Edition 20 June 2023

ICMS Highlights

THE COOL ART OF IMAGING THE ULTIMATE MOLECULAR DETAIL

PULLING THE TRIGGER ON THERMOSETS

EARLY-STAGE DRUG DISCOVERY WITH AI

ICMS
INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS

TU/e

INTRODUCTION

ICMS Highlights

We are in a year of celebration: 2023 marks 15 years of ICMS! We are very proud of the institute as it is today, but of course we have had our ups and downs. Just as each and every member of our community has experienced their highs and lows. Especially in the difficult moments we foster our atmosphere of learning from our failures, of comradeship and willingness to help each other, and being happy for someone else's success. This is what we celebrate in 2023!

Addressing complexity and molecular systems will remain our bread and butter. However, we have adjusted our strategy to address these topics. This was presented during our very pleasant Annual Symposium on March 30. In the future, ICMS will work from three distinctive science domains:
1. Foundations of Complex Molecular Systems;
2. Advanced Materials;
3. Engineering Life.

In the first domain we expand our knowledge on the mechanisms of how molecular interactions lead to function. This is strongly integrated with the other two domains, where the focus is on the exploitation of these functionalities. With this updated structure we expect to be more effective in responding to scientific opportunities and research needs that fit well within the scope of ICMS. This will also support decision-making when it comes to strategic investments.

As molecules that interact to create function, the ICMS community will continue to collaborate in the service of science and join forces that will further shape ICMS. In this issue of our Highlights magazine, we showcase examples of this scientific journey by our members and friends, which we hope you enjoy reading.

Jan van Hest
Scientific director

Monique Bruining
Managing director

Colophon

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.

EDITORIAL STAFF
Cindy Plompen (editorial assistant)
Harm Ikink

DESIGN AND PRINT
ECHT Marketingcommunicatie, Eindhoven

ILLUSTRATIONS AND COVER
ICMS Animation Studio

ARTICLE CONTRIBUTIONS
Marysa van den Berg, Steven Frolke, Leendert van der Ent, Roel van der Heijden, Harm Ikink, Dorine Schenk, Nicole Testerink, Marga van Zundert

PHOTOGRAPHY
Leonie Voets
Bart van Overbeeke

SECRETARIAL SUPPORT
Wendy Brouwers, Cindy Plompen

CONTACT
Eindhoven University of Technology
Institute for Complex Molecular Systems
P.O. Box 513, 5600 MB Eindhoven
The Netherlands
Telephone: +31 (0)40 247 5074
Email: icms@tue.nl

COVER "15 years of ICMS"

Content

FIFTEEN YEARS ICMS: A CATALYST FOR FUNDAMENTAL SCIENCE

SELF-LEARNING MATERIALS FOR SOLAR ENERGY

PULLING THE TRIGGER ON THERMOSETS

INVENTING MATERIALS FOR A GREEN FUTURE

08 DRUG DELIVERY WITH LIPID BUBBLES

10 THE COOL ART OF IMAGING THE ULTIMATE MOLECULAR DETAIL

12 & 32 NEWS, AWARDS & GRANTS

14 MERT ASTAM WINS THE ICMS PHD PAPER AWARD

15 CONNECTING THE ICMS PHD STUDENTS

18 FULL SPEED AHEAD ON A CRYSTAL CLEAR COURSE

20 OSCILLATING CHEMISTRY INSPIRED BY THE CELL

24 PHOTO IMPRESSION ICMS ANNUAL SYMPOSIUM 2023

26 EARLY-STAGE DRUG DISCOVERY WITH AI

29 KEY PUBLICATIONS

30 FINDING THE CLUES TO INFLAMMATORY OR HEALING CELLS

31 "IT'S COOL TO PITCH YOUR IDEAS TO THE MINISTER"

