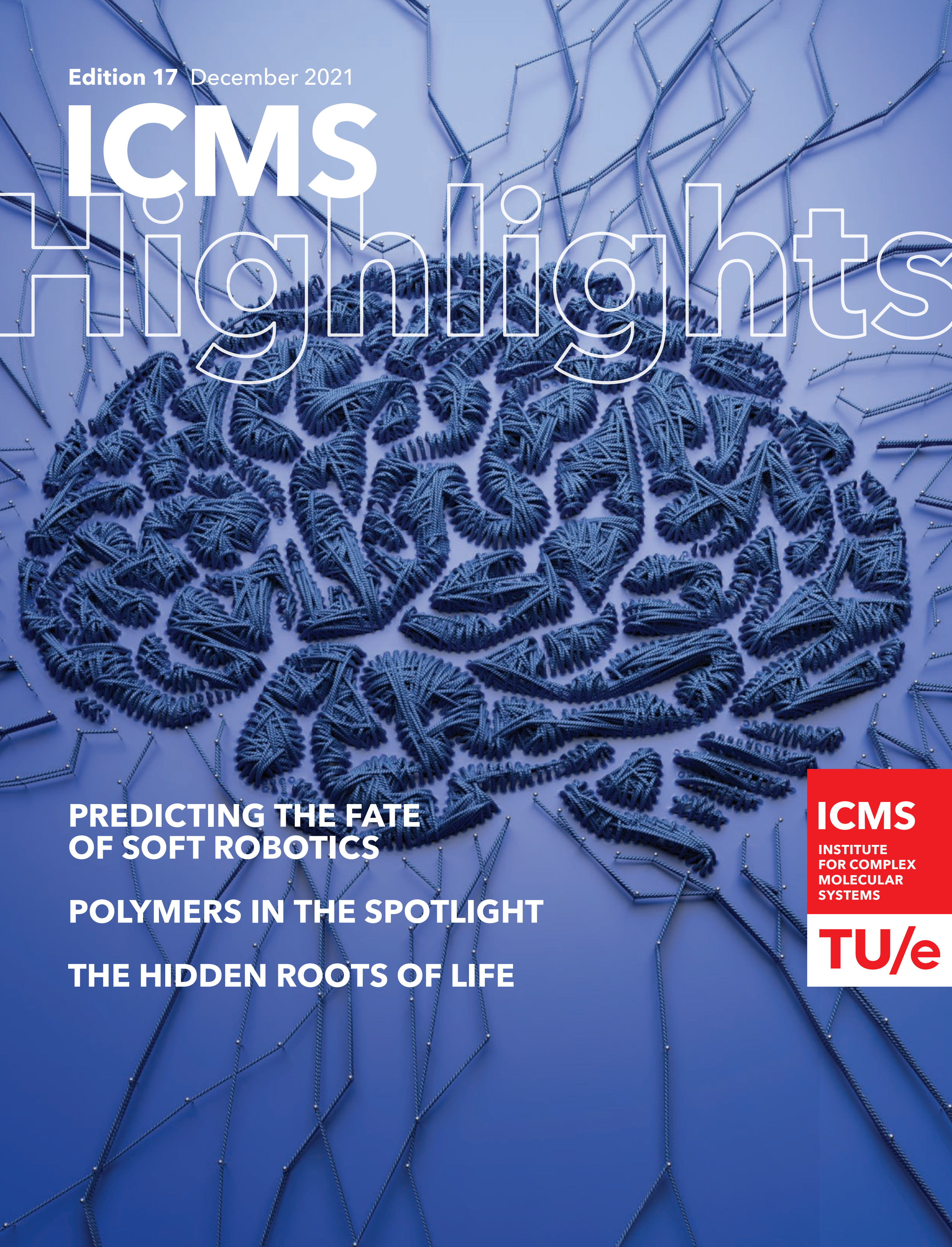
Edition 17 December 2021

ICMS Highlights



PREDICTING THE FATE OF SOFT ROBOTICS

POLYMERS IN THE SPOTLIGHT

THE HIDDEN ROOTS OF LIFE

ICMS
INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS

TU/e

INTRODUCTION

ICMS Highlights

Thirteen years ago, ICMS set out on a mission to go beyond the status quo in the field of complex molecular systems. Interdisciplinary science, curiosity-driven research and a vibrant community were identified as cornerstones, to facilitate fundamental understanding of molecular systems. Throughout the years, we learned that a strong community is the main element for growth and impact. Together we fall and together we rise. We truly value and embrace everyone in the ICMS community and we want to make new members feel at home. Therefore, we will kick-start the careers of incoming researchers by welcoming them to the ICMS family, through onboarding sessions.

In this edition, we showcase young scientists who discover their talents under the guidance of our senior researchers. These researchers participate in projects in which bridging disciplines is daily business. We welcome our new ICMS Fellow, Shikha Dhiman, and look forward to a pleasant collaboration.

Senior researchers play a key role in our community through their scientific expertise and the way they foster talent. A special word of appreciation to Dick Broer who contributed immensely to both aspects. Dick, you are a warm and inviting person who has contributed to science in an unprecedented way. We congratulate you with your royal distinction to become "Knight in the Order of the Lion of the Netherlands." We are confident that your findings will contribute to society for many years to come.

We hope you all will enjoy reading this edition of the ICMS Highlights.

For more information on our community, please visit our LinkedIn page.

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Scientific director

Monique Bruining
Managing director

Calendar

ICMS/SG lecture
prof.dr. Hans Heesterbeek
"How to understand a pandemic"
12 January 2022

Advanced Analysis #4
Xray techniques
14 January 2022

Onboarding session #1
18 January 2022

Advanced Analysis #5
Correlative approaches & conclusions
4 March 2022

IBEC – ICMS mini-symposium
23 March 2022

ICMS Annual Symposium
24 March 2022

ICMS - MPI-P mini-symposium
Grip on Complexity 2-day workshop
February tbd

ICMS Postdoc Paper event
13 May 2022

Please check our website for our upcoming events.
www.tue.nl/icms

EDITORIAL
ICMS Highlights is the half-yearly magazine of ICMS for ICMS members, colleagues, collaboration partners, policy makers and affiliated companies. ICMS Highlights is published twice a year.

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Content

COVER Artist impressions of complexity in networks (front) and hierarchical structure in a supramolecular fiber (back).

CHEMICAL BIOLOGY

Collaborating on cellular control

New Centre for Living Technologies engineers new properties into living cells

Tom de Greef

The Dutch “polder”-mentality – the ability to work together for the common good – happily permeates all walks of Dutch life, including scientific collaboration. Knowing that you can achieve more together than you can alone, has triggered a powerful new partnership: The Centre for Living Technologies. A collaborative synthetic biology research program that connects TU/e, Wageningen University Research (WUR), Utrecht University (UU) and University Medical Centre Utrecht (UMCU). Together, these four institutions aim to develop bio-based technologies to improve the health of people, animals and the environment by engineering new properties into living cells.

"MICROBES IN A MIX ARE A BIT LIKE TODDLERS AT AN UNSUPERVISED PARTY"

Tom de Greef, associate professor of Synthetic Biology, is leading this collaboration from the TU/e end. Using synthetic biology, the collaborators will work together to create materials that can mimic, enhance and increase the functionality of living cells. These materials can then be used in a therapeutic way in the body or to create advanced materials that can help solve environmental problems.

CELL AS COMPUTER

De Greef's lab specializes in biological computing within the synthetic biology field. "We engineer cells to perform the very familiar functions of a computer, such as logical reasoning, analytics, recording of signals and storage of data," he explains. The translational possibilities for this emerging field where synthetic biology and computing meet, are vast. Combining their joint strengths, the collaborators have chosen two topics that they believe may contribute to addressing challenges in the field of health and the environment: "Smarter cellular therapies" and "Policing the microbial soup."

SMARTER CELLULAR THERAPIES

Together with Lukas Kapitein, professor of molecular and cellular biophysics (UU), the first project focuses on elevating existing cellular therapies – treatments where living cells are engineered to fight disease and then are administered to patients – to the next level of sophistication. De Greef: "First-generation cellular therapies are in the clinic, but these are relatively simple. They are programmed to detect single antigens and, in a limited way, destroy diseased cells." The collaborators will focus on engineering designer cells to recognize and respond to multiple antigens resulting in targeted and more accurate therapies. This generation of smarter cellular therapies would be responsive and capable of tackling cancer cells that are constantly adapting to survive and outwit anti-cancer therapies. "It's a kind of engineered intellectual match between the therapy and the cancer cell," says De Greef.

POLICING THE MICROBIAL SOUP

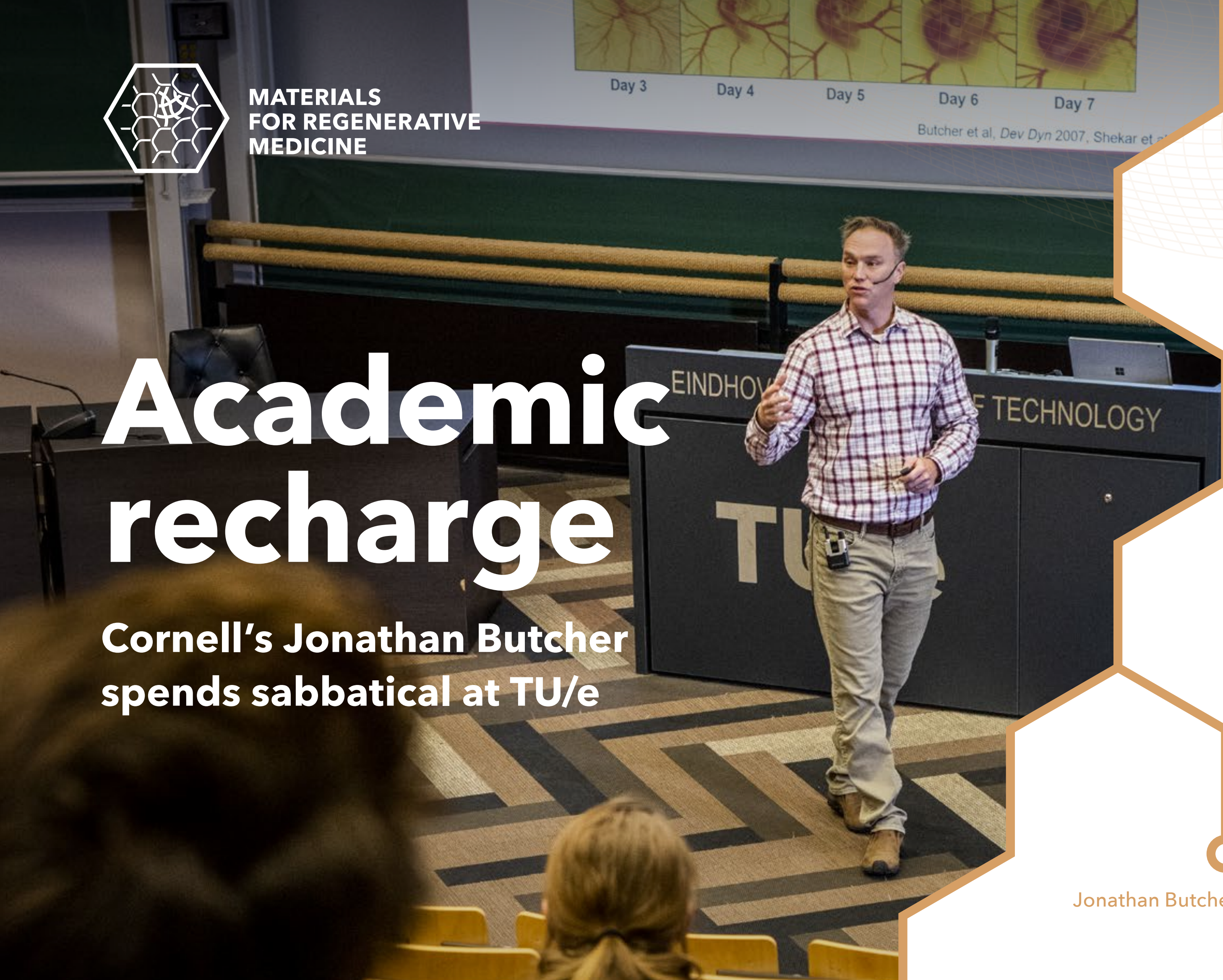
Humble and often overlooked microbes could help to solve the biggest problem facing humanity today: global warming. Professor of microbiology at WUR, Diana Machado de Sousa knows that a side effect of culturing certain microbes in a mix, is the conversion of greenhouse gases into biomass. Using such a microbial mix or microbial soup to "eat" carbon emissions and produce a sustainable biofuel could be an important tool in reducing atmospheric CO_2 levels and thus counter global warming.

