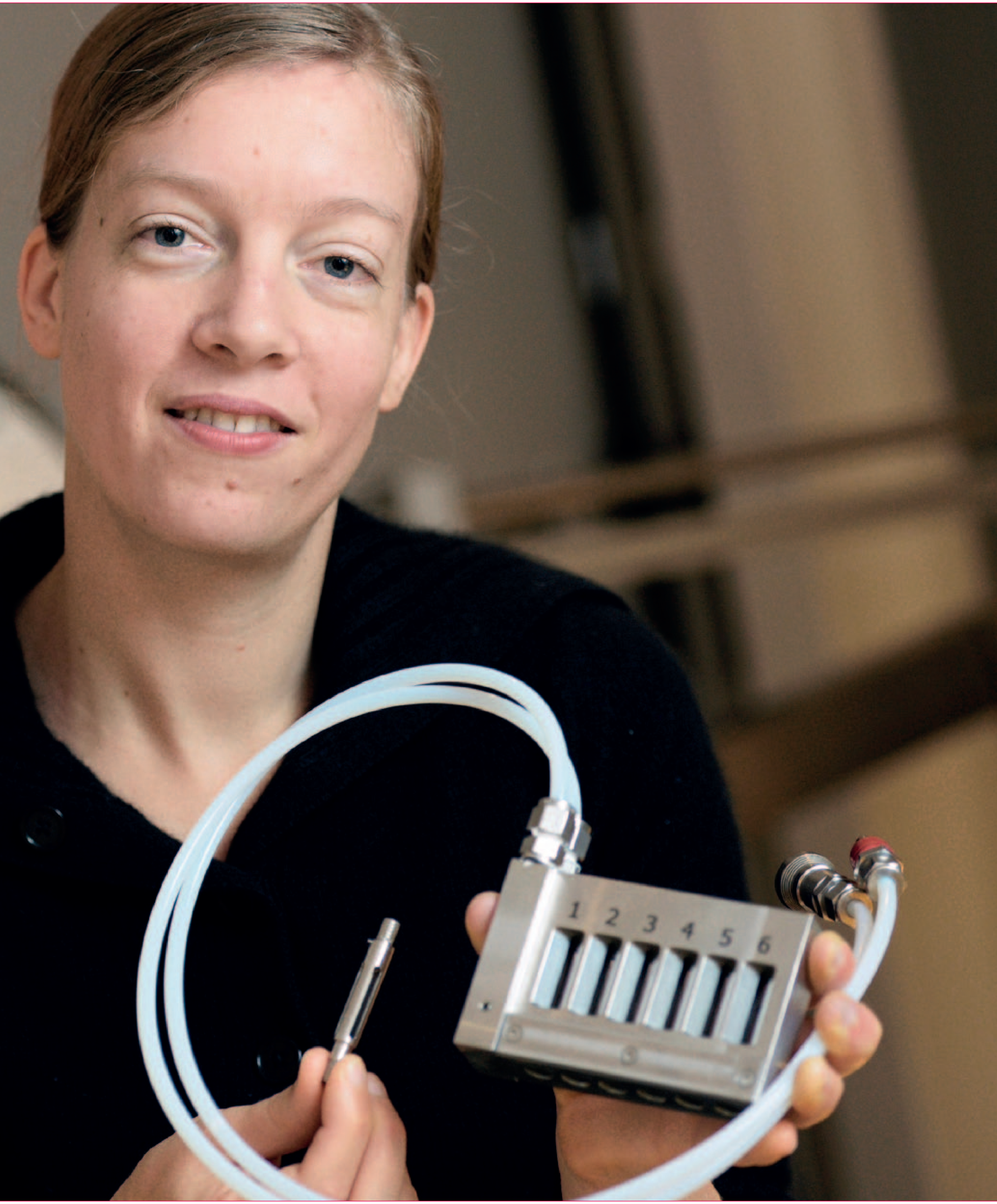
Edition 4
May 2015

/ Ilja Voets

Making materials that make themselves

PURE CURIOSITY, THAT'S HOW I GOT INTO THIS TOPIC

"I was working at the Adolphe Merkle Institute at the time and read an article about antifreeze proteins in snow fleas. This intrigued me. I found out that many freeze-tolerant species, such as polar fish, bacteria, and budworms, survive at subzero temperatures because of ice-binding proteins. I also discovered that no one really knows how these proteins do the trick. It seemed like a fascinating challenge to dive into, and indeed it is." says Ilja Voets.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“IN OUR RESEARCH, WE HOPE TO DISCOVER NEW WAYS TO MODULATE SELF-ORGANIZATION WITH MACROMOLECULES

In November of 2014, assistant professor and physical chemist Ilja Voets received a European Research Council Starting Grant for her research into the working mechanism of antifreeze proteins (AFP) and polymers. Her work shows there may be a bright future for macromolecular antifreezes in a range of applications, such as de-icing technologies and biomedicine. Voets: “Ice cream is the only product with antifreeze proteins on the market today. The proteins help to keep the ice cream soft and tasty by slowing down the growth of ice crystals. We want to learn how these antifreeze proteins work and use this insight to develop synthetic, ice-binding polymers that perform even better in complex environments. My dream is to engineer synthetic compounds that can be produced on large-scale to control the growth, size, and morphology of ice crystals. If we manage to tackle this formidable challenge, we could develop new routes to harness sensitive soft materials against freeze damage.”

Learning curve

Currently the AFP project is in its fourth year at TU/e and ICMS. Voets: “In my group, we work at the interface between chemistry, physics and biology.
We use a range of advanced experimental techniques to study macromolecules in action, with nanometer precision, even in complex environments like supercooled solutions. It’s an interesting and a challenging field of research ideally positioned at TU/e and the ICMS, that joins science and technology across the boundaries between classical disciplines. We also collaborate with scientists at other universities, such as Maastricht, Utrecht and Amsterdam, to learn more about the hydration of antifreeze proteins and to investigate potential applications in biomedicine.”

“We have already come a long way since we started four years ago. We no longer buy commercially available antifreeze proteins, but instead we produce our own proteins in the chemical biology laboratory.” In this way, the group investigates the impact of mutations of a single amino acid on the ice-binding site. The group also developed several standardized assays to measure the activity of the antifreeze proteins in a reproducible fashion. Voets: “Luuk Olijve is the first PhD student in my group who started working on this topic and he will defend his thesis later this year. His work has already led to several surprising new insights, but I’m sure there is more to come. One of the big breakthroughs was a recent study with our collaborators in Amsterdam in which we showed that certain antifreeze proteins actually have a thin ice layer on their surface already at room temperature. We speculate that this ice layer is crucial for the protein to bind to ice, but we still have to figure out precisely how this works.”

Challenge

The research of Voets is challenging and often requires the group to design and build specialized equipment and sample chambers.
Voets: “Most equipment is optimized for operation at room or body temperature, but we need to work at subzero temperatures with high precision. What we want to do is often very close to the limit of what is technically possible at the moment. Our next target is imaging individual proteins bound to ice. We hope that this enables us to answer the questions: Where does the protein bind? Is it stuck there or can it move on ice? Is the ice curved in between bound proteins? What is the binding density and how does it relate to the activity of the protein?”