34 UNDERSTANDING THE BEHAVIOUR OF "MINI-SPONGES"

36 INTRODUCING FOUR EUROTECH POSTDOCS WITHIN ICMS

38 THESES

40 OPENING UP NEW AVENUES IN GREEN CHEMISTRY

41 SMART, DYNAMIC, SUSTAINABLE: DESIGNING A NEW GENERATION OF POLYMERS

42 A BRAND NEW "BUTTON" TO CONTROL MOLECULES


Kees Storm


Patrick Anderson


Maarten Merkx

Remco Tuinier

Edwin van den Heuvel

Fifteen years ICMS: a catalyst for fundamental science

The Institute for Complex Molecular Systems (ICMS) is renowned for its research at the most fundamental level, driving future applications within materials, energy, mobility, health, and life itself. To make this happen, ICMS joins expert scientists from chemistry, biomedicine, mathematics, physics, and mechanical engineering. This year, ICMS celebrates its 15th anniversary. We asked five deans, representing their department in the ICMS advisory committee, to reflect on the past years and look ahead to the future of the Institute.

"I quite vividly remember the early days of ICMS," says Kees Storm, dean of the department of Applied Physics and professor of Theoretical Biophysics. "We were a group of young scientists just starting their career as individual researchers, including Tom de Greef, Patricia Dankers, and me. In the basement of what was then the university main building – now Atlas – we had these wonderful regular meetings with Bert Meijer, Mark Peletier, Rutger van Santen, and Sagitta Peters. Just a small bunch of people that got together to talk about joining forces and creating a future for interdisciplinary research at TU/e."

MORE THAN A HUNDRED SCIENTISTS

And they sure joined forces. The former boiler house was renovated to provide ICMS with a dedicated workspace. It is now called Ceres and houses more than a hundred scientists working closely together. "Bert Meijer recognized the importance of bringing people from different backgrounds together in a shared location," says Patrick Anderson, dean of the department of Mechanical Engineering and professor in Structure and Rheology of Complex Fluids. "There we can all meet each other, for instance at an ICMS lecture, and connections just form spontaneously," adds Remco Tuinier, who is vice dean of the department of Chemical Engineering & Chemistry and professor of Physical Chemistry. This great strength of ICMS is also underlined by Edwin van den Heuvel, dean of the department of Mathematics and Computer Science and professor of Statistics. "A lot of people from our department are working with ICMS scientists. For instance, people in probability research, analysis experts, and machine learning scientists."

INSPIRATION AND CONNECTIVITY

The combination of disciplines leads to various accomplishments. "I think one of the greatest recent achievements is acquiring the Gravitation program in Interactive Polymer Materials," says Anderson. "Usually, these programs don't go to just one university, but at TU/e, thanks to ICMS, we pulled it off." According to Maarten Merkx, dean of the department of Biomedical Engineering and professor of Protein Engineering, the examples of excellent multidisciplinary projects are numerous. "These include understanding the pathways of supramolecular self-assembly, the application of super-resolution microscopy to study single polymers and nanoparticles, the development of bionanomedicines, and various ways of molecular computing."

These achievements are without a doubt noticed within the rest of the Netherlands. "As an organizational model it certainly is an inspiration for other universities," thinks Storm. "ICMS is very good in selecting topics that we already are outstanding at, or have a real shot at becoming outstanding in. I think this also attracts a lot of talented young scientists." Companies also like to work with ICMS, explains Tuinier. "I used to work at DSM and remember that ICMS was particularly good at connecting us with researchers at TU/e. I think this works very much as a catalyst for advancing science."

AN ATTRACTIVE PARTNER

ICMS is also recognized from outside the Netherlands as an attractive partner, according to Merkx. "Well-known universities and institutes such as Northwestern University in the US, the Max Planck Institute for Polymer Science in Germany, and the Institute for Bioengineering of Catalonia (IBEC) in Spain consider ICMS as an excellent and inspiring peer institute." Through seminar series ICMS maintains this position. "We invite and talk to many people from abroad. This way the institute keeps being visible. And we make sure the impact of the research is labeled and connected to the institute," Anderson explains.

Another benefit from being part of ICMS is gaining access to advanced equipment. "Nowadays in the Dutch scientific landscape it's very difficult to get funding for this," says Tuinier. "With the help of ICMS we managed to get some really nice large-scale instruments that have a huge impact on our research, like equipment for new X-ray scattering and electron microscopy."