Unfortunately, the unstable nature of the mixture hampers large-scale application of microbial soups. De Greef: "Combining specific microbes produces this very welcome side effect, but their very co-existence also leads to each species influencing the other. That makes the combined culture unstable, destructive and volatile and thus unfit to be used at scale." He has an insightful metaphor at hand: "It's a bit like toddlers at an unsupervised party. It can all go great for a while, but at some point, things are pretty sure to take a turn for the worse." Together with Machado de Sousa, De Greef is engineering so-called policing microbes (comparable to parents at the party) who can control microbial interactions by detecting certain signals. "Receiving a signal that one species is growing too fast will trigger the policing microbe to send a stop signal, thus slowing down the overactive growth," explains De Greef. Adding such an engineered police force will result in a stable product that can be part of the toolkit to help combat global warming.

JUST AN ENGINEER

Without the deep commitment to collaboration and the structure provided through the living technologies collaboration, these projects would not be possible. "I am just an engineer," says De Greef. "I taught myself how to modify organisms, so for me it's easy to apply this to different societal problems." Beyond joint projects, this collaboration is also focused on training the next generation of scientists, sharing facilities and stimulating spin-off collaborations. The return on investment of a collaboration like this is predicted to be significant and long lasting with ripple effects that will spread across the scientific community and stimulate further advancements for society.

MATERIALS
FOR REGENERATIVE
MEDICINE



Jonathan Butcher

Academic recharge

Cornell's Jonathan Butcher spends sabbatical at TU/e

For twenty years, Jonathan Butcher (Cornell University, USA) and TU/e's Carlijn Bouten have been working together to further our basic understanding of the heart and develop innovative, regenerative therapies for cardiovascular diseases. Taking their professional association to a new level, Butcher is now three months into a one-year sabbatical at TU/e. In this article, we hear more about his research and what he hopes to gain from his year in The Netherlands. "I want to look at the TU/e model of partnerships and understand how PI's work together here."

At TU/e, Jonathan Butcher, professor of Biomedical Engineering at Cornell University (USA), is hosted by the Materials Regenerative Medicine group. Butcher's approach to studying regenerative medicine through a developmental mechanobiology paradigm is complemented by the deep knowledge of materials-driven engineering present in Eindhoven.

EMBRYONIC UNDERSTANDING

To understand how to regenerate human tissue and find therapies for diseases, Butcher tracks the biomechanical development of one of the body's most complex organs: the heart. Studying the heart in its embryonic stages, he aims to uncover the mechanics involved in the assembly and maturation of cardiac tissue. Studying and manipulating the mechanical forces at play in embryonic development of the heart is, in Butchers own words, "a kind of 'one-stop-shop method' for discovering information about how heart tissue grows, matures, stabilizes, becomes diseased and regenerates." To study this mechanobiological development in action, Butcher works with chicken embryos. "Within one week we can see the heart developing in the chicken embryo, it grows a hundred times in size from a simple tubular form to a fully formed heart." The sheer amount of engineering taking place within a week has never been replicated in the lab, says Butcher. "This window into dynamic cardiac development is transformational for our fundamental understanding of how the heart is engineered into existence."

COLLECTIVE CREATION

Understanding all the underlying, collective mechanical interactions of a developing and growing heart is an important focus area for Butcher. "With so much complex engineering happening within the embryonic heart, there are many parallel processing and feedback loops occurring that are not fully understood." Working at the mesoscale (one step up from the cellular level), Butcher's goal is to gain insight into the mechanobiological processes taking place in heart tissue so that he can paint a clearer picture of the mechanical interactions between the various components of the heart. He hopes that studying this fundamental collective mechanobiological behavior will reveal how the heart is able to develop with such speed and precision. It will also extend the already rich body of knowledge on how genetics play a role in heart development and health. Unlocking these mechanobiological developmental secrets will contribute to understanding which non-genetic mechanisms are involved in congenital heart defects and myocardial infarctions. Butcher is confident that his work can help guide the engineering of living replacement tissues and thus enhance the field of regenerative medicine. "We aim to develop therapies that can have an influence on the mechanobiology of the heart ensuring that its growth, maturation and stability are positively affected."

EXCHANGE PROGRAMS

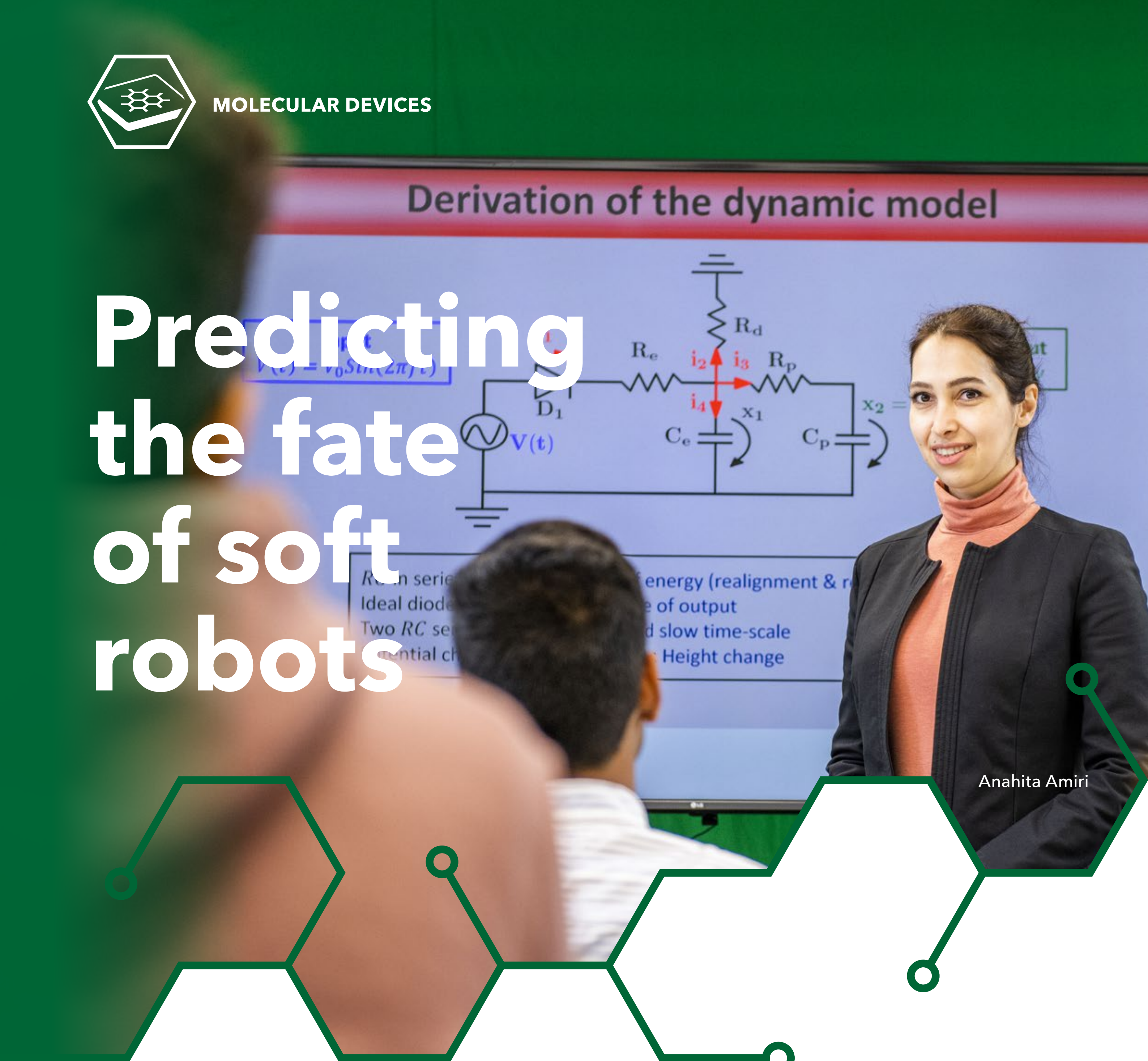
For Butcher, research is only one aspect of this sabbatical year. "Yes, I bring a developmental mechanobiology perspective to regenerative medicine that is complementary to the materials expertise of Carlijn and her team, but for me it is broader than that." He explains that part of the appeal of spending time at TU/e is experiencing the university's collaborative approach. "I want to look at the Eindhoven model of partnerships, understand how different PI's work together, witness the co-working between universities and explore how TU/e works with industry." Butcher also hopes to learn from the way education is organized at TU/e and he sees potential for setting up future exchange and semester-abroad programs with Cornell University. "As well as a researcher, I am also an educator with a deep interest in pedagogy and so I am thrilled to be exposed to the TU/e way of doing things." And last but not least, he explains how this sabbatical is an opportunity to recharge and reboot his academic batteries. Freed from the responsibilities he undertakes at Cornell, Butcher now has the space to be truly in the moment, absorb knowledge and share his expertise.

"I'M THRILLED TO BE EXPOSED TO THE TU/E WAY OF DOING THINGS"

Carlijn Bouten

MOLECULAR DEVICES

Predicting the fate of soft robots



Anahita Amiri

Soft robotics is an emerging field that aims to develop adaptive soft materials, often responsive to certain stimuli such as light or electricity. But how can we manipulate these materials to exhibit the right behavior? PhD student Anahita Amiri works at the interface of mechanical and chemical engineering to address this complex question. "The combination of smart materials and dynamic modeling can generate exciting applications."

In her PhD project entitled "Dynamic models for electro-active surface deformations in smart coatings," Anahita Amiri embarks on an interdisciplinary journey. Being involved both in the Dynamics and Control group at the Mechanical Engineering department and the Stimuli-responsive Functional Materials & Devices group in the Chemical Engineering department, Amiri has to keep an open mind about the different views of these two areas. "It is important to learn how to look at this topic from various angles without bias. The challenge of this multidisciplinary research lies in bringing the two views together."

Although it's not the first collaboration between the two departments, ICMS mediated the start of Amiri's research. Ines Lopez Arteaga, professor in the Dynamics and Control group, remembers the kick-off. "I had a meeting with Monique Bruining, managing director of ICMS, and she asked me if I would like to brainstorm about a possible collaboration with a researcher at the chemistry department who works on soft robotics. We quickly identified the possibilities to work together, and so the project began." That researcher is Danqing Liu, assistant professor in the Stimuli-responsive Functional Materials & Devices group. "I was happy to learn that someone was interested in the materials we developed in the past," says Liu, "it's nice to see how these materials can be optimized from a modeling perspective."

MISSING LINK

Taken together, the aim is to develop a dynamic model to control the behavior of smart surfaces for soft robotics. "If you look into traditional robotics, it's all about precision control," says Liu. "However, in materials science, the focus lies on the input and output. Precision control is missing. The idea behind this project is to create a link between robotics and materials science." Lopez Arteaga agrees: "That's exactly what we are trying to do here, to bridge the gap. From our perspective, the work starts after the development of a functional material. For the application in soft robotics, you need to be able to predict how a material will respond to a stimulus. For example, how much it will deform. For that, you need a model that can predict the material's behavior." She emphasizes that this will not happen in one go. "Most likely, the first model will not be perfect, so you need to measure what the motion actually is after you apply a certain input. This is an iterative process, going back and forth between model and experiment until you get the motion prediction right. And only then when you have this, you have a robot."

Anahita Amiri's background in polymer engineering contributes an essential perspective to this challenge. "It is very interesting to investigate materials science from a modeling perspective. Indeed, it feels really satisfying to see that we are bringing two fields of science together. Only then can you work towards a property you actually desire of a material," Amiri explains. "Scientists often develop responsive materials without knowing how to control their behavior upon a certain input. This makes it very difficult to turn into an application. The link between developing a smart material and developing a potential application lies in the dynamic modeling of the material."

ELECTRO-ACTIVE COATINGS

During her PhD, Amiri concentrates on a specific property. "Smart materials can be activated by many inputs such as light and electricity. For now, the material we have chosen to work on is an electro-active coating. Electricity is very interesting because it's clean, you can use it remotely and it can be automated. Additionally, you can easily integrate it in an electrical device, for example, in touchscreens." Electricity is also more convenient from an application standpoint, says Lopez Arteaga. "For many practical applications, such as the movement of a robotic hand, an electrical actuation is easier than the application of light. Since you want to develop a model that will help you control the movement, you need to think beforehand about what inputs are feasible in practice." But what is the perfect electro-active material? "In my opinion there is no perfect material," Liu states. "It really depends on the intended application. At the moment, we work mainly on liquid crystals, but we have different materials based on the desired properties. For example, if you want faster deformation, then you need to choose a more elastic material. If we need an anisotropic deformation, then liquid crystals are a good choice. This is how we start at a technical university; we consider the application we want."