Application

Currently, the team focuses on the fundamental aspects of AFPs, but plans to extend the research and investigate future application possibilities are on the horizon.
Voets: “Our work is almost always fundamental, curiosity-driven research, but we regularly get inspired through discussions with industrial partners aiming to

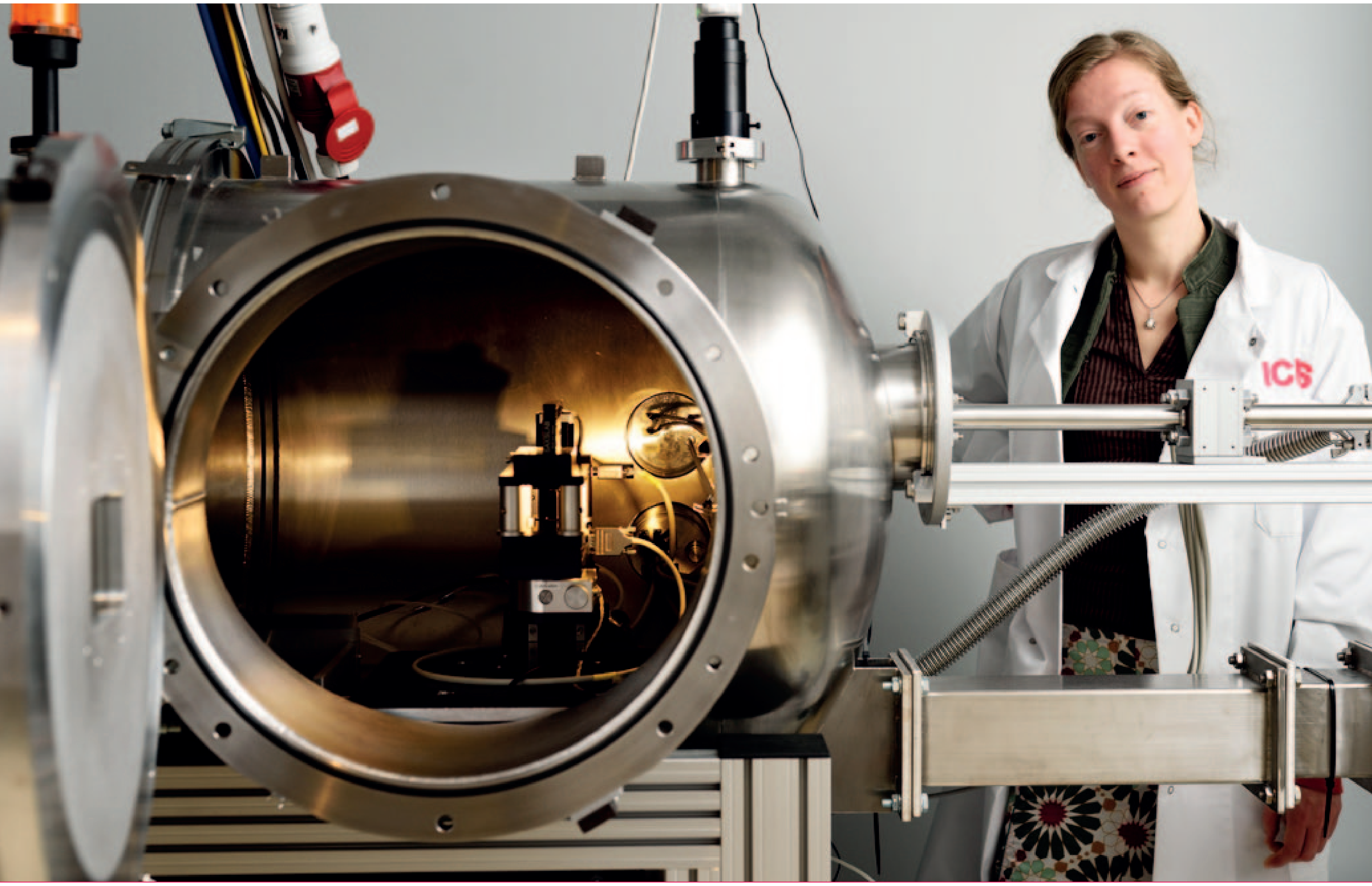
improve an existing product or better understand its production process or performance. In the end, what could be a better test of complete understanding of how a material works than to come up with a new design, build it, and find out whether you got it right and have made a new material that works even better?"

Voets: "I really enjoy working at the ICMS. It's an excellent place for great science that crosses boundaries. It brings people together from many different disciplines and organizations. This brings different viewpoints to a discussion which often results in new ideas. Actually, I think it is really important to continuously put yourself in a position where you are surprised. It gives you new perspective, inspires and excites to discover new things. The great thing about science is that there is plenty of room for creativity. Sometimes it's a small practical detail of an experiment, but it may be as big as developing a new strategy for years of research. Research is discovery, you never know in advance what you will find!"

Bio-inspired

"Nature is a continuous source of inspiration. Anyone interested in self-organization is amazed with the complexity and functionality of biological materials. As chemists, we can only dream of programming materials to reliably express desired architectures and functions. In our research, we hope to discover new ways to modulate self-organization with macromolecules and ultimately, to make materials that make themselves. That's an exciting goal that lies far ahead of us. But, each step that we make brings us closer."

The small angle X-ray scattering equipment at the ICMS offers a unique window into the structure of materials



Outreach Symposium 2015

In January 2015, the ICMS brought together around 200 scientists, students, and industry professionals to discuss topics including polymer and materials science, biomedical sciences, and functional molecular systems.

Showcasing recent scientific progress, the ICMS Outreach Symposium is designed to inspire collaboration and interdisciplinary research. A few reactions from the participants :

Prof. Clemens van Blitterswijk, University of Twente and Maastricht University

"ICMS is a kind of matrix placed over the TU/e research groups. Therefore we can easily establish short lines between groups, individual scientists but also the industry. To me, that's the strength of this institute. A symposium like this underlines this." *Bram Pape, PhD Biomedical Chemistry, TU/e*

Visited by around

200

scientists, students, and industry professionals

"Interesting and good lectures which I can surprisingly link to my research on stochastic processes for nanoparticles. I knew the ICMS already, but I particularly liked this symposium. It is also a nice opportunity to meet people." *Marco Decorato, TU/e*

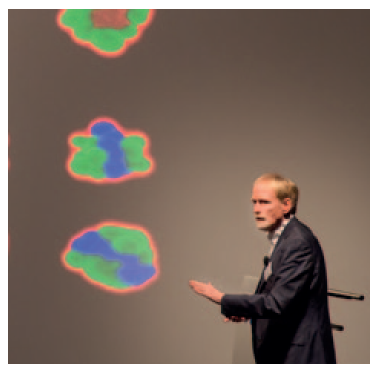
"I really liked the first talk of prof. Martin van Hecke, Leiden University and AMOLF on mechanical metamaterials. It looks rather simple, but is a whole new way of looking at materials, manipulating them by mechanically interrupting their structure. I think the talk fits ICMS, a place where people with diverse backgrounds gather and develop new ideas on the crossroads together." *Björne Mollet, PhD at ICMS, teacher at TU/e*

NEXT OUTREACH SYMPOSIUM

JANUARY 21 & 22 2016

"We at DSM Resins are heavily involved in creating new materials. Every time it is a challenge to make certain properties and to obtain stability. I visit the symposium from this perspective and also to establish interesting connections with the various universities and institutes present." *Mike Schellekens - DSM*

"It is a nice way to showcase scientific work. I love the multidisciplinary approach at ICMS anyway. The goal is to take complex systems and making them simple to solve the problems. By reaching out via symposia like this, we can further enhance that." *Matthew Baker, Post-doctoral researcher at ICMS*



/ Mikko Karttunen

Research by the true meaning of the word interdisciplinary

Starting in May, prof.dr. Mikko Karttunen is a newly appointed member of the Centre for Analysis, Scientific Computing and Applications (CASA) and the ICMS at TU/e. With his diverse background in physics, chemistry, biology, and mathematics, Karttunen thrives on an interdisciplinary approach to research.

Mikko Karttunen, is currently leading the computational biology & soft matter group in the Department of Chemistry at the University of Waterloo in Canada. His research is hard to grasp in a few lines. Karttunen: "One of the things I am currently working on is the behaviour of Intrinsically Disordered Proteins (IDPs). These are proteins that behave in a very different way than their textbook relatives. Normally, proteins fold into a structure, a 3D form, sheets, helices and so on, but these guys are a new class; they hardly fold to a particular structure (that's why they are named disordered) and bind to lots of things. With their versatility, IDPs play an important role in the transport of signals from the outside of cells to the inside and vice versa. They enable cells to function correctly, for instance telling them to grow or not, and initiate the right body responses if we, let's say, take in too much sugar or drink too much alcohol."