AN INFINITE NUMBER OF QUESTIONS

ICMS has always had a strong focus on fundamental science and Storm wants to keep it that way: "There are an infinite number of questions to be answered. Those answers also lay the foundation for future applications." As an example, he mentions the development of new polymer materials. "I think this is a very exciting future direction," he says. "There are also plans to expand the focus to regenerative health and energy materials," Tuinier adds. "This is needed to ensure a healthy and environmentally responsible future society."

Another development that the deans agree on is the increasing integration of disciplines. Van den Heuvel even thinks that boundaries might vanish at a certain moment: "We might then arrive at a kind of almost 'fluent' research area. This should advance the fundamental science of ICMS even further." What a nice perspective for the next fifteen years of ICMS!

Self-learning materials for solar energy conversion

Erik Garnett contributed to the ICMS Annual Symposium in March with a lecture on “Self-learning materials for solar energy conversion.” As a group leader at AMOLF and a professor at the University of Amsterdam, Garnett is very much interested in the intricacies of light-matter interactions. He works in fields as diverse as solar cells and light-controlled chemical reactors, taking a highly interdisciplinary approach. His research is motived by a desire to understand, but also to apply.

Erik Garnett

"I WANT TO EXPLORE FUNDAMENTALLY NEW CHEMISTRY, BUT I ALSO WANT IT TO BE PRACTICALLY USEFUL."

"I think any big important problem tends to be pretty interdisciplinary. That is probably why I like interdisciplinary science so much. I've always been motivated for renewable energy research, which of course is a really big, complex problem. You can't solve it with just physics, chemistry, or engineering. I find it really stimulating to put joint efforts in addressing the 'higher level' research questions to find real innovative solutions."

Garnett was educated in chemistry at the University of Illinois (Urbana-Champaign) and did his PhD at the University of California (Berkeley), working on nanomaterials for energy applications. During a postdoc at Stanford University, he further broadened his scope combining materials science, physics, and photovoltaic engineering. Garnett held a joint position at three different groups and acted as a kind of liaison, connecting all fields of expertise. It fitted him like a glove: "I found it particularly attractive to obtain insights from different perspectives. Not only does that advance your science, it is also helpful for creativity." And not to forget, the three labs each had their own dedicated instrumentation that he could make use of. "A broad technical infrastructure is very important for doing cutting edge research. But I think it is also very important that as a researcher you gain a broad hands-on experience and learn how to get things done in a lab."

SELF-LEARNING PEROVSKITES

In recently started research, for which he was awarded an ERC Consolidator grant, Garnett exploits the interaction of light and so-called mixed halide perovskites. This is a relatively new class of promising materials for efficient solar cells and other opto-electronic applications such as LEDs. One of their more intriguing properties is the migration of halide ions under illumination. In a more common solar cell or LED design this would decrease the conversion efficiency, but not for Garnett. He uses the halide migration to his advantage and makes the material work for him. "It is the proverbial turn your problem into a solution," he says.

In a recent paper in Advanced Functional Materials Garnett shows how light shining through nanophotonic microlenses can locally induce separation of iodide and bromide ions in the perovskite layer. The focal point becomes rich in iodides, which can be exploited in different ways. In an LED, the iodide-rich spots can turn into highly directional emitters, reversely mimicking the original light input. In a solar cell, the lenses can be used as solar concentrators. There, direct sunlight is captured by the iodide rich areas while at the same time, because of local bandgap differences, diffuse solar radiation can be collected through the iodide-depleted areas. This would substantially improve solar cell efficiencies. What's more, such a system is fully self-tracking since the iodide-rich focal spots move along the material, following the movement of the sun above.

To Garnett, that's the beauty of the concept: "We have in fact a self-learning system that adapts to a stimulus. Whether you could call this learning is up for debate, but it's not unlike what the brain does: it is quite plastic and remoulds upon a repeating stimulus. In our system, light changes the underlying chemistry of the perovskite material in a comparable responsive manner. So what we effectively do is train the material to display a certain behavior."

LIGHT-DRIVEN CHEMISTRY

Another focus in Garnett's research is using light to drive chemical reactions. The rationale is that future chemistry must not be based on burning fossil fuels, but on using renewable energy. Electrical heating would be an obvious solution, but Garnett thinks using light from LEDs or lasers could be a more effective, targeted way to sustainably "power" chemical conversions. "I want to explore what light can deliver that you can't get by normal thermochemistry. For instance, you can create enormous gradients in temperature, both in space and in time, resulting in chemistry that is very far from equilibrium. From a fundamental point of view that's super exciting because it's a different regime than all of the history of chemical reactions."