SIZE MATTERS?

"The electro-active coating itself is a few micrometers thick," specifies Amiri. "However, the deformation of the material can be as small as hundreds of nanometers. The scale matters, but it doesn't necessarily need to be observable by the eye. The deformation just needs to be enough to trigger a feedback." Translating these small changes to a bigger scale is a different challenge, according to Amiri. "You can simulate the scaling up of this material, but in practice it is more difficult." Lopez Arteaga knows why. "If you increase the coated surface, there are additional aspects to consider. For example, you need to know how uniform the material really is." And with this, future research incentives are created. Liu: "How you use the simulation to model the scale of this material is rather interesting. I would like to later discuss that with you both." But first things first. "We are really at the beginning of this kind of research," explains Lopez Arteaga. "First, we need to see that the model we have is working for the scale we are investigating."

Solving puzzles to find solutions

Dick Broer

It already started as a festive day. On September 16, the Functional Materials and Devices research group celebrated its 10-year anniversary with a big reunion. A great way for former students and researchers to catch up on old times and exchange current ideas and activities. But the day turned into a truly extraordinary event when, after his closing lecture, professor Dick Broer was presented with a royal distinction to become "Knight in the Order of the Lion of the Netherlands." The oldest and highest Dutch civilian order of chivalry.

You didn't see it coming?
"Oh no, it was an absolute surprise. I was the last speaker of the day and I did notice that there were many questions from the audience and it seemed as if this was actively stimulated, more than usual. And then the mayor walked on stage and suddenly I saw my family in the audience and on the screen behind me, from Canada, and then I knew something was going on. I was overwhelmed and it was very touching to realize that so many people took the effort to make this happen."

A recognition of a distinguished research career in both industry and academia that spans almost fifty years. What do you see as the main differences between these two worlds?
"Freedom and money. Here at the university, the upside is that you are completely free to pursue your own research interests, but you also have to realize the funding for every single project. That is a serious downside because it means a high administrative workload on top of the actual scientific work. Another difference is the endpoint of the research. In academia, you aim for a proof-of-principle, publish a nice paper in a top journal and that's usually where it ends. Whereas in industry, the track goes on and you can easily take the next steps towards, for example, development of a prototype. That is what I missed at the university, this whole environment that you have in industry to take your findings to the next level."

When it comes the science, what is on your mind these days? What kind of questions grab your attention?
"I'm still fascinated by the idea of communication between materials and systems. How can we transduce signals from one material to other? Can we realize neural networks in our materials? The key issue remains whether and how a material can perceive a signal and formulate a response."

Why are you intrigued by this question?
"It is no so much the question, but the search for solutions that I find interesting. New puzzles pop up again and again and I like solving those. It's like a crypto puzzle."

And you're a crypto fan?
"Yes, I get to work every Saturday when the newspaper arrives."

ICMS Fellowship for Shikha Dhiman

Shikha Dhiman

"Trying to understand nature and translate it into synthetic systems" – from the moment Shikha Dhiman was introduced to supramolecular chemistry during her master studies in India she knew she wanted to build a career in that field. Dhiman joined the ICMS community in 2020 as a postdoc in the group of Bert Meijer to work on the design of supramolecular biomaterials as extracellular matrices. In September 2021, she was awarded an ICMS Fellowship.

Dhiman aims to develop synthetic supramolecular materials that stabilize stem cells and steer their differentiation towards, ultimately, organoids and even organs of interest. "Supramolecular materials are very dynamic and hard to study," says Dhiman. But luckily for her, the necessary technology is nearby in the group of Lorenzo Albertazzi (Biomedical Engineering). "I am using superresolution microscopy to look at the interface and first point of interaction between the supramolecular extracellular matrices and the cells."

SEE THE INTERACTIONS

Over the years, many synthetic ECM systems that failed to stabilize stem cells have been discarded, without ever really knowing what went wrong. The new microscopy approach can offer more insight. "We can now see, on the molecular level, how the synthetic supramolecular biomaterial and the cell surface interact. That provides a better understanding of the materials." First, Dhiman is testing the supramolecular ECM with a supported lipid bilayer, a cell surface mimic. "We need dynamic materials with ligands that can rearrange, as the receptors on the cell surface are in constant motion." She will next test her materials using stem cells; a collaboration with the Technical University Munich, made possible by the Eurotech fellowship she was granted this year.

September 2021, Dhiman was granted an ICMS Fellowship, a special recognition from the institute and a great opportunity to start building the academic career she dreams of. She immediately experienced the vast networking possibilities this distinction affords. "The very moment I became an ICMS fellow, people started reaching out to me." According to Dhiman, the exchange of ideas is a key element in the ever more professionalized academia. "The ICMS fellowship also includes grants to travel for research and conferences and the organization of events where I will have responsibilities." A range of activities that Dhiman hopes to use for both personal and scientific growth.

ADVANCED ANALYSIS OF COMPLEX MOLECULAR SYSTEMS

High-level support for visualization issues

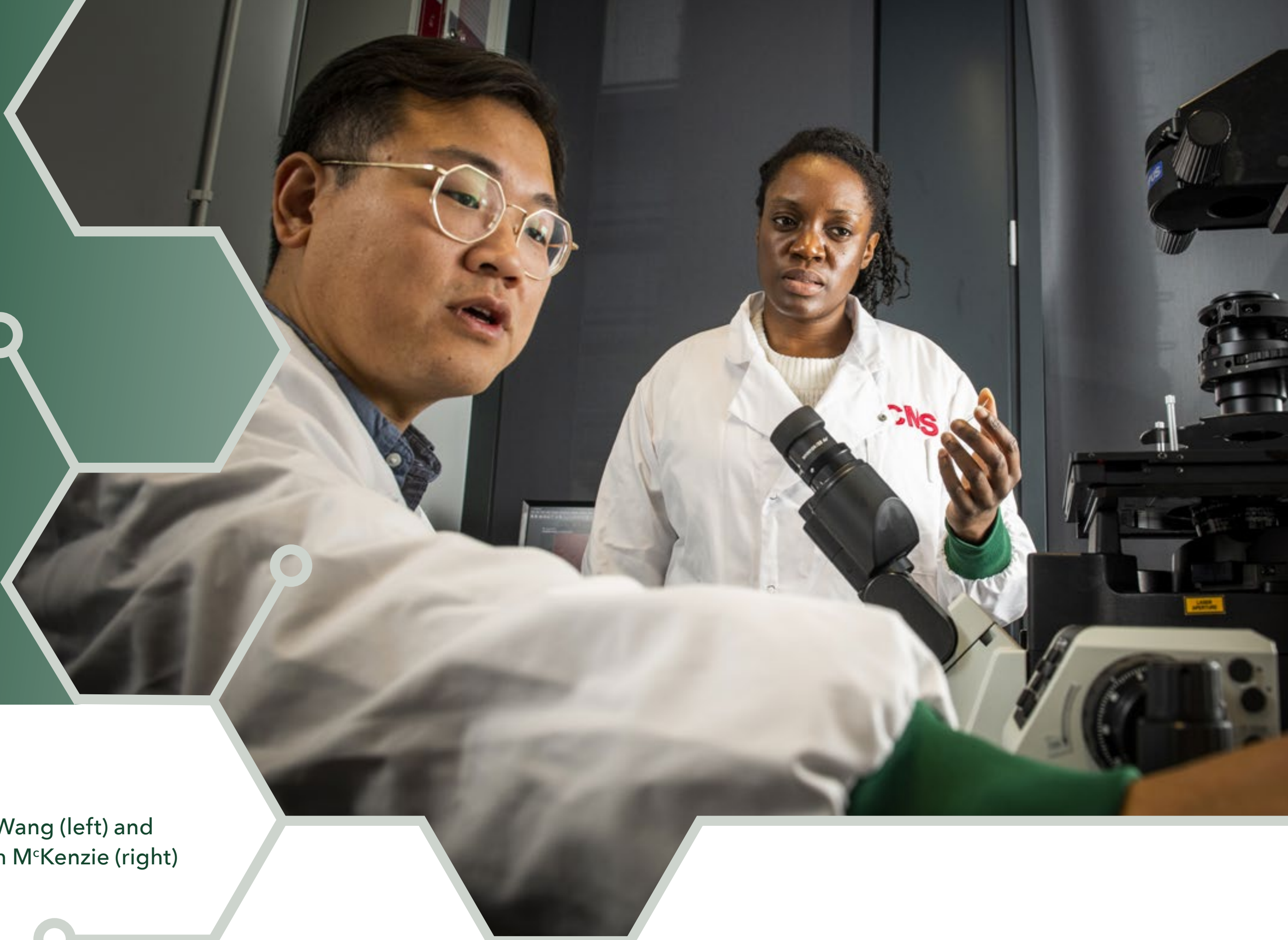
Yuyang Wang is the new Microscopy Facilities Manager

Advanced Analysis of Complex Molecular Systems is a fundamental part of the ICMS activities. It is destined to provide a new, advanced toolbox for all researchers working on advanced materials. Both within and outside ICMS. By working on research challenges that ICMS researchers are facing, current visualization techniques will be pushed forward. Yuyang Wang and Elizabeth McKenzie explain the need for this new facility and why we need higher resolution – spatial and temporal. "What we need is a correlative approach that allows us to connect the information gathered from different techniques."

"Simply put, at ICMS it is all about fiddling on the molecular level," Elizabeth McKenzie kicks off. "Everyone here is trying to understand how events at the molecular level lead to the properties and behavior we observe in materials. To achieve that, you really need to see what is happening on the molecular scale." To accommodate these needs, the ICMS portfolio has a dedicated focus area: Advanced Analysis of Complex Molecular Systems, in which cutting-edge visualization techniques play a leading role. "This is an integral part of ICMS, because it enables the research in all the other focus areas," says McKenzie, who as Business Engagement and Research Development Manager is closely involved in embedding these activities internally as well as in reaching out to industrial parties to show what ICMS has to offer.

DYNAMIC ENTITIES

The new effort will be spearheaded by Yuyang Wang, who was recently appointed as the Microscopy Facilities Manager. "Every group within ICMS works on different systems, different materials and different questions, but they all need visualization techniques," he says. Wang emphasizes that although a very detailed view of the structure, shape and composition of materials is essential, truly deep understanding of molecular behavior is impossible without considering the dynamics on the molecular scale. "Molecules are not static, but highly dynamic entities and those dynamics determine their behavior on much larger scales. You need to visualize the dynamics as well. So, next to ongoing technology development to improve spatial resolution, we need serious improvements in temporal resolution." McKenzie points out that technology development is at the heart of the new facility. "A massive part of this effort is about pushing the technology further, not only to improve spatial and temporal resolution, but also to 'stitch' the different scales together. How does what we observe on the nanoscale translate to behavior on the micron scale? These are key issues that we aim to address."



Yuyang Wang (left) and
Elizabeth McKenzie (right)

CONNECT INFORMATION

That will require the design of both hardware and software that allows such stitching. One way to achieve that is to develop ways to use the same sample in different equipment, so you are really looking at the exact same spot with different techniques. But that is not always feasible, because some techniques are quite destructive. That is why Wang focuses on another way to extract more information from various measurements. “What we need is a correlative approach that allows us to connect the information gathered from different techniques. For example, cryoEM offers extremely high resolution, but the sample is frozen which means there is no information on the dynamics. Super-resolution microscopy can reveal the dynamics, but offers lower resolution. We need to figure out how to combine the outcomes of the two techniques in such a way that we get a robust, reliable view of both the spatial properties and dynamics. As if the two were measured together.”

MORE FUN

Clearly, these are multidisciplinary issues that Wang cannot tackle on his own. The idea is that through collaboration with various groups within ICMS, Wang gains input to continuously push the technology ahead. But can anyone just drop a question? Is there a selection procedure? “At the moment, it is all quite informal,” says Wang. “Researchers get stuck with a problem that requires some form of advanced visualization, they get in touch and then we start talking. They tell me about their research, I share what the technology has to offer, we exchange data and ideas. It is really about communication. Together, we devise a pilot plan to see what could be possible and depending on the outcomes, we take the next steps. But talking openly is really important to get to the heart of the large problem.” For Wang, this way of working means that he is exposed to a high variety of research topics. Which happens to be exactly what he likes best.

“WE NEED SERIOUS IMPROVEMENTS IN TEMPORAL RESOLUTION”

“I am very interested in the multidisciplinary nature of science. Research gets more and more specialized, but I really like to talk to people with different backgrounds on different questions. To me, that is more fun than devoting all my time to one specific subject.” According to McKenzie, this is exactly what ICMS is about. “We like to keep the pot stirring and stimulate exchange. Also with external parties. We want to position ourselves as the ‘go to’ partner in advanced analysis and characterization, which is to become an integral part of everything. It is the new toolbox. If we want to improve existing materials and design and create new ones, we need to take on this technological challenge.”