FACT

The Dutch connection: Dutch chemist GERARDUS MULDER was the first to describe the chemical composition of proteins in 1838

> BRINGING TOGETHER DISCIPLINES, LIKE ICMS DOES, IS THE KIND OF INTERACTING WHERE THE BIG BREAKTHROUGHS AND THE PROPAGATION WILL COME FROM

Find a systematic

Karttunen: “This is a new field in many ways. Due to their small size and disordered state, finding proper characterization methods and behavioural models for IDPs is quite a challenge. Normally, one would start by shooting x-rays and getting the structure. Due to the lack of well-defined folded structures, the first step doesn’t work here like it does with the textbook proteins. In order to come up with answers and questions even, one has to effectively combine information from lots of different sources. Fields like polymers, disordered systems, fundamental interactions, biology, maths; all come together. This is research by the true meaning of interdisciplinarity. At this moment we put a lot of time and effort in computer simulations and mathematical modelling. This is a powerful way to define structures, change them and see how these changes influence behaviour. When we find a systematic, we can start thinking about manipulation of these proteins.”

Application directions

Potentially, IDPs enable us to influence very small events in the body. This can offer significant advantages in diagnostics and possibly the treatment of diseases, such as cancer and diabetes. Karttunen: “We work towards applications with experimental collaborators. By translating our research to the design of new structures we envision for example creating highly efficient drugs. Via IDPs we could realize targeted delivery of drugs, for example by carriers that release their active substance when encountering cancer cells (with high concentrations of the targeted proteins and enzymes) in the body. Furthermore, when we can control the switch-like behaviour of IDPs we can also work towards the blocking of events in vivo, the generation of tumour-cells for instance. This can have an enormous impact.”

Moving to Eindhoven

Professor Mikko Karttunen will begin working at TU/e in mid May 2015. He will make his mathematical and computational expertise of use at CASA, while his broad background in physics, chemistry, polymers and proteins will be very interesting for the ICMS. Karttunen: “I am very excited about my new position. I think moving to Eindhoven is a great opportunity. Being European myself, I have been tempted to come back to the old continent for some time now. And also, from a science perspective this is an interesting move. There seems to be a serious push for science in Europe today and there is definitely a lot of interesting stuff going on at the TU/e. I have visited twice and both times I was very positively taken by the place. It has an excellent atmosphere; the research is promising and the people have a good attitude. It was not just words I met, but a group of truly enthusiastic scientists working in fields I like.”

Looking forward

Karttunen: “If you look back the past decade, there has been a lot of talking about interdisciplinarity. However there has been a slow convergence. The real merger of scientific disciplines will break the usual boundaries of departments. This is the kind of interacting I like and where, in my opinion, the big breakthroughs will come from and science can propagate. ICMS is directly working from this perspective on a range of interesting topics. I am looking forward to new and interesting collaborations!”

THE CHARACTER OF INTRINSICALLY DISORDERED PROTEINS

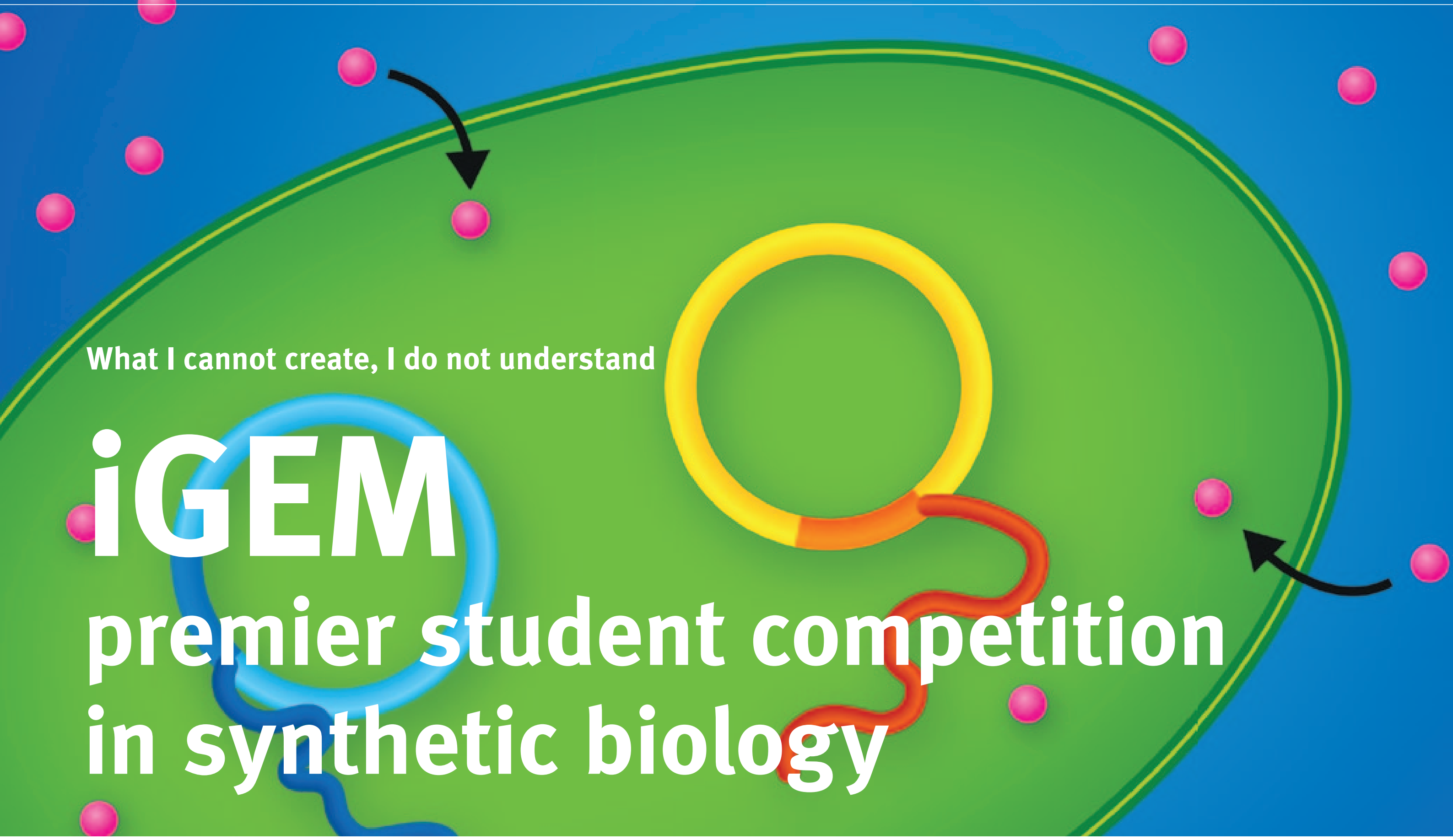
IDPs comprise ~30% of the proteins in our bodies and have key roles in protein-protein interaction networks. Studies have shown that the structural properties of IDPs are crucial to the protein-protein interactions they participate in. Despite their name, IDPs do not adopt completely random conformations – many IDPs have conformational propensities. These segments are called Linear Motifs (LMs), and typically consist of continuous 5-25 amino acid stretches.

IDPs versus globular proteins

- IDPs have more charged residues
- More polar residues
- More structure breaking residues (glycine & proline)
- Less aromatic content
- Less hydrophobic content
- Linear motifs, crucial for binding

Advantages of IDPs versus globular proteins

- Specificity without excessive binding strength
- Fast, switch-like, binding
- One-to-many signalling: Protein Hubs



What I cannot create, I do not understand

iGEM
premier student competition in synthetic biology

Started a decade ago at MIT, the International Genetically Engineered Machine competition (iGEM) is the premier Synthetic Biology competition for students. The project design and competition format provides an exceptionally motivating and effective learning environment. TU/e has participated in iGEM for several years. Let's hear about some experiences from the student team captains and their mentors.

The 2013 experience

As part of the iGEM competition, teams are given a kit of biological parts at the beginning of the summer from the Registry of Standard Biological Parts. Working at their own universities, teams use these parts as well as new parts of their own design to build biological systems and operate them in living cells. At the end of the summer, the teams present their studies, findings, and new biological creations at the iGEM Giant Jamboree in Boston, USA.

Pieters: "This is a competition about creating new functionality with BioBricks and ultimately delivering some new BioBricks to the Registry for future teams as well as scientists in general to work with."

Van der Linden: "What I like the most about iGEM is that it is an intense learning environment. Teams choose the projects themselves and conduct all the experiments. It is really a deep dive into hands-on science. During iGEM, we only partially succeeded in achieving our goals. The time was very limited, of course."