Another exciting opportunity arises from the combination with operando spectroscopy, that can provide feedback to change the light input in real time. Garnett envisions producing a range of chemicals from the same feedstock, simply by tuning the characteristics of the light. "The dream is already there. But of course, to realize it there's still a huge amount of work to do. I find this super inspiring. I want to explore fundamentally new chemistry, but I also want it to be practically useful. I would not be excited if in the end it doesn't lead to something new."

Drug delivery with lipid bubbles

Pieter Cullis

Pieter Cullis (University of British Columbia, Canada) is world-renowned for his pioneering research on lipid nanoparticle drug delivery systems. His decades of work proved crucial for the development of the Pfizer and BioNTech COVID-19 vaccines. What started as fundamental research on lipids in cell membranes "evolved, unplanned, into something that had a big impact on a global scale."

Lipid nanoparticles have been injected into millions of arms in the last few years. The COVID-19 mRNA vaccines illustrate the relevance of the revolutionizing lipid-based drug delivery system that Pieter Cullis has been working on for nearly half a century. Along the way, he co-founded several biotech companies and accumulated an impressive list of awards and honors.

CANCER DRUGS AND NUCLEIC ACIDS

Cullis completed a PhD in physics at the University of British Colombia (Canada) before moving to the University of Oxford in 1973. There, as a postdoc, he studied lipids. "You have about thirty trillion cells in your body. Each has a membrane around it that is held together by lipids," he explains. "In order to study these lipids, you have to make so-called model membranes – which are essentially lipid nanoparticles with a diameter of about 100 nanometers." Cullis and his colleagues developed a technique to make these model membranes. After three years in Oxford and a postdoc stint at Utrecht University, he returned to his alma mater where he was appointed full professor in 1985.

Around that time the idea arose to load the lipid nanoparticles with cancer drugs. The nanoparticles are like bubbles that encapsulate the cancer drugs and transport them to a tumor site. Cullis co-founded a company and in the 1990s two cancer drugs were developed that eventually were approved for clinical use. "In the mid-1990s we started working on delivering bigger molecules, such as the nucleic acids DNA and RNA, using these lipid nanoparticles,"

Pieter Cullis was scheduled to give a talk during the ICMS Annual Symposium 2023 but unfortunately, due to a busy traveling schedule and a canceled flight, he could not make it to Eindhoven.

"YOU HAVE ABOUT THIRTY TRILLION CELLS IN YOUR BODY"

says Cullis. However, to encapsulate nucleic acids, which are negatively charged, positively charged lipids were needed. The existing ones were too toxic for therapeutic use. "Luckily, in some of our basic work on membranes, we had synthesized a lipid called an ionizable cationic lipid. These lipids are neutral and nontoxic at physiological pH-values but are positively charged and can encapsulate nucleic acids at low pH."