Introducing three EuroTech postdocs within ICMS

EuroTech Postdoc: **Mariia Efremova**

As a EuroTech postdoc, Mariia Efremova will develop a platform based on designer synthetic antiferromagnetic nanoplatelets (SAF-NPs) for targeted and remote magneto-mechanical actuation of ion channels involved in cancer progression. The project, called ChannelControl, is a collaboration between the Physics of Nanostructures group of Reinoud Lavrijsen at TU/e, and the Neurobiological Engineering group of Gil Westmeyer at the Technical University of Munich. The key to successful implementation of ChannelControl is to deploy the synergy between the reproducible nanofabrication of SAF-NPs actuated by original 3D magnetic field setups at TU/e and the unique expertise in mammalian cell bioengineering at TUM. ChannelControl is expected to create synergy with, in particular, the Immunoengineering program but also in the network of ICMS.

During her PhD research at Lomonosov Moscow State University, Efremova acquired expertise in the synthesis, characterization, and biomedical application of magnetic nanoparticles. In 2019-2021, she was a Humboldt Research Fellow at the Technical University of Munich and Helmholtz Zentrum Munich. There, she developed genetically controlled magnetic nanocompartments in living cells and got skilled in bioengineering and cell and molecular biology.

EuroTech Postdoc: **Eva Judy**

Eva Judy completed her PhD at the Indian Institute of Technology Bombay, where she worked on understanding the partitioning and encapsulation of drugs in micellar and vesicular systems and explored their interactions with biomolecules. These insights facilitated her in understanding how drugs and model drug delivery systems interact. Building on the experience gained, Judy focused on the development of targeted drug delivery systems composed of protein biomolecules aimed for chemotherapeutics. In her EuroTech project, Judy aims to develop protein based nanocarriers conjugated with cancer targeting peptides, which can show enhanced

retention and sustainable release of drugs as well as target-oriented delivery of chemotherapeutic drugs. To enhance the biocirculation of the systems and increase the efficiency polymers will be included in the systems. The work will also involve a combination of biophysical and biochemical assays. The project is a collaboration between the groups of Remco Tuinier at TU/e and Christine Papadakis at the Technical University Munich, who contributes expertise in development of drug delivery systems and their analysis.

Shikha Dhiman

Recently appointed ICMS Fellow Shikha Dhiman is also a EuroTech postdoc; read more about her research on page 11.

Key publications

APRIL 2021 – OCTOBER 2021

01. A PLUG-AND-PLAY PLATFORM OF RATIOMETRIC BIOLUMINESCENT SENSORS FOR HOMOGENEOUS IMMUNOASSAYS
Y. Ni, B.J.H.M. Rosier, E.A. van Aalen, E.T.L. Hanckmann, L. Biewenga, A.-M. Makri Pistikou, B. Timmermans, C. Vu, S. Roos, R. Arts, W. Li, T.F.A. de Greef, M.M.G.J. van Borren, F.J.M. van Kuppeveld, B. Bosch, M. Merkx
Nat. Commun. 12, 4586 (2021)

02. BIODEGRADABLE POLYMERSOMES WITH STRUCTURE INHERENT FLUORESCENCE AND TARGETING CAPACITY FOR ENHANCED PHOTO-DYNAMIC THERAPY
S. Cao, Y. Xia, J. Shao, B. Guo, Y. Dong, I.A.B. Pijpers, Z. Zhong, F. Meng, L.K.E.A. Abdelmohsen, D.S. Williams, J.C.M. van Hest
Angew. Chem. Int. Ed. 60, 17629-17637 (2021)

03. BOTTOM-UP DE NOVO DESIGN OF FUNCTIONAL PROTEINS WITH COMPLEX STRUCTURAL FEATURES
C. Yang, F. Sesterhenn, J. Bonet, E.A. van Aalen, L. Scheller, L.A. Abriata, J.T. Cramer, X. Wen, S. Rosset, S. Georgeon, T. Jardetzky, T. Kreys, M. Fussenegger, M. Merkx, B.E. Correia
Nat. Chem. Biol. 17, 492-500 (2021)

04. CORRELATING SUPER-RESOLUTION MICROSCOPY AND TRANSMISSION ELECTRON MICROSCOPY REVEALS MULTIPARAMETRIC HETEROGENEITY IN NANOPARTICLES
T. Andrian, P. Delcanale, S. Pujals, L. Albertazzi
Nano Lett. 21, 5360-5368 (2021)

05. DETERMINANTS OF LIGAND-FUNCTIONALIZED DNA NANOSTRUCTURE-CELL INTERACTIONS
G.A.O. Cremers, B.J.H.M. Rosier, A. Meijs, N.B. Tito, S.M.J. van Duijnhoven, H. van Eenennaam, L. Albertazzi, T.F.A. de Greef
J. Am. Chem. Soc. 143, 10131-10142 (2021)

06. DUROTAXIS OF PASSIVE NANOPARTICLES ON ELASTIC MEMBRANES
I. Palaia, A. Paraschiv, V.E. Debets, C. Storm, A. Saric
ACS Nano 15, 15794-15802 (2021)

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S. Vermeulen, F. Honig, A. Vasilevich, N. Roumans, M. Romero, A. Dede Eren, U. Tuvshindorj, M. Alexander, A. Carlier, P. Williams, J. Uquillas, J. de Boer
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12. MACHINE LEARNING OF QUASIPARTICLE ENERGIES IN MOLECULES AND CLUSTERS
O. Caylak, B. Baumeier
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13. ONCOGENIC RAS INSTRUCTS MORPHOLOGICAL TRANSFORMATION OF HUMAN EPITHELIA VIA DIFFERENTIAL TISSUE MECHANICS
A. Nyga, J.J. Munoz, S. Dercksen, G. Fornabaio, M. Uroz, X. Trepat, B. Baum, H.K. Matthews, V. Conte
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14. PHOTOACTIVATED NANOMOTORS VIA AGGREGATION INDUCED EMISSION FOR ENHANCED PHOTOTHERAPY
S. Cao, J. Shao, H. Wu, S. Song, M. Teresa De Martino, I.A.B. Pijpers, H. Friedrich, L.K.E.A. Abdelmohsen, D.S. Williams, J.C.M. van Hest
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15. REVERSIBLE COVALENT IMINE-TETHERING FOR SELECTIVE STABILIZATION OF 14-3-3 HUB PROTEIN INTERACTIONS
P.J. Cossar, M. Wolter, L. van Dijck, D. Valenti, L.M. Levy, C. Ottmann, L. Brunsveld
J. Am. Chem. Soc. 143, 8454–8464 (2021)

16. ROBUST ANGULAR ANISOTROPY OF CIRCULARLY POLARIZED LUMINESCENCE FROM A SINGLE TWISTED-BIPOLAR POLYMERIC MICROSPHERE
O. Oki, C. Kulkarni, H. Yamagishi, S.C.J. Meskers, Z. Lin, J. Huang, E.W. Meijer, Y. Yamamoto
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17. SPIN FILTERING IN SUPRAMOLECULAR POLYMERS ASSEMBLED FROM ACHIRAL MONOMERS MEDIATED BY CHIRAL SOLVENTS
A.K. Mondal, M.D. Preuss, M.L. Sleczkowski, T.K. Das, G. Vantomme, E.W. Meijer, R. Naaman
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18. SUPRAMOLECULAR ENHANCEMENT OF A NATURAL 14-3-3 PROTEIN LIGAND
X. Guillory, I. Hadrovic, P.J. de Vink, A. Sowislok, L. Brunsveld, T. Schrader, C. Ottmann
J. Am. Chem. Soc. 143, 13495–13500 (2021)

19. THE CURRENT LANDSCAPE OF NUCLEIC ACID THERAPEUTICS
J.A. Kulkarni, D. Witzigmann, S.B. Thomson, S. Chen, B.R. Leavitt, P.R. Cullis, R. van der Meel
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20. TORSIONAL FRACTURE OF VISCOELASTIC LIQUID BRIDGES
S.T. Chan, F.P.A. van Berlo, H.A. Faizi, A. Matsumoto, S.J. Haward, P.D. Anderson, A.Q. Shen
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21. TRANSLATING 2D DIRECTOR PROFILE TO 3D TOPOGRAPHY IN A LIQUID CRYSTAL POLYMER
P. Lv, Y. You, J. Li, Y. Zhang, D.J. Broer, J. Chen, G. Zhou, W. Zhao, D. Liu
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22. WAVELENGTH-SELECTIVE PHOTOPOLYMERIZATION OF HYBRID ACRYLATE-OXETANE LIQUID CRYSTALS
D.C. Hoekstra, B.P.A.C. van der Lubbe, T. Bus, L. Yang, N. Grossiord, M.G. Debije, A.P.H.J. Schenning
Angew. Chem. Int. Ed. 60, 10935-10941 (2021)

New ICMS member: Francesca Grisoni

Francesca Grisoni (Como, Italy) joined TU/e early 2021 as assistant professor in the Chemical Biology group (Biomedical Engineering), where she leads the Molecular Machine Learning team. Grisoni studied environmental sciences with a focus on molecular modeling. During her masters studies, she got into chemometrics and statistical learning – what we now call "machine learning." She went on to use these methods in her PhD to predict various molecular properties such as toxicity for prioritization purposes. After briefly working as a data scientist for a startup and as a biostatical consultant for a pharmaceutical company, she joined ETH Zürich as a postdoc. There, she started applying machine learning to drug discovery, particularly to design molecules with tailored biological properties.

Her research focuses on Artificial Intelligence (AI) for drug discovery. "My work targets the initial phases of drug discovery. I develop and apply methods to efficiently navigate the vast chemical universe, containing up to 10^{60} molecules that could potentially be synthesized and tested. By training the models on available molecular data, they 'learn' to generate new promising molecules and/or predict their biological targets. The goal is to augment human intuition by designing better molecules faster, compared to traditional laboratory-based trial and error."

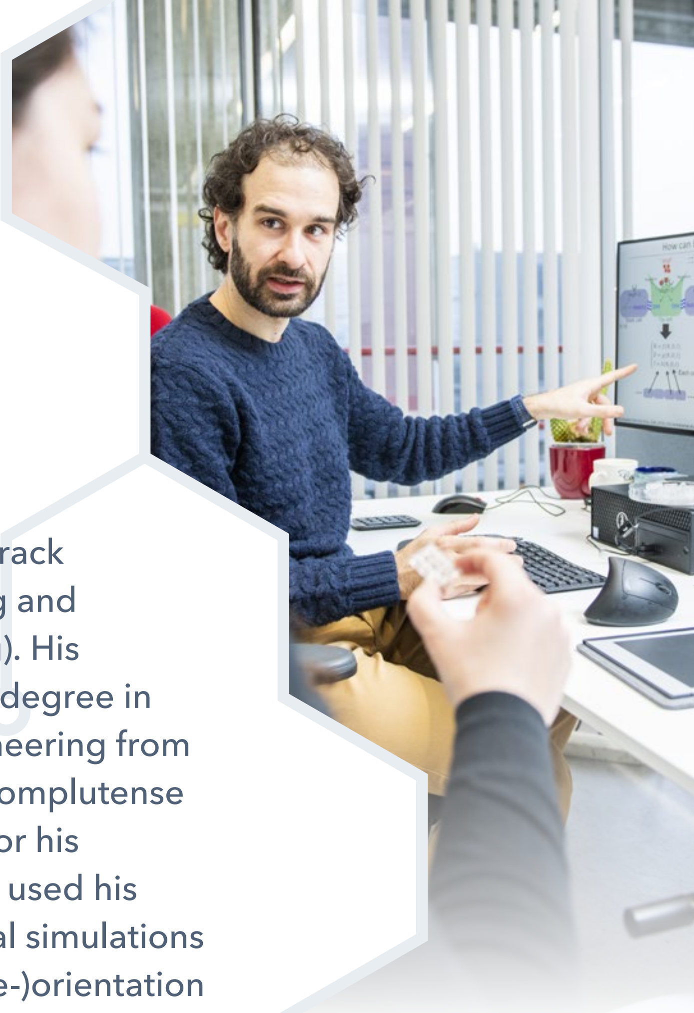
In the future, she aims to collaborate with experimentalists to improve and validate the new algorithms for specific disease applications. "For instance, together with Luc Brunsveld, we will apply these AI approaches to aid the design of novel bioactive molecules for relevant drug targets such as nuclear receptors."