Pieters: "We succeeded in generating MRI contrast with our system but didn't achieve the specific targeting of cancer cells. However, our team passed the European preliminaries. We produced new BioBricks, and we were awarded a gold medal a gold medal at the European preliminaries (Lyon). We subsequently participated in the Giant Jamboree in Boston."

The 2014 experience

Cremers: “I was looking for an extra challenge in my studies and wanted to find out if research is my thing. iGEM really exceeded my expectations. We were actually conducting research beyond our initial capabilities, so we developed as scientists along the way. Working with a lab coat on is the definition of science to me.”

Boschman: “iGEM was a perfect challenge for me. Using our knowledge to create and to steer something in the direction we want is great. We had quite a large team. This may seem advantageous, but complicates the situation as well. It was like running a small organization. We worked long days and nights and really put effort into this challenge. We were lucky everything went right the first time.”

Cremers: “We executed a proof-of-principle and got a lot of attention for our Click Coli system. A lot of research groups and professors attended the poster presentation, and our presentation was well-received.”

Boschman: “We won the category of ‘best new application’ for undergraduate teams. That is nice. And currently, three TU/e students are further researching our project as a bachelor graduation project. So we really contributed as well.”

The mentors

Dr. Maarten Merkx: “I think iGEM is an excellent way to make students connect with knowledge in another way and at an early stage in their studies. They have very limited time to get to know the biological field and try to create something new and original. The students go deep and have to get everything

Team 2013

MRIGEM

Captains: Ardjan van der Linden, Pascal Pieters

Abstract

Our project presents an alternative solution to the use of heavy metals in MRI contrast agents. The most commonly used heavy metal, gadolinium, may be involved in the induction of diseases and may be toxic if the patient has kidney failures. There is an alternative. Within CEST imaging, proteins enclosing exchangeable hydrogen atoms can generate high quality images. Escherichia coli are used to express CEST proteins when the bacteria sense a hypoxic environment via a promoter designed for this purpose. Thus, the bacteria works as both a production and delivery system for the CEST MRI contrast agent. A rapidly evolving research area in the field of oncology is focused on bacterial based cancer therapies, in which bacteria like E. Coli and Salmonella are used to induce cancer cell death. Based on this type of cancer therapy, and considering that hypoxic regions are related to tumors, our eventual goal is to use this system to target and image tumors in humans by injecting the bacteria into the bloodstream. A secondary application is the tracking of bacteria in bacterial infection studies. For iGEM, the proteins were expressed ex-vivo in both aerobic and anaerobic conditions.

Check the MRIGEM wiki page:
http://2013.igem.org/Team:TU-Eindhoven

> “It is really *a deep* dive into **HANDS-ON SCIENCE.”**

Team 2014

Click Coli

Abstract
A fundamental problem in utilizing genetically modified bacteria is their limited ability to survive in non-natural environments, such as the harsh conditions in industrial reactors or due to the immune system also in the human body. We report a “Plug-and-Play” system that allows the introduction of chemical anchors on cell membranes, that are subsequently used to attach a functional coating. The anchors consist of azidophenylalanine, which couples covalently with molecules containing the strained alkyne DBCO in a so-called "click" reaction. We obtained proof-of-concept that our Clickable Outer Membrane Proteins (COMP) enable this fast and effective click reaction. We applied it to create a safe “clicked-on” coating that allows E.coli to be used in the human body for healthcare purposes. Furthermore, we have designed microfluidic devices that give increased control over the click reaction and single cell coating. We believe our “Plug-and-Play” system is a versatile tool that provides numerous possibilities for engineering the outer membranes of bacteria.

Check the Click Coli wiki page:
http://2014.igem.org/Team:TU_Eindhoven/Abstract

“We were actually conducting *research* beyond our INITIAL CAPABILITIES.”

Captains: Glenn Cremers, Anke Boschman


Mentors: Tom de Greef, Maarten Merkx

right. It fits the famous quote of Feynman: ‘What I cannot create, I do not understand’.

Dr.ir. Tom de Greef: “We use our time effectively. We start with team formation and idea generation in January. Students decide what project they want to participate in. We do not steer but only guide the decision-making. For instance, we help the team transition ideas into realistic plans that are possible at our university. And along the way we guide the teams as much as possible.”

Merkx: “It is amazing to see how much the students develop in just a year. You could ask yourself if this is the perfect form of education. However, it wouldn’t be practical for large numbers of students, and it may not be effective for every student. You need a lot of motivation and enthusiasm to participate.”

De Greef: “It is great to see a team grow. You can already experience that with our 2015 team. They are currently figuring out which idea to work on. One idea builds on the Click Coli project; the other idea is to use specific bacteria as a biosensor. I think iGEM fits TU/e like a glove. Synthetic biology is mostly an engineering science. Our 2013 and 2014 teams did great, so the sights are set high!”

NEWS, AWARDS & GRANTS

PETER KOREVAAR

wins the KNCV 'Challa Polymer Award 2015'

The KNCV Challa Polymer Award is presented every two years to a young scientist under 30 that defended his / her PhD thesis at a Dutch University in the broad field of polymer science and engineering. The award will be presented to Peter Korevaar at the annual Dutch Polymer Days in Lunteren. The scientific publications of Peter as well as his PhD thesis are judged as being outstanding contributions to polymer science.

PATRICIA DANKERS

joins The Young Academy (De Jonge Akademie)

Patricia Dankers was selected by The Young Academy as one of the ten new, young top scientists to add to its ranks. In addition to their proven research excellence, members of the Young Academy take a broad interest in science and in science communication.

Koninklijke Nederlandse Akademie van Wetenschappen (KNAW) has nominated her to be a member of the Young Academy, starting November 26th 2014 for the duration of 5 years. She has accepted the membership and has been officially installed on March 26th 2015 in the members meeting of The Young Academy.

ERC Starting grant for

ILJA VOETS

Ilja Voets was successfully granted an ERC Starting grant on her research on anti-freeze proteins and materials. The European Research Council starting grant is worth 1.66 million Euros and gives Ilja Voets the opportunity to study in detail the working mechanism of antifreeze proteins and polymers.

FRANKS BAAIJENS HAS BEEN APPOINTED AS NEW RECTOR MAGNIFICUS

Prof.dr.ir. Frank Baaijens will replace prof.dr.ir. Hans van Duijn as rector magnificus of the TU/e starting May 1st 2015.

Consequentially, he will terminate his work at the department BME, as a professor of Soft Tissue Biomechanics and Tissue Engineering, vice dean of the department and associate scientific director of the ICMS.

We wish Frank success as the new rector and we like to thank him for his input, work and continuous support for ICMS.

Farewell note by Frank Baaijens

Dear reader,

ICMS unites scientists from various departments in a unique setting that aims to stimulate intellectual interaction in an informal but dedicated environment. Scientists sharing ideas, expertise, and infrastructure. Challenging each other to push the frontiers of our knowledge. All in an effort to perform world-class research.

The ICMS boasts a unique leadership necessary for maintaining focus on the core mission of ICMS: scientific excellence. By its very nature, it also contributes to the education of the next generation of top scientists. It works, and it pays off in a big way.

Despite my change in career path, I aim to continue my participation in some of the outstanding meetings at the ICMS. I am confident that the ICMS will continue to make important contributions to science and to the scientific community of the TU/e in particular.

Frank Baaijens

MENNO PRINS

new Associate Scientific Director of the ICMS

We are very pleased to announce that Menno Prins is the new Associate Scientific Director of the ICMS as the successor of Frank Baaijens starting April 1, 2015. Menno will also be responsible for our research line “Bio-Inspired Engineering”; which he will chair together with Patricia Dankers.