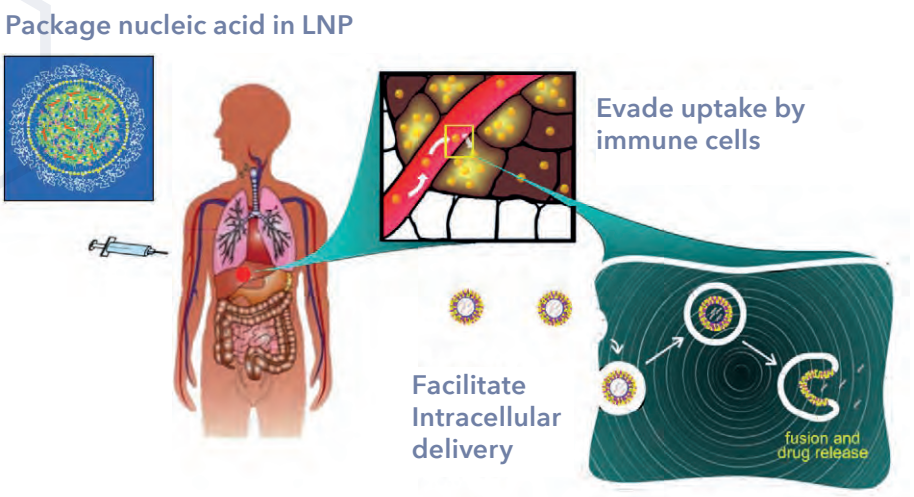
VACCINES AND MRNA

That gene therapy research led in the 2000s to a collaboration with the American company Alnylam Pharmaceuticals. It worked on using small interfering RNA (siRNA) to shut down the production of a particular protein in cells. The collaboration showed that lipid nanoparticles containing ionizable cationic lipids were able to get siRNA into the interior of cells in the liver. It resulted in a treatment for the condition transthyretin-induced amyloidosis which entered clinical trials in 2012 and was later approved by the FDA. Cullis and co-workers then started working on delivering messenger RNA (mRNA) in a next venture, Acuitas Therapeutics. That caught the attention of Drew Weissman, immunologist at the University of Pennsylvania, who worked on mRNA vaccines. "We initially looked at a vaccine for the Zika virus, consisting of lipid nanoparticles containing mRNA which codes for a protein on the outside of the Zika virus," says Cullis. "We got spectacularly good results. It is very likely that it will be turned into a commercial vaccine soon."

Those results brought Acuitas to the attention of the German company BioNTech. Five years ago, they started working together on an influenza mRNA vaccine. When the pandemic hit, in 2020, all efforts switched to COVID-19, says Cullis. Acuitas' lipid nanoparticles turned out to be a perfect fit and got incorporated into BioNTech and Pfizer's mRNA COVID-19 vaccines. "That is how basic work on membranes led to COVID-19 vaccines. It was not a planned process and we had challenges along the way, for example with drugs that did not get approved by the FDA," concludes Cullis. "But that is the way science works, it is not a linear process." According to Cullis, organizations like ICMS, putting people and resources together for example to start a company to commercialize discoveries, play a vital role in developments like lipid nanoparticles.

TARGETING

Now well past retirement age, Cullis still does research, for example on targeting. "It would be nice to have drug systems that target particular cells, to treat only those and leave the rest of the body alone." This is not easy. "As soon as you put targeting information on the outside of the lipid nanoparticles, you run into horrendous problems." However, Cullis is not ready to give up. "It is hard. But this targeting process could make diseases like sickle cell anemia, leukemia, cystic fibrosis and heart failure treatable. So, it is important that we find a way to develop this next generation of lipid nanoparticles."



Heiner Friedrich

The cool art of imaging the ultimate molecular detail

The TU/e Center for Multiscale Electron Microscopy (CMEM) acquired a ThermoFisher Glacios Cryo Transmission Electron Microscope. It provides a complete solution for macromolecular structure determination. Cryogenic TEMs are widely used in life sciences research. The use for material science applications is a rare Eindhoven specialization – one that provides valuable additional insights.

Samples have to be stable in vacuum in order to be studied in a Transmission Electron Microscope (TEM). But what when your object of study is only present in a liquid, such as water or an organic solvent? Drying is no option, as the original structure could change. "We prepare a very thin film of liquid and cool it at very high speed," CMEM head Heiner Friedrich explains. "Then the liquid becomes like glass in which the sample's structure is fully preserved." This is not an easy technique, but it is widely used in life sciences, for instance to study biological macromolecules, viruses and cellular structures. Friedrich: "The cryogenic approach enables studying the subtlest of chemical and structural changes in soft materials, such as particles for drug transport or complex assemblies of synthetic macromolecules. It brings you as close as possible to what is actually happening – as long as you know what you are looking at." According to research specialist Anne Spoelstra: "Before we started using cryogenic sample preparation, all kinds of treatments were in use. But the conclusion is clear: everything you do can change the sample – except when you literally freeze it in time. That is why we have been applying CryoTEM in chemistry for twenty years now."