ENHANCE HUMAN INTELLIGENCE

Grisoni joined ICMS as soon as she started at TU/e. With her background in molecular machine learning, chemo informatics and (bio)chemistry, and as a new PI building an interdisciplinary group at the interface between chemistry, biology and computer science, she fits right in. "AI is becoming increasingly relevant. Scientists have been collecting enormous amounts of high-quality data in the past decades. Now is the time to use that data to build models that can generate solutions faster and cheaper, both in the biomedical field and beyond." She is looking forward to collaborations within the institute at the interface between experiments and computations. "AI bears the potential to enhance human intelligence in navigating complex high-dimensional data and to provide innovative answers to specific research questions."

Francesca Grisoni

New ICMS member:
Tommaso Ristori



Tomasso Ristori

Tommaso Ristori has been appointed as tenure-track assistant professor in the Soft Tissue Engineering and Mechanobiology group (Biomedical Engineering). His background is in mathematics; he earned a joint degree in theoretical mathematics and mathematical engineering from the University of Florence and the Universidad Complutense de Madrid. Ristori moved to Eindhoven in 2013 for his PhD. Under the supervision of Frank Baaijens, he used his theoretical background to work on computational simulations of cell-mediated collagen remodeling and cell (re-)orientation in response to mechanical and topographical stimuli. As a postdoc, he was awarded the NWO Rubicon Fellowship and the Marie Skłodowska-Curie Global Fellowship, which enabled him to expand his research with experimental work. In the group of Christopher Chen at Boston University, he performed experiments with endothelial cells on 2D substrates and in 3D microfluidic devices, to mimic angiogenesis *in vitro*.

His current research at TU/e builds upon his postdoctoral experience. "Controlling angiogenesis is important in both regenerative medicine and in cancer therapy. In the first case, we want to stimulate physiological blood vessel formation, but in the other we want to prevent it. My goal is to develop experimentally-informed and validated computational models that can predict vascular formation under different conditions. In the future, I aim to use machine learning as a tool to combine models and experiments to predict this process."

Besides unravelling the most important parameters to consider when trying to spatially control angiogenesis via micro-contact printing of cell-cell signaling proteins, he is also working to understand the temporal dynamics of the signaling pathways involved, both with experiments and simulations.

VESSEL TOPOLOGY

Ristori has been involved in ICMS since he started his PhD project in 2013 and is now part of the ICMS immunoengineering program.

"What connects me to ICMS is complexity. This is an essential aspect of angiogenesis, as it is a process that is influenced by several factors and small variations can lead to large differences in vessel topology." Furthermore, as in ICMS, multidisciplinarity is central in his research. "I work at the interface of mathematics, mechanics, and biology and ICMS offers me the possibility to interact with other members and establish future collaborations across these disciplines."

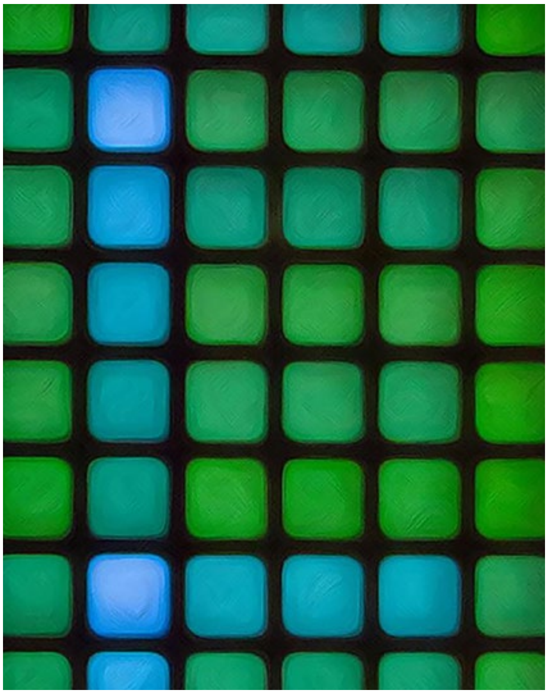
News, awards & grants

Nanostructured siloxane-based materials for novel plastics and microelectronics

BRIGITTE LAMERS DEFENDED HER PHD THESIS ON THE INTERPLAY OF PHASE SEGREGATION AND SUPRAMOLECULAR INTERACTIONS.

The self-organization of molecular components into hierarchically ordered nanostructures is an essential part of the development of new materials for emerging nanotechnologies and sustainable plastics. Brigitte Lamers investigated the complex interplay between molecular driving forces in bulk assembly to find structure-property relationships in the area that merges block copolymers and liquid crystals. She defended her PhD on June 23rd.


Brigitte Lamers


Source: Bas Rosier and Maarten Merkx (TU/e).

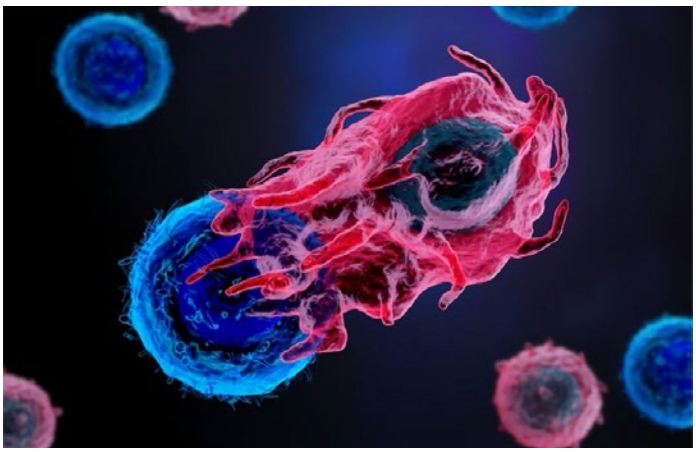
A molecular traffic light for infectious diseases

NEW SENSOR WITH BIOLUMINESCENT PROTEINS INDICATES PRESENCE OF ANTI-DRUG ANTIBODIES AND MOLECULES ASSOCIATED WITH COVID-19 IN BLOOD.

Home test kits to check for COVID-19 spike proteins and anti-COVID-19 antibodies are fast and simple to use, but lack the sensitivity and accuracy of laboratory tests. Researchers from Eindhoven University of Technology and Utrecht University have developed a new type of sensor that combines the sensitivity and accuracy of current laboratory-based measurements with the speed and low-cost of current home tests. The new sensor uses a “glow-in-the-dark” signal to indicate the presence of tiny amounts of proteins and anti-drug antibodies, as well as COVID-19 spike proteins and antibodies in blood. The results have been published in Nature Communications (see key publication 1).

Machine learning helps to predict when immunotherapy will be effective

IMMUNOTHERAPY AND MACHINE LEARNING JOIN FORCES TO HELP THE BODY'S IMMUNE SYSTEM CRACK ONE OF ITS GREATEST MYSTERIES – HOW TO FIND HIDDEN TUMOR CELLS IN THE HUMAN BODY.



Source: Shutterstock

Our immune system is tasked with a key role – find and eliminate foreign invaders such as bacteria or viruses, but it also tackles threats inside the body such as cancer. But cancer cells have developed clever ways of avoiding destruction by switching off immune cells during their search. Immunotherapy can reverse the process, but it doesn't work for all patients and cancer types.

Researchers at Eindhoven University of Technology have turned to machine learning to solve the riddle. Thanks to a small trick, they've created a model to predict if immunotherapy will work for a patient. The model even performs better than current clinical approaches. This innovative new work has been published in the journal Patterns.

TU/e to acquire top electron microscope

"THIS DONATION FROM DAF PACCAR WILL ENHANCE TU/E ADVANCED RESEARCH AND DEVELOPMENT IN THE LIFE SCIENCES AND MATERIALS SCIENCES."

DAF President Harry Wolters (left) hands over a framed illustration to TU/e President Robert-Jan Smits, for the 65th anniversary of TU/e. The illustration, an image created with an electron microscope, symbolizes the donation of DAF to TU/e. Photo: Odette Beekmans.

The TU/e is pleased to announce a generous donation from DAF Trucks and the PACCAR Foundation to acquire a world-class electron-microscope for soft matter research.

Robert-Jan Smits, president of the Executive Board of Eindhoven University of Technology shared: "The university thanks DAF Trucks and the PACCAR Foundation for its generous donation, which will enhance TU/e advanced research and development in the life sciences and materials sciences. The acquisition of the sophisticated soft matter electron-microscope and technical laboratory equipment is very important as universities and medical centers accelerate research to develop solutions to global health and material issues. DAF founder Hub van Doorne was among the early leaders to recognize the benefits of establishing TU/e. The university was founded in 1956 and is celebrating 65 years of excellence."

Monique Bruining

ICMS Onboarding sessions:

Off to a good start

A warm welcome to new members of the ICMS community. With that in mind, Monique Bruining and the ICMS team initiated the onboarding sessions. Starting in January 2022, this initiative will take place twice a year to facilitate the integration of new members into the ICMS family.

The onboarding sessions are designed to get researchers engaged in the ICMS community right from the start of their career. “New masters, PhDs, postdocs and tenure track researchers come in throughout the year,” explains Bruining. “Building a community and making good connections is an essential part of scientific careers. We want to create a welcoming, dynamic and creative environment where scientific ideas can thrive, especially for young researchers at the start of their career.” However, the onboarding sessions are not only designed for newcomers. “I also see many people who have been here for years who are interested in joining the initial sessions to get an overview of what is happening within ICMS.”

BOTTOM-UP SCIENCE

ICMS seeks to unify researchers and support them in navigating different scientific challenges together. “The entire ICMS team is passionate about facilitating bottom-up science. It’s the beating heart of our university: without strong science and support, there is nothing.” And with this vision as the starting point, the process of scientific matchmaking begins. A successful example of scientific collaboration is the partnership with IBEC in Barcelona, a bottom-up initiative of ICMS researchers. “Other examples include the collaboration between chemical engineers that develop responsive materials and mechanical engineers that employ them.”

OPEN DOORS

With the onboarding sessions, renewed energy will be invested into bridging different research areas. “It takes consistent effort to facilitate connections between scientists of different disciplines, and we take ownership of that process. In general, we facilitate connections in a very informal setting. After all, making new connections is fun.” To Bruining, ICMS is first and foremost a community of people. “Being part of ICMS should be something people are proud of, even young people who just joined.” And there is always room to grow and innovate, Bruining emphasizes. “After the first onboarding session, we are very open to hearing what people think so we can continuously improve our program. We have an open-door policy. Just come in and share your ideas.”

First ICMS PhD Paper Award for Aysegul Dede Eren

Aysegul Dede Eren is the winner of the first-ever ICMS PhD Publication Award. Dede pitched her paper "Self-agglomerated collagen patterns govern cell behavior" published in Scientific Reports, to earn the recognition of the jury and the first place from the total of eleven submissions. Dede performed her PhD research on tendon tissue engineering in the Biointerface Science group of Jan de Boer (BME). Her exploration of collagen topography production by droplet evaporation for cell shaping has delivered remarkable initial results which are resonating with tissue engineers and other scientists.

Tendons largely consist of a highly organized collagen-based extracellular matrix (ECM). This strong collagen organization gives tendons the mechanical strength required to cope with the high loads they are subjected to. Cozily embedded between the collagen fibers are the tenocytes, which are in charge of collagen production and maintenance. Disruption of the collagen architecture provokes tenocytes to lose their characteristic elongated shape. In turn, this has a dramatic effect as changes in gene and protein expression lead to a decline in the production of proteins necessary for collagen production and maintenance. As a result, tenocytes no longer function properly.

To understand how the collagen organization impacts tenocyte shape and behavior, Dede engineered platforms with artificial topographies: patterned surfaces that mimic the structure of natural collagen ECM. Such topographies are used to study how tenocytes respond to exposure to different landscapes. On this occasion, Dede used the very type of collagen tendons are made of to generate topographies. She was also looking for a facile technique to do that and tried droplet evaporation of a collagen solution. The results were stunning.

MULTIPLE COLLAGEN TOPOGRAPHIES

Upon liquid evaporation, collagen self-assembled into three distinct topographies, with patterns in the micro- to nanometer scale. Arranged in a concentric fashion, at the center of the stain the collagen is isotropic, at the periphery it adopts V-shaped patterns and, in between those two domains, well-ordered concentric-ring shaped collagen patterns were observed. To achieve isotropic and anisotropic well defined ordered collagen topographies, let alone three of them at once, is an accomplishment worth noting. Droplet evaporation requires little time and barely any equipment. "You just need a pipette, a glass support and a chamber for humidity control," Dede explains, "this can be reproduced in any laboratory in the world."

The platform is proving to be a success in cell steering. Dede: "Tenocyte shape is drastically different in each region." Having three markedly different collagen topographies on one single substrate is also highly convenient in that it can help address other questions posed by the natural tendon like tenocyte migration between domains or tenocyte behavior in those parts of the tendons where they transition to bone or muscle. Although still in its initial stages this platform promises interesting insights that can aid tissue engineers to fully comprehend how tendons work and how to design biomaterials that will adequately interact with tenocytes in the body.