ICMS TOP PUBLICATIONS

September 2014 – April 2015

1. *K.H. Hendriks, W.W. Li, G.H.L. Heintges, G.W.P. van Pruissen, M.M. Wienk, R.A.J. Janssen*
Homocoupling defects in diketopyrrolopyrrole-based copolymers and their effect on photovoltaic performance
J. Am. Chem. Soc., 136, 11128-11133 (2014)

2. *K.H. Hendriks, W.W. Li, M.M. Wienk, R.A.J. Janssen*
Small-bandgap semiconducting polymers with high near-infrared photoresponse
J. Am. Chem. Soc., 136, 12130-12136 (2014)

3. *I.A.W. Filot, R.A. van Santen, E.J.M. Hensen*
The optimally performing Fischer-Tropsch Catalyst
Angew. Chem. Int. Ed. 53, 12746-12750 (2014)

4. *N.A.J.M. Sommerdijk, M. Cusack*
Biomineralization crystals competing for space
Nat. Mater. 13, 1078-1079 (2014)

5. *K. Meister, S. Strazdaite, A.L. de Vries, S. Lotze, L.L.C. Olijve, I.K. Voets, H.J. Bakker*
Observation of ice-like water layers at an aqueous protein surface
Proc. Nat. Ac. Sci, U.S.A., 111, 17732-17736 (2014)

6. *P.J.M. Smeets, K.R. Cho, R.G.E. Kempen, N.A.J.M. Sommerdijk, J.J. de Yoreo*
Calcium carbonate nucleation driven by ion binding in a biomimetic matrix revealed by in situ electron microscopy
Nat. Mater. Published online (2015)

7. *T.F.E. Paffen, G. Ercolani, T.F.A. de Greef, E.W. Meijer*
Supramolecular buffering by ring-chain competition
J. Am. Chem. Soc. 137, 1501-1509 (2015)

8. *S.N. Semenov, A.S.Y. Wong, R.M. van der Made, S.G.J. Postma, J. Groen, H.W.H. van Roekel, T.F.A. de Greef, W.T.S. Huck*
Rational design of functional and tunable oscillating enzymatic networks
Nat. Chem. 7, 160-165 (2015)

9. *J.J. van Franeker, M. Turbiez, W. Li, M.M. Wienk, R.A.J. Janssen*
A real-time study of the benefits of co-solvents in polymer solar cell processing
Nat. Commun. 6, 6229 (2015)

10. *J.J. van Franeker, D. Westhoff, M. Turbiez, M.M. Wienk, V. Schmidt, R.A.J. Janssen*
Controlling the dominant length scale of liquid-liquid phase separation in spin-coated organic semiconductor films
Adv. Mater., Published online (2015)

11. *W. Li, K.H. Hendriks, A. Furlan, M.M.Wienk, R.A.J. Janssen*
High quantum efficiencies in polymer solar cells at energy losses below 0.6 eV
J. Am. Chem. Soc., Published online (2015)

12. *B.M.G. Janssen, M. van Rosmalen, L. van Beek, M. Merkx*
Antibody activation using DNA-based logic gates
Angew. Chem. Int. Ed, 8, 2530-2533 (2015)

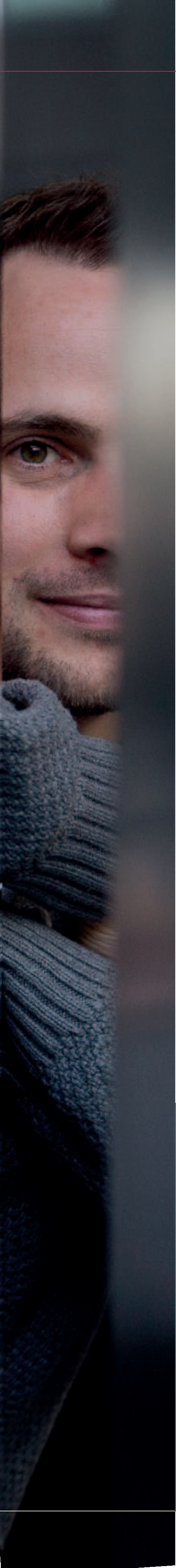
This overview lists publications in high end journals with ICMS as affiliation.

/ Erik Steur

The robustness of dynamic networks

Erik Steur is joining ICMS as a postdoctoral fellow within the complexity hub chaired by prof.dr. Rutger van Santen and prof.dr. Mark Peletier. His research aims to help us understand why the dynamics of our brain is so robust. As a brain grows and learns, its structure changes, but it continues operating in more or less the same way. Insights into this system may help keep autonomous cars on track.

The human brain has much more structure than can be dictated by mere DNA. This means that the blueprint for the nearly 100 billion neurons in the brain and their 100 trillion interconnections is not drawn beforehand. While growing, the brain develops its optimal structure. It is this growth process that Erik Steur analyzes. New experiences bring dynamics into play, as they must eventually be incorporated into the brain structure. For example, connections are reinforced between cells that fire synchronously. Erik has simulated this in a computer model in which he establishes new connections between co-firing neurons.



Erik did postdoctoral research at the Laboratory of Experimental Psychology in Leuven, where he had access to neuroimaging data that shows various synchronizations between neurons. A similar dynamic, one where connections are built up and strengthened, may be found in other networks. Erik is planning to extend the application of his insights to, for example, networks of self-steering vehicles.

The brain is organized into local clusters. Each cluster performs its own functions but is also connected to other clusters. Therefore, Erik modeled the brain as a modular network. Unique to his model is the way he accounts for time delay in information transfer. This is crucial, as it takes some time for the brain to transmit a signal from one cell to another. A delay makes the model mathematically much more difficult. “It is tempting to rely immediately on a computer simulation that shows how a network behaves. All sorts of patterns may form, but you will learn little about how they might arise,” says Erik. “For that, you will have to look at the mathematical relationships. That reveals the mechanisms of the network dynamics.”

Erik's model still is a simplification; in reality there are several mechanisms that strengthen connections, he says. However, it appears that the different ways in which the brain can learn and grow produce similar results. “We want to understand why that is,” says Erik. “In addition, the network of neurons in each person is different. So it is important to understand why the building mechanisms continue to work well even when the networks are distinct.”

That robustness is also important for autonomous vehicles. For example, what happens if a car cannot drive fast enough or is limited in its ability to communicate with others? Would that upset a whole road of autonomous vehicles?

“That's really still an open question,” says Erik.

More about this research

N. Jarman, C. Trengove, E. Steur, I. Tyukin, and C. v. Leeuwen. Spatially constrained adaptive rewiring in cortical networks creates spatially modular small world architectures. Cogn Neurodyn (2014) 8:479–497. doi:10.1007/s11571-014-9288-y

E. Steur, W. Michiels, H. Huijberts, and H. Nijmeijer. Networks of diffusively time-delay coupled systems: Conditions for synchronization and its relation to the network topology. Physica D (2014) 277:22–39. doi:10.1016/j.physd.2014.03.004

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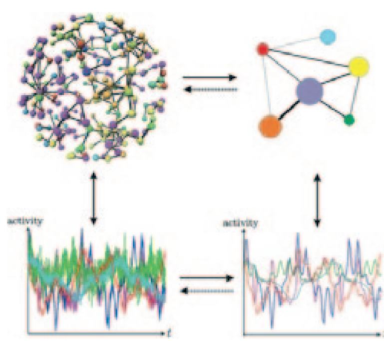


THE ROBUSTNESS OF THE BRAIN, IN SPITE OF ALL ITS DYNAMICS, MAY TEACH US HOW AUTONOMOUS CARS CAN COOPERATE

EPL Update

Frank Bates on polymer science

The future lies in combining materials to capture multiple functionality

It is not every week you have a chance for a tête-à-tête with one of the world's most renowned polymer science experts. In mid-March, Regents Professor at the University of Minnesota and member of the DSM science advisory board, Frank Bates, paid a visit to the Netherlands. EPL seized this opportunity and welcomed Bates for a lecture and a series of meet-ups with its scientists. Needless to say, the discussions concentrated on the challenges in polymer science and how to cope with them.

Frank Bates: "The polymer market is large, about 400 billion USD per year worldwide, and the materials go everywhere. Any advance in this area has a big economic impact. However, over the past decades the developments have mostly focussed on just a few types of materials. The future lies in combining these materials into products that capture multiple functionality. For example, products that contain stiff elastic properties and toughness, or electric conductivity while being fully sustainable.

Today we benefit from remarkable advances made over the past two decades in synthetic chemistry and an enhanced understanding of polymer engineering. We can design and make multiblock polymers with new molecular architectures and all kinds of exciting properties. However, we hardly know what to make. We have so many possibilities; we don't know how to anticipate structure and properties theoretically.