MORE VITAL DETAIL

The new machine contains the latest generation of electron counting detectors, a Falcon 4i. Friedrich explains: "Frozen water is vulnerable to the electron beam. The newest detector has the highest sensitivity achievable. This means the maximum signal to noise ratio. It gets the most out of each electron we put in to image the sample." Other features include automated data acquisition, which together with the latest software results in vastly higher throughput. "For instance, following assembly processes will also improve," Friedrich remarks. "More samples can be frozen and looked at, which enables us to look at all different stages of a process and thus provide more vital detail. That is also the big bonus for using this technology in chemistry research; it provides insights that you otherwise wouldn't get." TEM education and research officer Rick Joosten adds: "It's not only the device; to get the max out of the technology, sample preparation is all-important. You have to make very thin, electron transparent samples in order to get the desired results. We have developed quite unique capabilities to get the utmost out of the instrument."

ANOTHER NOVELTY

A new type of camera and the possibility to perform scanning transmission electron microscopy provide an exquisite combination for both life sciences research and material sciences research. Spoelstra: "The specific feature set allows us to accommodate a broad field of applications. The new microscope will be used for research as well as education, enabling students to get familiar with the latest technology."

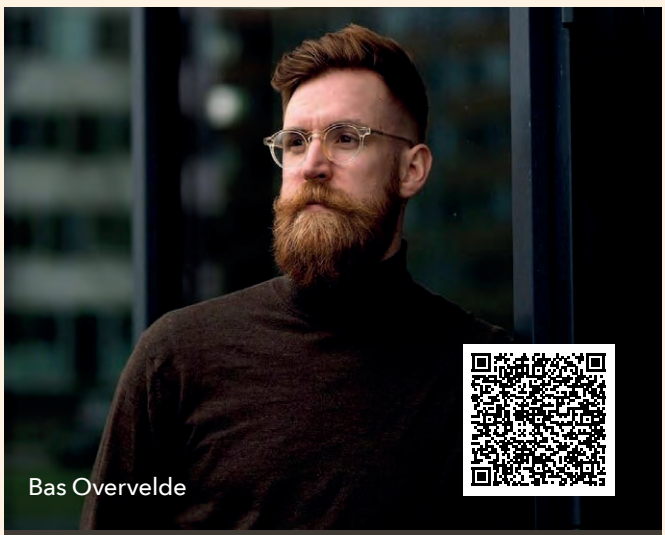
Friedrich adds: "There are very few centers with this focus, bridging life sciences and materials sciences in chemistry, the latter including for instance polymer assemblies. The new instrument will immediately be able to prove its added value in the recently awarded NWO Gravitation research program for Interactive Polymer Materials. The automation part of the CryoTEM system enables 24/7 data acquisition. This will accommodate quick progress for large amounts of samples for the various faculties."

NEWLY UPGRADED LAB OPENS MAY 30

The TU/e Center for Multiscale Electron Microscopy (CMEM) is located in Eindhoven. Although ThermoFisher has a production location at Eindhoven, the new Cryo-TEM was manufactured in Brno, Czechia. The proximity of the ThermoFisher location still has its benefits, as technical support arrives rapidly at CMEM. Both parties are currently working on a framework agreement that will be signed during the opening event of the upgraded microscopy laboratory on May 30. Cryogenic TEM is a clear focal point for CMEM. The same goes for quantitative 3D and in-situ EM such as Scanning Electron Microscopy (SEM) in environmental humidity conditions, as well as liquid-phase TEM imaging. CMEM is the flagship node for these specializations within the Netherlands Electron Microscopy Infrastructure (NEMI).

News, awards & grants

Scan the QR codes to read the full articles

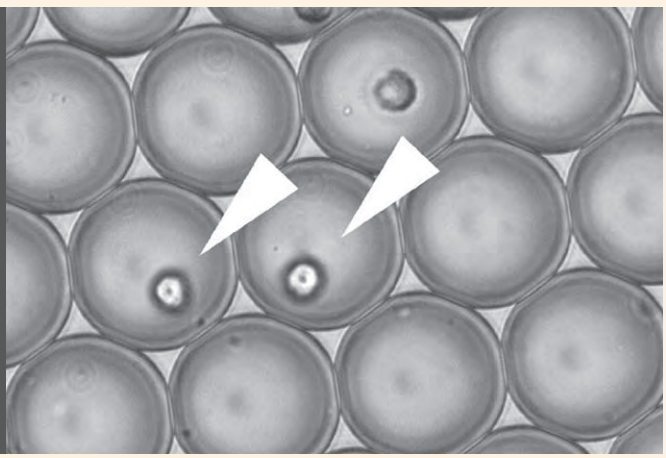


Early career award for pioneering research on soft robotics

RESEARCHER BAS OVERVELDE RECEIVES EARLY CAREER AWARD FROM KNAW.