Aysegul Dede Eren

Left: Ana-Maria Olteniceanu
Middle: Maurik Engelbert van Bevervoorde
Right: Maurits Flos

Understanding echo chambers may help to counter fake news

Our societies become increasingly interconnected, both on the level of people and the devices they use. The TU/e Honors Academy addresses the challenges these developments pose in its “Networked society” track. One of those challenges is the rise of fake news and misinformation. Participating bachelor students within ICMS are now focusing on echo chambers in social media and how their formation can be understood through modeling. “Once you know how echo chambers arise, you may also be able to prevent them.”

Universities are increasingly offering all kinds of programs for students that show an outstanding performance and are up for an additional challenge on top of the standard curriculum. For this small, but highly motivated group, ICMS organizes a two-year "Networked society" – track for bachelor students. Participants spend ten hours a week on studying the complexity of our hyper-connected societies where social media link people from all over the world and "smart" devices are chatting over the internet – from thermostats in our homes to self-driving cars. The track, which started in the previous academic year, is part of the TU/e Honors Academy and the ICMS Grip on Complexity-program.

DELVING DEEPER

Assistant professors and ICMS members Pim van der Hoorn (Mathematics) and Erik Steur (Mechanical Engineering) coordinate the track. "Complexity science is a multidisciplinary effort, so we are excited to have attracted students from different disciplines," says Van der Hoorn. "Their backgrounds range from chemistry to computer science and from math to data science." The first group of four students started more than a year ago by diving into a broad range of topics that fit the overall theme the networked society. Most of the were brought up by the students themselves. By delving deeper into these issues, they created a better understanding of the most important research questions. For example, on the topic of pandemics, they interviewed Hans Heesterbeek, professor of infectious diseases at Utrecht University. Early next year, on January 12, Heesterbeek is a guest speaker in Eindhoven at the Studium Generale and he will talk about the spread of viruses in a networked society.

CRITICAL MINDSET

The students also attended courses on graph theory, one of the tools they could use in their research. "We narrowed the overall theme down to three separate subjects," says computer science student Ana-Maria Olteniceanu, one of the participants. "We decided on navigation, climate change and fake news. These topics all seemed very relevant to us and we thought network theory can contribute to increasing our understanding of them. For instance, graph theory is still a new approach in climate research, despite all the research that is happening." Her fellow participant, Maurik Engelbert van Bevervoorde, who studies both chemistry and mathematics, explains more about their approach. "We discussed scientific articles in the Journal Clubs, to gain more insight in our subjects. At first, you just summarize what the article is about. But because of all the questions that come up, you start asking more and more questions yourself. Are the conclusions of the author justified? Are the methods correct? What argues against it?" According to Van der Hoorn, the students turned into scientists with a critical mindset. "It was very rewarding to see this rapid development. That is also the intention of the Honors Academy."

EMERGING ECHO'S

The students eventually managed to single out one topic and define a research question. "We chose to investigate the emergence of echo chambers in social media," says Olteniceanu. "Good mathematical work has already been done there, on which we can build to make a model. We also see opportunities to obtain data so that we can test the model." The students are now assessing the possibility to download large amounts of data via an application programming interface (API), a possibility that various social media offer. There are also databases for research purposes that the group could use, she thinks.

"For modeling, it is also necessary to define exactly what an echo chamber is," adds Van Bevervoorde. "An intuitive definition is not enough to develop a model." The division of tasks within the group is along the lines of their backgrounds. The data scientist is busy obtaining data, the mathematicians define the model, the computer scientists are looking at how to implement it. Exactly as it is in a multidisciplinary research team. During this second year of their honors program, the students will be conducting their actual research. "We hope to add something to the knowledge about echo chambers," says Van Bevervoorde. "Once you know how they arise, you may also be able to predict and prevent them." Sharing that knowledge is also part of the project. "Once we have results, it would be great if we could publish them as a scientific paper," says Olteniceanu. "We are also looking forward to presenting the results to the ICMS community."

The hidden roots of life

George Church

Just before summer, gene editing pioneer George Church presented a lecture entitled "Engineering life" at TU/e's Studium Generale. Church is professor at Harvard University and MIT and his lecture was part of the ICMS "Complexity" series . Following the lecture, Jan van Hest, scientific director of ICMS, continued the discussion with Church on topics like the evolution of life and potential interventions in living organisms.

Van Hest: How far are we when it comes to engineering organisms, can we bring them to a higher level?
Church: "We are now able to read, write and edit DNA. That is very powerful. DNA produces RNA, proteins, other polymers, cells, organs and ecosystems. But we are still in a very primitive stage of using this. We don't know how to make things from scratch. We are also very bad at morphology. If you want something with a certain form or function, you wouldn't know what DNA you need to make it. You can make small changes in existing genomes. You may call them micro-evolutionary changes. But we can't make larger leaps, for now. But not for long, the field is developing fast."

Do we need new tools for it, or do we need new knowledge to use our tools more effectively?
"In this field, there is little difference between science and engineering. Tools are improving, and so is our knowledge. We will primarily need new software, that models how a one-dimensional DNA structure builds a 3D structure. We also need rapid testing to improve the internal rules of this software."

What role can machine learning play? Is it just a tool to distill the right information out of the increasing amount of data? Or does it also add something new?
"Machine learning is not fundamentally different from cluster analysis, neural nets or other computational tools. But what is special about machine learning is its ability to build large libraries of data. We can catalog up to a trillion different genomes and then test the millions, billions or trillions of functionalities with high throughput. That will be key to further rapid improvement in synthetic biology."

At what kind of problem would you direct this effort?
"Every project we initiate should have a really cool philosophical question. But we should also ask what the benefits for society could be. We have matured, so that we combine pure and applied science in one project. The science and engineering community has largely outgrown pure curiosity. One of our first challenges on a genome scale was to make an organism resistant to essentially all viruses. We tinkered with the genetic code and made it resistant to 92 percent of all virus categories. We are now working to make an organism completely resistant to all naturally occurring viruses, thousands of different viruses. That project is profound enough in basic science terms and also very relevant to society. Still more challenging is differentiating cells, so that they make different tissue types. This is all epigenetics. We just published papers with about 300 recipes for different cell types with different transcription factor combinations. This is very much the result of trial and error. We try a switch and see what it does, and then try it in combination with other switches. We aim at a million combinations in one experiment."

How far are we from creating life from inorganic materials?
"We still don't know what the first forms of life looked like. Some scientists think the easiest way to make a minimal cell is to start with a living organism, cutting away the modern parts of it. It is easy to get started that way, deleting a thousand genes. It is very hard to continue, going all the way back. Today we have highly evolved organisms, which might have thrown away the scaffolding that was essential in earlier stages of evolution. We don't know what it was and how to bring it back. It is far more interesting trying to make life bottom-up, starting with plausible prebiotic soup. It is a more fundamental approach and it is also easier."

"WE TRUST THAT WE WON'T NEED AN AX."

Are modern species better at adapting?
"If an organism gains robustness in a particular category, it loses robustness in other categories. The most abundant photosynthetic organism in the world is Prochlorococcus, very small marine cyanobacteria. When you bring them into the laboratory they are extraordinarily finicky and picky about how you simulate the ocean. If there is just a part per million too much copper or too little iron they give up and die. They have lost their adaptability because the ocean from their viewpoint is very constant. It's like humans who used to carry around all weapons that were needed to survive. A modern citizen walks around in shorts and a cellphone. We trust that we won't need an ax. This extreme specialization makes us versatile, but vulnerable to larger changes. Our societies are, for example, not adapted to temperature rise. We have lost that flexibility. Maybe we should train some people to recreate civilization from dirt."

Theses

APRIL 2021 – OCTOBER 2021

Advanced optical materials for light control: on the road towards smart greenhouses
GILLES TIMMERMANS
April 6, 2021
PhD advisors:
A.P.H.J. Schenning
M.G. Debije

The search for synergy in laboratory data
SASKIA VAN LOON
April 8, 2021
PhD advisors:
V. Scharnhorst
U. Kaymak
A. Boer

Phase behaviour of mixtures of structurally complex colloids and polymers
VINCENT PETERS
April 21, 2021
PhD advisors:
R. Tuinier
M. Vis

Protein-engineered cowpea chlorotic mottle virus-like particles as a drug delivery platform
DAAN VERVOORT
April 23, 2021
PhD advisors:
J.C.M. van Hest
M. Merkx

Photonic materials and soft actuators from oxetane liquid crystals
DAVEY HOEKSTRA
April 28, 2021
PhD advisors:
A.P.H.J. Schenning
M.G. Debije

Bringing coating surfaces to life: electric field-driven surface dynamics of PDMS
FABIAN VISSCHERS
April 30, 2021
PhD advisors:
D.J. Broer
A.P.H.J. Schenning
D. Liu

Modeling novel thermal transport phenomena in semiconductor nanowires
SUBASH GIREESAN
April 30, 2021
PhD advisors:
P.A. Bobbert
E.P.A.M. Bakkers

Unlocking the adaptivity in supramolecular biomaterials via chemistry and processing
DAN JING WU
April 30, 2021
PhD advisors:
P.Y.W. Dankers
C.V.C. Bouten

Engineering nanoreactors for catalytic cascades in-flow
MARIA TERESA DE MARTINO
May 3, 2021
PhD advisors:
J.C.M. van Hest
L.K.E.A. Abdelmohsen

Magnetic micromixing: for point of care diagnostics
ERIOLA-SOPHIA SHANKO
May 10, 2021
PhD advisors:
J.M.J. den Toonder
P.D. Anderson
Y.B. van de Burgt

A study of partial synchronization in networks of delay-coupled systems
LIBO SU
May 11, 2021
PhD advisors:
H. Nijmeijer
W. Michiels
E. Steur

Cowpea chlorotic mottle virus-like particles for oligonucleotide delivery
CHIARA PRETTO
May 25, 2021
PhD advisors:
J.C.M. van Hest
A. Urtti

Exploring the multiscale hierarchy of natural and synthetic materials
DENIZ EREN
May 27, 2021
PhD advisors:
G. de With
H. Friedrich

Mapping ultrafast electric fields using terahertz microscopy
NIELS VAN HOOF
June 3, 2021
PhD advisors:
J. Gómez Rivas
I. Tafur Monroy

Nature-inspired biomaterials discovery for tendon tissue engineering
AYSEGUL DEDE
June 9, 2021
PhD advisors:
J. de Boer
J. Foolen

Supramolecular charge transfer systems
ANDREAS RÖSCH
June 21, 2021
PhD advisors:
E.W. Meijer
A.R.A. Palmans

Exploring allosteric modulation of the nuclear receptor RORγt from a drug discovery perspective
FEMKE MEIJER
June 23, 2021
PhD advisors:
L. Brunsveld
R. Doveston

Nanostructured siloxane-based materials: on the interplay of phase segregation and supramolecular interactions
BRIGITTE LAMERS
June 23, 2021
PhD advisors:
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A.R.A. Palmans
G.M.E. Vantomme

Numerical methods for pattern and bifurcation analysis in complex networks
KIRILL ROGOV
June 25, 2021
PhD advisors:
H. Nijmeijer
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A.Y. Pogromskiy
E. Steur

Functional drawn polymer composites: for thermal management and actuators
XINGLONG PAN
June 29, 2021
PhD advisors:
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C.W.M. Bastiaansen

Structural characterization and ligandability exploration of 14-3-3 protein-protein interactions to investigate small-molecule stabilization
FEDERICA CENTORRINO
July 1, 2021
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Identification of molecular glues of 14-3-3 protein-protein interactions
LORENZO SOINI
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Multifunctional polymeric nanovesicles as vaccine delivery platform
PASCAL WELZEN
July 8, 2021
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M.I. de Jonge

Temperature responsive photonic coatings based on siloxane liquid crystals
WEIXIN ZHANG
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G. Zhou

Perovskite solar cells on steel substrates
BENJAMIN FELEKI
September 2, 2021
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M.M. Wienk

Network control and estimation under restrictions on channel capacity
QUENTIN VOORTMAN
September 3, 2021
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J. Richard
A.Y. Pogromskiy
D. Efimov

Topology and non-Fermi liquids in two-dimensional materials
NIELS DE VRIES
September 3, 2021
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C.F.J. Flipse
R.A.J. Janssen

Engineering microcompartmentalized cell-free synthetic circuits
PASCAL PIETERS
September 9, 2021
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T.F.A. de Greef
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Controlling the length of supramolecular polymers
ELISABETH WEYANDT
September 17, 2021
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E.W. Meijer
G.M.E. Vantomme

A phenomenological model for morphology development of disperse polymer blends in complex flows
WING-HIN WONG
September 22, 2021
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P.D. Anderson
M.A. Hulsen

Liquid crystalline particles prepared from dispersion and precipitation polymerization
XIAOHONG LIU
September 23, 2021
PhD advisors:
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M.G. Debije
J.P.A. Heuts

Folding behavior of elastic origami metamaterials
AGUSTIN INIGUEZ RABAGO
September 28, 2021
PhD advisors:
B. Overvelde
H. Nijmeijer

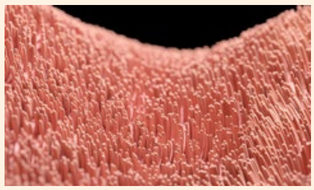
Stabilizing metal halide perovskites by computational compositional engineering
JUNKE JIANG
October 14, 2021
PhD advisors:
P.A. Bobbert
S. Tao

Attractive soft matter: polyelectrolyte assembly for the design of functional materials
CHRISTIAN SPRONCKEN
October 26, 2021
PhD advisors:
I.K. Voets
P.Y.W. Dankers

News, awards & grants

Artificial ultra-tiny "hairs" open up future small-scale applications

OUR RESEARCHERS HAVE DEVELOPED A NEW WAY TO MAKE MAGNETIC ARTIFICIAL CILIA COMPARABLE IN SIZE TO REAL CILIA THAT COULD BE USED IN FUTURE MICROFLUIDIC DEVICES AND SENSORS.