In my work I get many of the most important ideas from working with companies. There, you will find complicated and interesting problems that help to define what materials to work on. When you start to explore, to understand in detail, you discover fascinating applications that ultimately drive again fundamental research. I spent the first seven years of my career at Bell Laboratories, an incredible invention factory that thanks its success to blending theory and experimentation. Bell scientists and engineers had tremendous freedom to pursue issues across a wide range of topics. That is an important requirement for scientific discovery; however, this freedom needs to be placed in an environment that addresses societal need and practical applications. There is always a balance to be struck.

To me, the next steps in polymer science and the transfer of knowledge into new materials and applications, requires an interdisciplinary approach. It is like peeling an onion. There are levels of complexity to be understood and peeled off one by one. I think we are just at the beginning of developing new interdisciplinary approaches to understanding the fundamental scientific phenomena that are subsequently translated into engineering principles. In the end I believe every game-changing discovery is a product of serendipity. The trick is to create an environment that enhances this process. So you need places where seemingly disparate disciplines can meet, where there is freedom to explore and important and often practical targets to work on. In the academic setting this comes with the simultaneous challenge to blend research and discovery with a rigorous and coherent educational platform for students as well. After all, it is inevitably the students and postdocs who come up with fresh ideas to overcome the most challenging materials problems.

I don't know enough about the Dutch science and engineering community to make comprehensive comments and in-depth remarks, but the part I am familiar with, most notably the ICMS, is very impressive. There is an exciting level of sophistication in synthetic chemistry, coupled to physical, structural and property relationships that strikes a commendable balance, which is obvious and important.

Guiding the next generation of students and post docs to develop the right attitude towards research and discovery, emphasizing an interdisciplinary approach, will lead to creative and productive scientists and engineers. And as a dividend we will generate knowledge that helps to advance fundamental understanding that ultimately drives industrial progress."

"It was a fantastic opportunity to have Frank Bates visiting. His work exemplifies the modern, interdisciplinary approach in materials science, and it is inspirational to see how mechanical, electrical and chemical functionality are designed, combined, and actually made in the lab. Aside from his scientific accomplishments, I admire also the way in which Bates has transformed Chemical Engineering and Materials Science at his own university in Minnesota - at the ICMS and the EPL in Eindhoven we are working hard to realize a similarly collaborative and interdisciplinary environment, which I believe is an absolute must for continued excellence in polymer science and engineering. Frank Bates has shown us that these are truly exciting times to be a polymer scientist!"

dr. Cees Storm
Associate professor in the group Theory of Polymers and Soft Matter in the department of Applied Physics and Board Member EPL

/ Patricia Dankers

Dreaming of a first-in-man study

Associate professor Patricia Dankers is driven to contribute to longer and healthier lives. Her interest in drug discovery and drug development started as a child. However, eliminated by numerus fixus for Medicine, she studied Chemistry instead. Now she puts her knowledge and skills to work at ICMS in developing biomaterials for use in regenerative medicine. The level of sophistication in her scientific work is well recognized. Dankers received an ERC Starting Grant for her research, and in March 2015 she was inducted into De Jonge Akademie of the KNAW (Dutch Royal Academy of Sciences), an organization that brings together top scientists to advocate for science in society.

Elastomers and hydrogels

Dankers: “In our research group ‘Supramolecular biomaterials for translational biomedical science’, we synthesize supramolecular materials based on, for example, the supramolecular ureidopyrimidinone (UPy) moiety which was developed by prof.dr. Bert Meijer and prof.dr. Carlijn Bouten. We aim at the development of various biomaterial types based on this supramolecular chemistry, varying from elastomers to hydrogels. We draw inspiration from the extracellular matrix, which is a natural and complex supramolecular material that surrounds the cells in our body. This natural, highly dynamic and bioactive material instructs cells to function properly. Therefore, our main goal is to introduce dynamics and bioactivity in our synthetic supramolecular materials in a way such that they are able to interact with cells and that these materials are able to instruct cells.”

Biomedical applications

“In close collaboration with prof.dr. Carlijn Bouten, we develop our supramolecular elastomeric materials into vascular access grafts. Today, access grafts for kidney patients that need regular dialysis are rigid and increase the chance of infection and thrombosis. We aim at the development of a vascular graft that attracts cells in situ and eventually form a new autologous vessel. Our research on supramolecular hydrogels focuses on the delivery of several drugs to the heart after a myocardial infarction via minimally invasive catheter injection. Our dream is to prepare a first-in-man study with one of our supramolecular biomaterials.”

At home

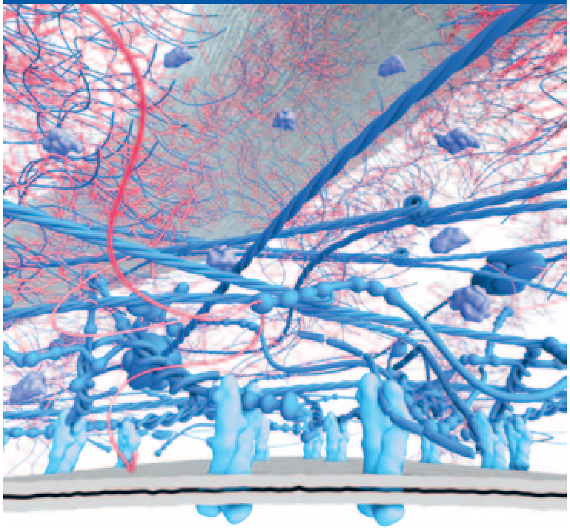
“In our research we cover many fundamental aspects, but it does not stop after studying and understanding how molecules aggregate. We truly aim to translate one of our materials and to prepare a first-in-man study. At TU/e and ICMS, we are fortunate to be able to cover various disciplines such as chemistry, biology and engineering - that’s quite unique and fulfilling! However, preparation of a first-in-man study will take years. Many experiments still have to be performed, and we have to comply with all the necessary regulatory requirements. So we have to work hard to achieve all this! This is good since we work from a clear ambition.”

Childhood dream

“There is an obvious need for technology in keeping people healthy and possibly extending life. To me, biomedical engineering has a bright future. On the issue of ethics, I hardly encounter resistance and fear in our field. In fact, I receive many supportive e-mails. People can directly see the advantages of regenerative medicine. That brings me pretty close to my childhood dream: cure people, make them healthy.”

> “We aim at the ***development*** of various **biomaterial** **TYPES** based on this supramolecular ***chemistry*** varying from **ELASTOMERS** to **HYDROGELS**.”

SCHEMATIC REPRESENTATION OF THE NATURAL EXTRACELLULAR MATRIX: OUR SOURCE OF INSPIRATION TO MAKE SUPRAMOLECULAR BIOMATERIALS



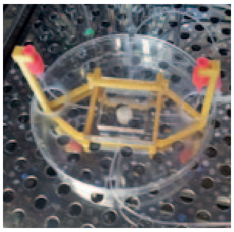
FACTS

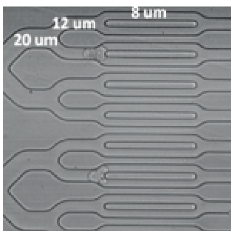
More than
200 different
cell types in the human body

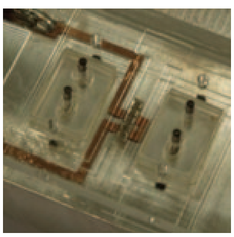
More than
2500 different
proteins in the ECM

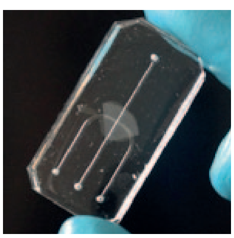
Microfab Lab

Officially opening in July 2015, the brand-new "Microfab Lab" will be a shared TU/e-wide microfabrication facility and part of the ICMS infrastructure. It will be a state-of-the-art facility for efficient and flexible manufacturing of fully functional microsystem prototypes both for scientific research and for education.









Typical examples of devices that will be made possible with the new Microfab Lab, illustrating the range of accessible materials and length scales.