Source: Shutterstock

Cilia are tiny hairs used in transport and sensing in the human body. Many scientists are trying to make artificial cilia for applications in microfluidic devices and sensors, but to date, they are much larger than biological cilia. Researchers at Eindhoven University of Technology and EPFL in Switzerland have solved this issue by designing a new way to make magnetic artificial cilia with the same maneuverability and size of biological cilia.

In the biological world, the ultimate micro-controllers are cilia. These tiny hairs can be found on the surface of microorganisms and help propel them through liquids. Cilia also line the walls of our airways and transport mucus out of our lungs, while in our kidneys, cilia act as sensors.

Unraveling the cell's sweet spot

Sugars interact with the cell surface through sugar-binding proteins called lectins. These interactions play a fundamental role in many of the cell's biological processes. One important function is the modulation of the immune response towards an outside threat. In a recent Nature chemical biology paper, ICMS researchers Roger Riera and Lorenzo Albertazzi team up with researchers from Leiden University to unravel the interactions of individual sugar molecules with cells using super-resolution microscopy.

Assembling materials using charged polymers

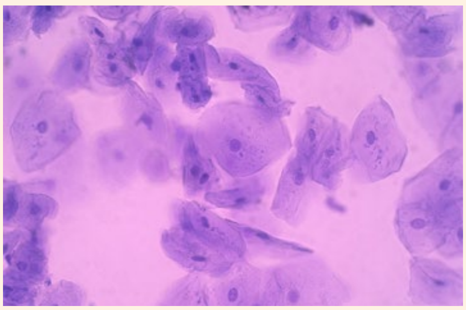
CHRISTIAN SPRONCKEN DEFENDED HIS PHD THESIS ON OCTOBER 26TH AT THE DEPARTMENT OF CHEMICAL ENGINEERING AND CHEMISTRY.

Soft matter can be found in many everyday materials, such as food, cosmetics, and the cells in our own bodies. The structure of these tiny, soft materials is determined by various interactions, one of which is electrostatic interaction. For his PhD research, Christian Sproncken used electrostatic interactions to assemble soft materials into various structures consisting of charged polymer chains. These materials may be used in responsive coatings for photonic microchips, or in materials to stop ice growth on car windshields or airplane wings.

Christian Sproncken

Tissue physics plays a key role in tumor growth

NEW RESEARCH SHOWS HOW TISSUE PHYSICS HELPS THE RAS GENE TO DRIVE EARLY TUMOR DEVELOPMENT.



The physics of tissues plays a role in cancer progression. Photo: Choksawatdikorn via Shutterstock

Cancer is a difficult disease to treat and to study, and can be caused by a range of genetic mutations. For instance, the mutated RAS gene causes a loss of structure in epithelial tissue, a tissue type that lines the outside of organs. To better understand this process, researchers at TU/e along with colleagues from IBEC in Spain and UCL in the UK have studied how the RAS gene leads to tumor growth in 2D layers of epithelial cells. Results indicate that tissue physics play a key role in tumor growth, suggesting that mechano-therapies might help to combat tumors in future treatments.

A new "twist" to viscoelastic bridges

SCIENTISTS AT TU/E AND THE UNIVERSITY OF OKINAWA HAVE FOUND A NEW METHOD TO IMPROVE DISPENSING OF VISCOELASTIC FLUIDS LIKE KETCHUP, SILLY PUTTY AND TOOTHPASTE.

Photo: Sofiamcfly, CC BY-SA 3.0

If you've ever tried to lift a pizza slice covered in hot, melted cheese, you've no doubt encountered the long, cheesy strings that bridge one pizza slice to the next. Keep lifting the pizza slice and these cheese bridges eventually break, covering the plate, table (or even your lap) in long, thin strands of cheese. While this is just a minor inconvenience with pizza, it is a longstanding problem in industry, where liquids with similar properties to melted cheese – dubbed viscoelastic fluids – need to be cleanly and speedily dispensed.

Now, scientists from the Polymer Technology group at the department of Mechanical Engineering have teamed up with a research group at the Okinawa Institute of Science and Technology Graduate University (OIST) in Japan. Together they developed a new technique that uses rotation to break these liquid bridges. Their findings, published in the Proceedings of the National Academy of Sciences (see key publication 20), could improve the speed and precision of dispensing viscoelastic fluids, in applications ranging from circuit board production and food processing to tissue engineering and 3D printing.

Werner en Fleur

iGEM'21

A living sensor for inflammatory bowel disease

Engineered bacterium creates bubbles for ultrasonography

The Eindhoven iGEM'21 team designed and synthesized a plasmid (circular strand of DNA) that may enable monitoring of inflammatory bowel disease (IBD) with ultrasound. It acts as a living sensor that does not require fasting, laxative agents or unpleasant procedures like an endoscopy, where a camera is inserted in the intestines. Clinical application is not yet in sight, but their efforts did earn the team a gold medal at the iGEM Jamboree in Paris.

"Hectic and highly educational" is the concise description of Fleur Kalberg of her time as a member of the TU/e iGEM2021 team. She gained the hands-on lab experience she wanted, but also qualified for a biosafety certificate, pitched for an audience of a few hundred people, made lava lamps with a class of ten-year olds and talked to business managers, GMO- and ethics specialists, gastrologists and patients. And she skipped her summer holidays. "I graduated young and was looking for something extra to do, something serious and interesting," says Kalberg, a master student in medical engineering. "Because of the pandemic, I didn't get a lot of lab experience. The iGEM competition seemed a chance to do just that."

After discussing options such as wound healing patches and a "health recorder pill," the team decided to focus on a non-invasive method for monitoring inflammatory bowel disease (IBD), which affects almost seven million people worldwide and that number is increasing. Kalberg became "captain human practices." "My main task was outreach: collecting feedback on our idea from patients, scientists and potential investors, to generate an optimal design." However, because the team was small (eight people), and the team manager fell ill, Kalberg performed all kinds of tasks from creating biodoodles in a fun challenge, to planning the team's work in the final month and arranging trouble shooting meetings every two weeks with the iGEM team from Vienna that happened to work work on a somewhat similar idea. Kalberg: "I definitely developed a lot of soft skills, and above all I learned the value of sound communication."

LAB CAPTAIN

Like the other team members, Kalberg spent time in the laboratory creating the bacterium they needed. The experiments were designed and prepared by Werner Doensen, BSc in biomedical engineering, and one of the three "lab captains." Doensen joined the team after enthusiastic stories of a friend who participated in a previous Eindhoven iGEM team. "I worked a lot in student groups on different assignments, but an iGEM-project is far more realistic both in scientific terms and in team work," Doensen shares. "We were exploring our own idea with unknown obstacles to overcome." He feels the project was a success, but with ups and downs. "We succeeded in preparing the correct plasmid and we delivered proof-of-concept. Our bacteria create gas bubbles that can be detected with ultrasound in the presence of IBD-markers."

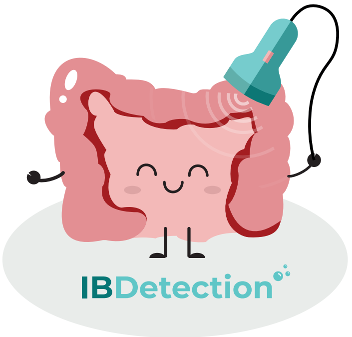
The new plasmid, which provides the required genes, is a clever combination of two existing plasmids. The first one causes the bacterium *E. coli* to produce a green fluorescent protein in the presence of tetrathonate, a biomarker for (the severity of) intestinal inflammation. The second plasmid enables the production of vesicles in bacteria that collect gas from their environment, creating "bubbles" that can be detected using ultrasound. After overcoming a few "surprises" in the functioning of the off-the-shelf-plasmids and delivering proof-of-concept for the ultrasound detection of the bubbles, the big puzzle started: copying and pasting parts of the two plasmids together into one new plasmid that would provide a sensing system for IBD. Doensen: "We needed to determine the right cutting places and make sure that recombining doesn't happen backwards. It took weeks to design the optimal strategy." The actual lab work takes three to four days, from cutting the DNA and isolating the necessary parts to "gluing" them together in the correct manner. Doensen: "You can't really see what you are making. You just follow the protocols. Only at the end when your bacteria grow, you know that you actually succeeded." The desired plasmid is now ready, but the team hasn't seen it in action, because the iGEM-deadline for experiments passed. A first task for a new Eindhoven start-up company?

After all, the team was awarded a gold medal and six nominations at the final iGEM-jamboree in Paris in November. Doensen: "Under the current laws, such a GMO-product unfortunately has no market potential." Kalberg agrees: "The whole bacterium is commercially a no-go, but there may be potential in a pill containing enzymes." However, the students both have other plans. Doensen and Kalberg will soon start their master thesis project.

iGEM team

The International Genetically Engineered Machine (iGEM) competition is an annual worldwide synthetic biology event that started in 2004. Teams of students (graduate, undergraduate or high school) compete by designing and realizing an idea that includes synthetic biology. Previous teams for example engineered *E. coli* to produce banana scent, but also a therapeutic recombinant enzyme to treat celiac disease. The competition resulted in several start-ups, including e.g. Ginkgo Bioworks (flavors, fragrances), Opentrons (liquid handling robots) and Puraffinity (ultrafiltration membranes). Since 2012, Eindhoven University of Technology participates in the iGEM competition. In 2020, the competition was cancelled due to the pandemic.

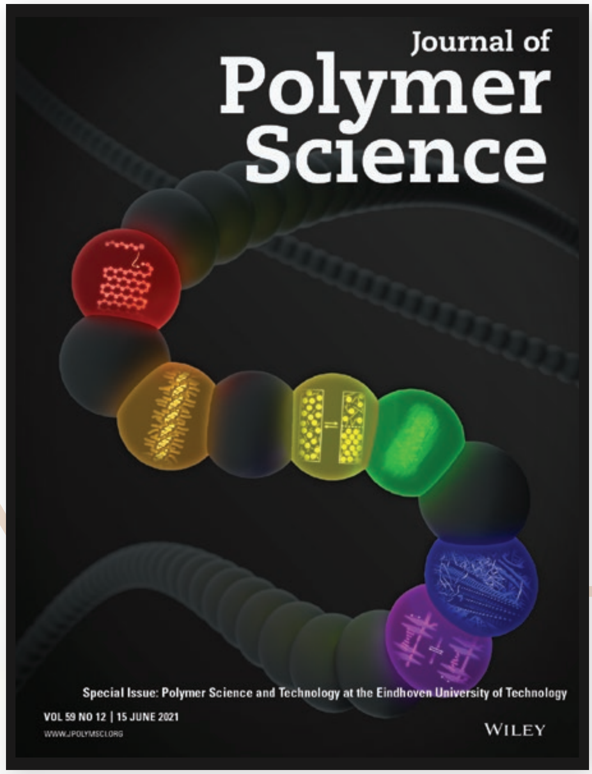
"IT TOOK WEEKS TO DESIGN THE OPTIMAL PLASMID CUT-AND-PASTE STRATEGY"

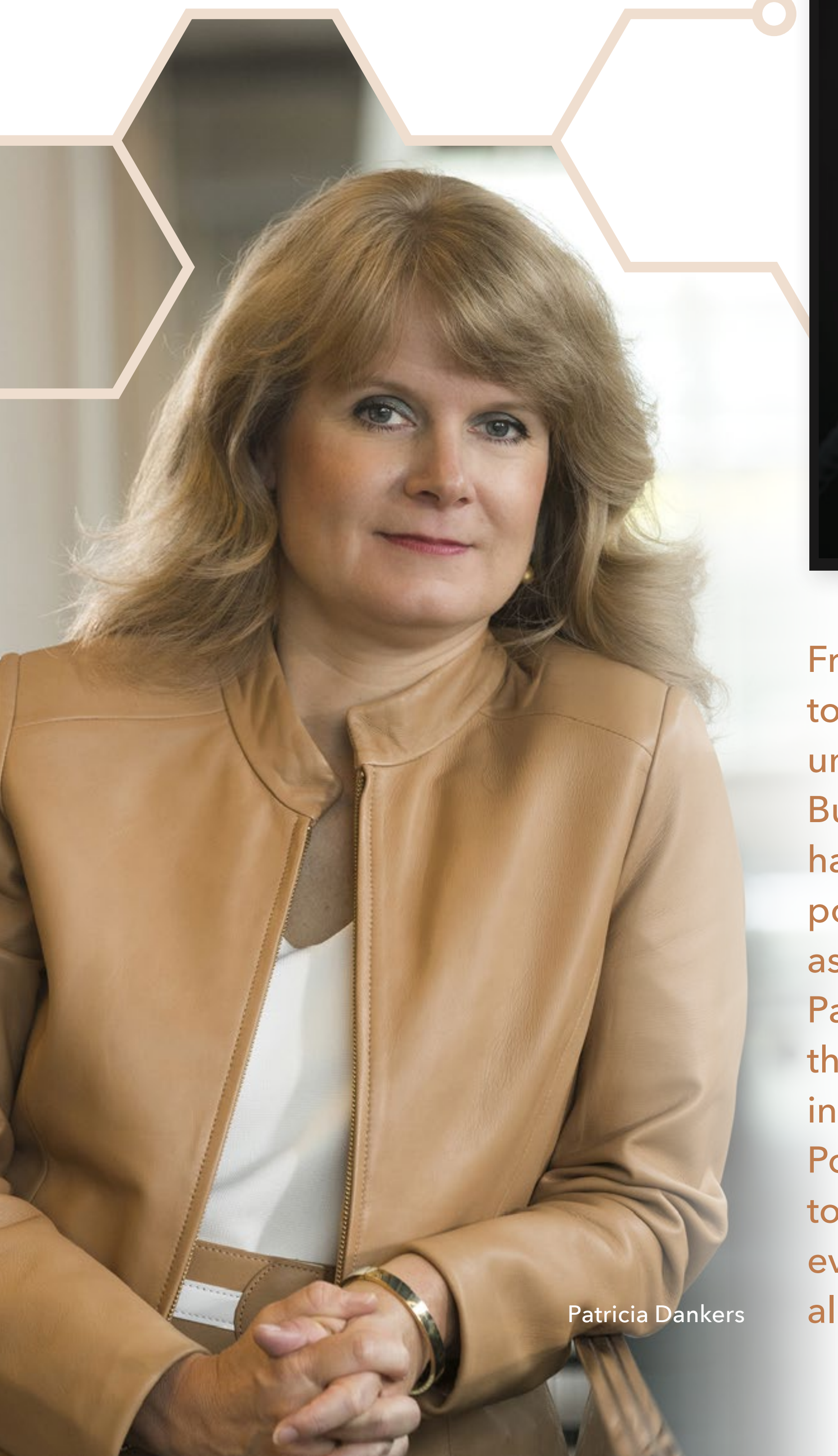


POLYMER SCIENCE AND TECHNOLOGY

Polymers in the spotlight

Special issue of Journal of Polymer Science showcases TU/e research




Patricia Dankers

From separate discipline to essential toolbox – polymer science has undergone quite a transformation. But to the outside world, that may have led to a hazy picture in which polymer research is not as visible as it used to be. Jan van Hest and Patricia Dankers decided to counter that image and that has resulted in a special issue of the Journal of Polymer Science devoted entirely to research at TU/e. “Polymers are everywhere and polymer science is alive and kicking in Eindhoven.”

"THERE ARE SOME URGENT ISSUES THAT WE NEED TO TACKLE"

Over the past few years, something strange occurred in the world of polymer science. While the importance, the variety and the applications of polymers keep on expanding, the visibility of polymer science as a cutting-edge discipline has waned. "For decades, TU/e was known as an internationally leading center on polymer chemistry and polymer technology, but now outsiders sometimes wonder whether we still do polymer research here", says Jan van Hest, scientific director of ICMS. "Which is quite unnerving, considering that polymer science is very much alive and kicking here in Eindhoven. We have twenty research groups working on polymers and polymer science has become strongly embedded in many different fields, ranging from soft biomaterials for regenerative medicine to innovative coatings for solar cells. Polymers are everywhere." Polymer science has become a toolbox that enables the development of groundbreaking, innovative materials for all kinds of applications. "Just like synthetic organic chemistry turned from a separate activity into an indispensable enabler of all molecular sciences", Van Hest explains.

CHAIN OF KNOWLEDGE

It is an interesting paradox: when a scientific area becomes more common and embedded and thus gains importance, it also often loses visibility and sometimes even recognition. Time to change that narrative, says Patricia Dankers, professor of Biomedical Materials & Chemistry. "There are very few hubs in the world that cover so many different aspects of polymer science as we do here in Eindhoven. We have a lot to offer to academic groups and industrial parties." Together, Van Hest and Dankers decided to get the message out and contacted the editorial board of the Journal of Polymer Science to see whether they were interested in producing a special issue on polymer research in Eindhoven. "They were immediately in favor of the idea", says Dankers. "Next, we invited all research groups active in polymer science to submit a paper on recent work and that generated a lot of enthusiasm." Van Hest emphasizes that they were not involved in the selection and review process. "No, this was a completely independent process conducted by the JPS editors. All submissions went through the normal, peer review process." That resulted in fifteen original research articles and two perspectives. None of the submissions were rejected. "We were very pleased with the number of papers and the quality of the work presented", says Dankers. She and Van Hest provided an editorial and the team at the ICMS Animation Studio designed a beautiful cover depicting the Eindhoven "chain of knowledge". They are both very pleased with the final result. Van Hest: "To me, this special issue provides a very good overview of our research here and I hope that readers will be surprised by the variety and quality of our polymer activities at TU/e."

RECYCLING

Next to showcasing what Eindhoven has to offer when it comes to polymers, Van Hest hopes that this special issue will also stimulate researchers to consider polymers with renewed interest. "There are some urgent issues that we need to tackle and the main one is of course recycling. Until recently, polymers were always developed for just their intended application, but those days are gone. Already during the design of a polymer do we need to consider how the material will eventually be discarded and recycled. A major bottleneck that we face is the lack of chemical methods to enable sustainable degradation and re-use of building blocks. That is an important and interesting challenge for polymer chemists." A challenge that is a perfect fit for the expertise at TU/e, says Dankers. "Just think about all the work we do here on supramolecular chemistry that provides a wealth of opportunities for creating dynamic, adaptive materials. And then add to that all the other aspects of polymer science that we address. The challenges that lie ahead require a multidisciplinary approach and I'm glad that we now have this JPS special issue to demonstrate our capabilities in this field."


Jan van Hest

ALLIANCES

ICMS and MPI-P: natural partners in materials science

The Max Planck Institute for Polymer Research (MPI-P) in Mainz, Germany and ICMS have a close and successful scientific collaboration in the field of materials science. We talked to four PhD students that take part in joint ICMS - MPI-P projects. What is the topic of their project and how do they experience the cooperation?

ICMS and MPI-P are natural partners when it comes to materials science. Both institutes integrate chemistry, materials science, physics, biology, mathematics, and molecular engineering to address important scientific and societal challenges. Both focus on research areas where polymers, often combined with other molecular building blocks, are applied in a much broader interdisciplinary context. The cooperation is based on complementarity in knowledge as well as and infrastructure, combined with shared scientific themes and challenges.

Imke Krauhausen

@ICMS: Microsystems, Neuromorphic Engineering (Yoeri van de Burgt)
@MPI-P: Organic Neuromorphic Electronics (Paschalis Gkoupidenis)

Imke Krauhausen studies the use of neuromorphic organic devices for brain-inspired smart robotics and sensors. The devices contain organic "artificial synapses" capable of creating synaptic connections similar to the human brain: as a result of an external stimulus a permanent change in electrical conductivity occurs. Krauhausen investigates their use in robotics for learning purposes. She just finished a project at MPI-P where she has equipped a path-finding robot with a neuromorphic device and taught the robot how to proceed at an intersection inside a maze.

Thanks to the device, the robot ultimately was able to exit the maze on its own. Earlier this year she moved to Eindhoven to start a new, related project trying to integrate neuromorphic organic devices with a robotic arm. While being at one location, she tries to keep up with meetings and other activities of the partnering group. That is challenging but well worth it, she says. "You can double the input for your research and obtain different perspectives to the same issue." And it's also helpful on a professional level: "I experience the struggles of the researchers in Eindhoven as well as in Mainz, and from that I get to learn a lot."

Riccardo Bellan

@ICMS: Biomedical Materials and Chemistry (Patricia Dankers)
@MPI-P: Synthetic Life-Like Systems (David Ng, Tanja Weil)

Riccardo Bellan works on the synthesis of novel supramolecular polymers. He is developing a new kind of monomer that is capable of selective assembly in living systems. "It's all about combining and controlling the assembly behavior of molecules in a biological environment", he says. "At MPI-P, the focus is on polymers that aggregate in another fashion than the molecules we use here in Eindhoven. We are now looking for ways to combine the two types of chemistry. We hope to create a new type of monomer that assembles in a novel fashion that combines the two approaches." According to Bellan, the collaboration brings out the best of both groups. "For me personally, the feedback and input from MPI-P really enables me to improve my work." Bellan expects to go to Mainz in the near future. "This is a very dynamic collaboration, we have not 'programmed' any exchange visits. But I can go over there whenever that seems relevant." He adds that the cooperation is not only about developing knowledge. "I also learn a lot from experiencing different cultures. Of course, being Italian, going to Eindhoven already broadened my horizon. But being in a project in which two internationally renowned institutes cooperate also adds to my personal growth."

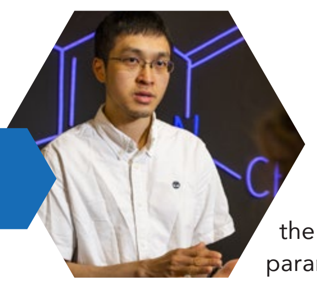
René de Bruijn

@ICMS: Soft Matter and Biological Physics (Paul van der Schoot)
@MPI-P: Molecular Electronics (Jasper Michels)

René de Bruijn is trying to unravel the processes that determine the morphology of thin polymer films. These films are applied, for instance, in organic solar cells or flexible transparent electrodes. Using theoretical modeling, he tries to pinpoint and understand the relevant aspects of the production technology that is applied, such as spin-coating or meniscus-guided coating. "It is relatively poorly understood how these production processes affect the emerging morphology, which hampers a rational material design", he says, adding that the cooperation with MPI-P really improves his work. "I get input from different technology experts so that we can incorporate many aspects in a state-of-the-art model description." The cooperative setting was a main driver for applying for this PhD position, also because it provided De Bruijn the opportunity to experience another working environment. He has just moved to Mainz for a three-month period and enjoys his stay there. "I really enjoy building a theoretical model that can be used to either design experiments or guide experiments. It really motivates me to understand the workings of complex systems or processes to arrive at a certain function."

Zhongquan Chen

@ICMS: Computational Quantum & Molecular Dynamics (Björn Baumeier)
@MPI-P: Organic Neuromorphic Electronics (Paschalis Gkoupidenis)



Zhongquan Chen performs computational modeling on neuromorphic organic devices that are designed to functionally mimic the human brain. In particular, he hopes to establish how the device operation – by means of electric field effects – is related to the processes within the material, such as electron transfer. For this, he uses a multi-scale simulation approach including first principle calculations and molecular dynamics as well as macroscopic simulations. This work benefits hugely from the collaboration with MPI-P, which according to Chen has really advanced expertise in the field of neuromorphic devices. "The experimental work on neuromorphic devices at MPI-P very nicely complements my theoretical modeling. Their characterization of the devices helps to establish the parameters and boundary conditions for the simulations, and it provides us with a check on our computational results." He finds that particularly relevant since what motivates him in his modelling efforts is their physical relevance. Also, the interdisciplinary setting of the cooperation adds to his delight: "In organizations, we work in different groups and different departments. But to solve problems of science and technology you have to go beyond those boundaries."


"SERVING YOUR
INNOVATION NEEDS"