New opportunities

In a number new and rapidly expanding areas of science and technology, the use of micro-devices and -systems is of paramount importance. Examples are the fields of microfluidics, biosensing, tissue engineering, chemical synthesis, synthetic biology, chemical reactions, lab-on-a-chip, optofluidics, organ-on-a-chip, novel material development, and micro-actuators and –sensors. These are active fields of research in research groups at the TU/e distributed over various departments, and especially within ICMS. The availability of a TU/e-wide state-of-the-art microfabrication facility, currently lacking, will create new opportunities to advance the research in these fields.

In addition, such a facility will give opportunities for education, since students of various departments can gain hands-on experience with a range of microfabrication methods.

For these reasons, the central board of the TU/e decided in 2014 to invest in setting up a brand-new micro-fabrication facility, and it is almost ready: the Microfab Lab.

The facilities

The Microfab Lab will be housed in building Gemini-Noord, and will consist of a number of different sections covering a total area of over 600 m2. The controlled microfabrication section, a cleanroom-like environment, has all that is needed to do basic lithography: spincoaters, thin film deposition, surface modification techniques like plasma treatment and UV-ozone treatment, UV-curing systems, a mask aligner, and chemical benches. In this section, soft lithography can be done as well. The laser fabrication section has a number of advanced lasers to precisely machine, and analyze materials. In another section, a basic cell lab can be used for biological experimenting. There is general fabrication section that houses 3D-printers, a CO_2 laser cutter, an excimer laser and mechanical micromachining, for quickly and conveniently making prototypes. Finally, there is an experimentation lab in which microfluidic, physical, and micro-mechanical testing can be done to carry out tests the devices made in the other sections of the lab.

The uniqueness of the lab is the availability of all these different technologies in one location, that can be combined to machine different material types from polymers to silicon, with resolutions of microns or larger. The Microfab Lab is complementary to the Nanolab@TU/e, which is an advanced cleanroom aimed at sub-micrometer resolution in strictly controlled environment, aiming at much higher resolutions than in the Microfab Lab.

A meeting place

The Microfab Lab will be accessible to all research groups at TU/e, and to our project external partners. The lab will be managed by the Microsystems group of Jaap den Toonder, core member of ICMS. Essential will be that the facility has a low threshold to access for all researchers and students, naturally after having received a thorough introduction into safety and way-of-working in the lab. One of the important missions is to create a natural meeting place and stimulate cross-disciplinary and cross-departmental collaboration, completely in line with the philosophy of ICMS.

THESES ICMS

September 2014 – April 2015

1 **Responsive polymer photonics**
Jelle E. Stumpel

November 6, 2014
PhD advisors:
prof.dr. A.P.H.J. Schenning
& prof.dr. D.J. Broer

2 **Protein-protein interaction fine-tuning by estrogen receptor post-translational modification**
Inga M. Tharun

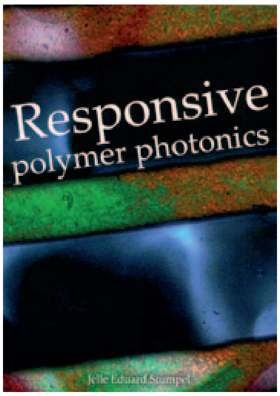
November 6, 2014
PhD advisors:
prof.dr.ir. L. Brunsveld
& dr. C. Ottmann

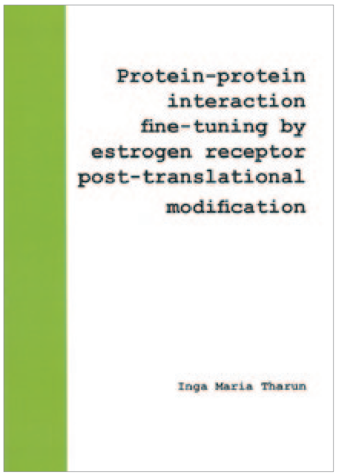
3 **Modulating the inflammatory response to biomaterials by mechanical stimuli: implications for in situ cardiovascular tissue engineering**
Virginia Ballotta

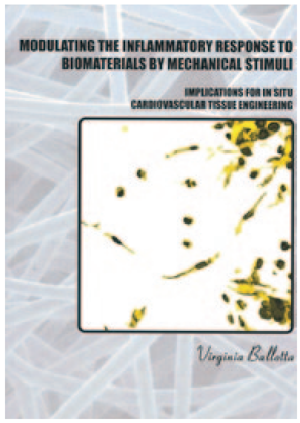
September 29, 2014
PhD advisors:
prof.dr.ir. F.P.T. Baaijens
& prof.dr. C.V.C. Bouten

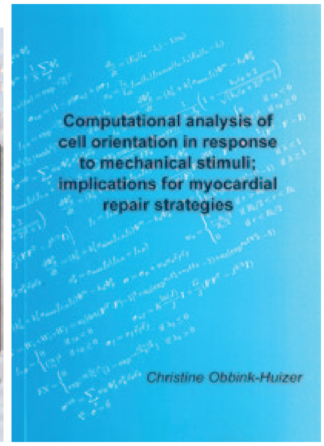
4 **Computational analysis of cell orientation in response to mechanical stimuli; implications for myocardial repair strategies**
Christine Obbink-Huizer

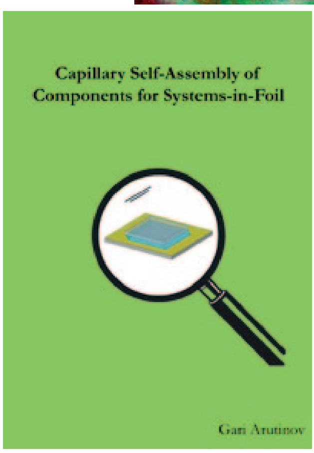
October 30, 2014
PhD advisors:
prof.dr.ir. F.P.T. Baaijens
& prof.dr. C.V.C. Bouten

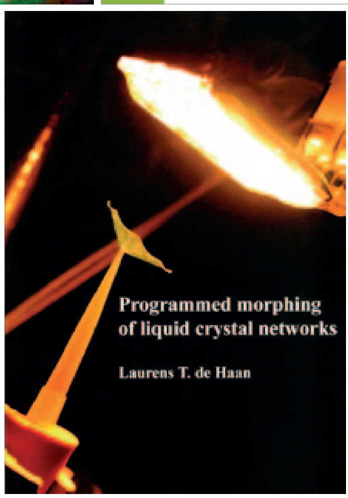


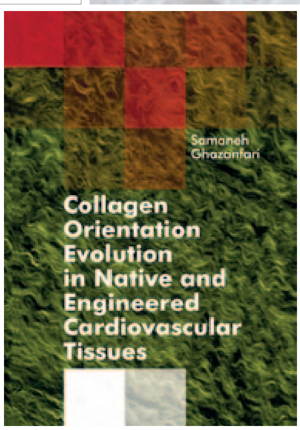


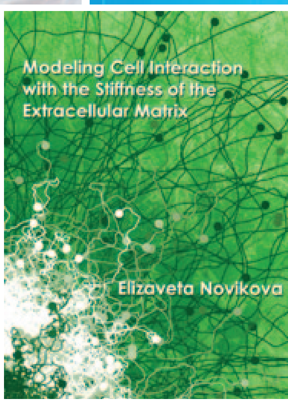












5 **Capillary self-assembly of components for systems-in-foil**
Gari Arutinov

November 10, 2014
PhD advisors:
prof.dr.ir. J.M.J. den Toonder
& prof.dr. A.H. Dietzel

6 **Programmed morphing of liquid crystal networks**
Laurens T. de Haan

November 13, 2014
PhD advisors:
prof.dr. A.P.H.J. Schenning
& prof.dr. D.J. Broer

7 **Collagen orientation evolution in native and engineered cardiovascular tissues**
Samaneh Ghazanfari

December 1, 2014
PhD advisors:
prof.dr. C.V.C. Bouten
& prof.dr.ir. F.P.T. Baaijens

8 **Modeling cell interaction with the stiffness of the extracellular matrix**
Elizaveta Novikova

December 15, 2014
PhD advisors:
prof.dr. M.A.J. Michels
& dr. C. Storm

9 **Supramolecular surfaces for cell adhesion**
Pauline Neirynck

January 19, 2015
PhD advisors:
prof.dr.ir. L. Brunsveld
& dr. L.G. Milroy

10 **Supramolecular biomaterials based on ureido-pyrimidinones**
Björne B. Mollet

January 29, 2015
PhD advisors:
prof.dr. E.W. Meijer
& dr.dr. P.Y.W. Dankers

11 **Local effective volume changes in fused silica by femtosecond laser irradiation**
Audrey Champion

January 26, 2015
PhD advisors:
prof.dr.ir. J.M.J. den Toonder
& prof.dr. Y.J. Bellouard

12 **Responsive materials from adaptive supramolecular constructs**
Isja de Feijter

February 24, 2015
PhD advisors:
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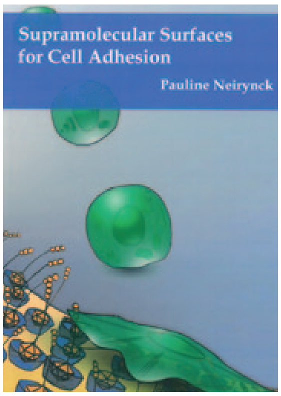
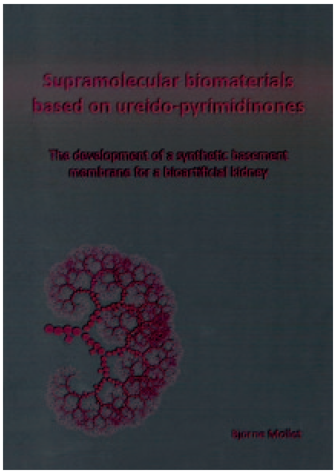
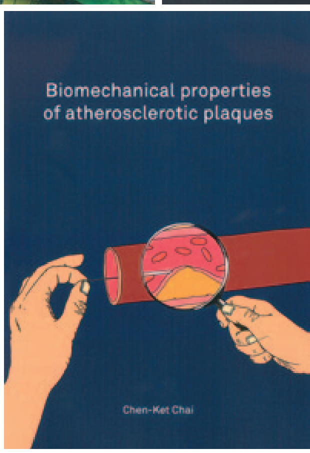
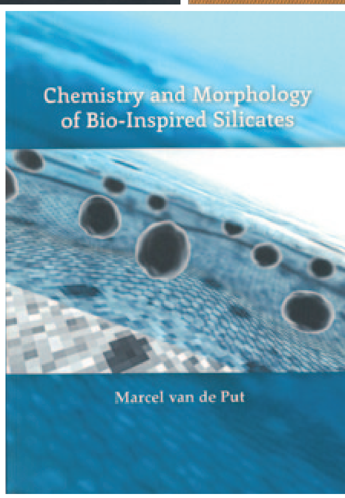
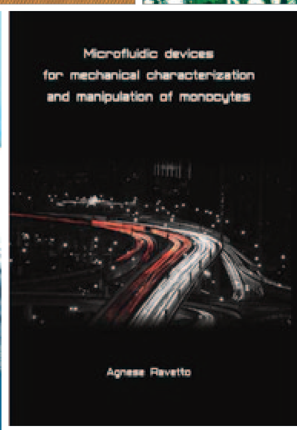
& dr.ir. I.K. Voets

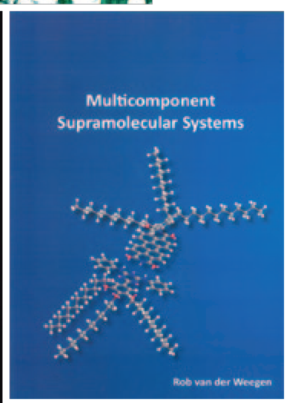












13 **Biomechanical properties of atherosclerotic plaques**
Chen Ket Chen

March 26, 2015
PhD advisors:
prof.dr. G. de With
& prof.dr. N. Sommerdijk

14 **Chemistry and morphology of bio-inspired silicates**
Marcel van de Put

March 26, 2015
PhD advisors:
prof.dr. G. de With
& prof.dr. N. Sommerdijk

15 **Microfluidic systems for mechanical characterization and manipulation of monocytes**
Agnes Ravetto

April 7, 2015
PhD advisors:
prof.dr. C.V.C. Baaijens
& prof.dr.ir. J.M.J. den Toonder

16 **Multicomponent supramolecular systems**
Rob van der Weegen

April 9, 2015
PhD advisors:
prof.dr. E.W. Meijer
& dr.ir. A.R.A. Palmans

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. M.W.J. Prins en dr.dr. P.Y.W. Dankers)
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 5074 with specific questions or remarks.

ICMS IN PRESS

Editorial
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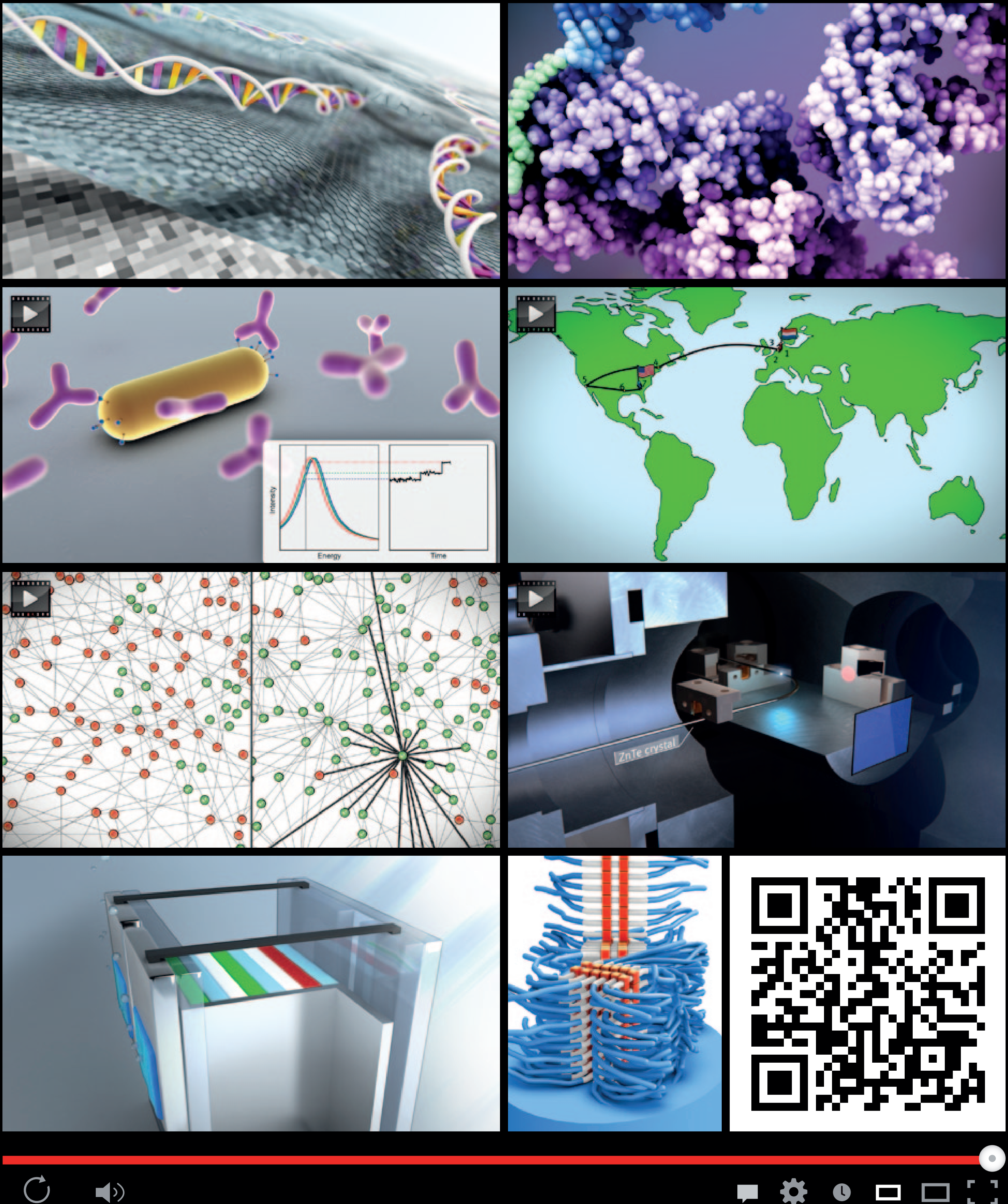

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