How do cells spread word upon a viral infection?

Individual immune cells encapsulated in droplets imaged using a regular microscope
(Photo: Laura Eyndhoven).



ERC Advanced Grant to chase the holy grail of "drugging the undruggable"

RESEARCH LED BY LUC BRUNSVELD ON NEW TECHNOLOGICAL CONCEPTS FOR DRUG DEVELOPMENT IS AWARDED A PRESTIGIOUS ERC ADVANCED GRANT WORTH 2.5 MILLION EUROS.

Luc Brunsveld.

Mechanical Engineering dean Patrick Anderson.
Photo: Bart van Overbeeke

NEW MECHANICAL ENGINEERING DEAN PATRICK ANDERSON

A catalyst for connection in a growing department

Mert Astam winner of the 3rd ICMS PhD Publication Award!

Mert Astam wins the ICMS PhD Paper Award

Mert Astam

Last November, Mert Astam of the department of Chemical Engineering and Chemistry received the ICMS PhD Paper Award. He also won the public vote for the pitch of his paper "Self-regulating electrical rhythms with liquid crystal oligomer networks in hybrid circuitry". In it, he describes a material that could eventually be applied in soft robotics.

In his paper, published last year in the journal Soft Matter, Astam exploits the thermal behavior of liquid crystals. Based on the phenomenon that a polymerized liquid crystal quickly contracts when exposed to heat, he built a self-regulated oscillator with frequencies between 0.08 and 0.87 Hz. He used a clever design where a thin film of polymerized liquid crystal diacrylate spans a gap. The film contains an electrical heating wire and at the bottom of the gap lies an electrode. Without heating, the film sags until it hits the bottom electrode. This activates the heating wire so that the material quickly contracts. As the contact with the electrode is lost, the power to the heating wire is cut off: then a new cycle of cooling and heating begins. “We have thus translated the thermal behavior of the polymerized liquid crystal into an oscillating motion,” Astam explains. He foresees using the set-up as an actuator, or as a sensor that produces a signal when a certain temperature is reached. “Think of a very simple sensor for consistent temperature control in a heater,” Astam says. He also mentions the possible application in small soft robotics for handling delicate objects, although this is still distant future.

ENGAGE WITH THE AUDIENCE

The jury praised the effectiveness and energy of Astam’s pitch. He also won the public vote. Does he have any tips? “Engage with the audience and use analogies people can relate to. For example, when talking about self-regulation, I mentioned a Roomba, an automatic vacuum cleaner. Also, use very simple slides with just one or two pictures and preferably no text, so people are really paying attention to you.”

Connecting the ICMS PhD students

From left to the right: Mert Astam, Juul Verbakel, Fatuma Omar, Shayan Zarin-Bal, Selina Janssen, Aref Saberi, Derek van Tilborg. Not in this photo: Roos van Hoffe

Doing a PhD can be a struggle and sometimes even feel a bit lonely. The ICMS PhD Outreach Committee tries to connect the 200 PhD students of ICMS, amongst others by organizing social events and handing out a prize for the best scientific paper.

For starting PhD students, the ICMS "onboarding session" serves as an introduction to the institute, and an opportunity to get to know each other. After that, many PhD students continue within their own research group, losing sight of fellow students at other groups. "Our goal is to keep the interaction going," says Shayan Zarin-Bal, a first-year PhD student in the department of Biomedical Engineering. He recently joined the PhD Outreach Committee, helping to organize social events like barbecues, game nights, and of course "borrels". "It's all about relaxing and having a nice time with other ICMS members. Not thinking about your research, but having fun with other people that live the same life as you," says Selina Janssen, also a first-year PhD student in the department of Biomedical Engineering and a new committee member.

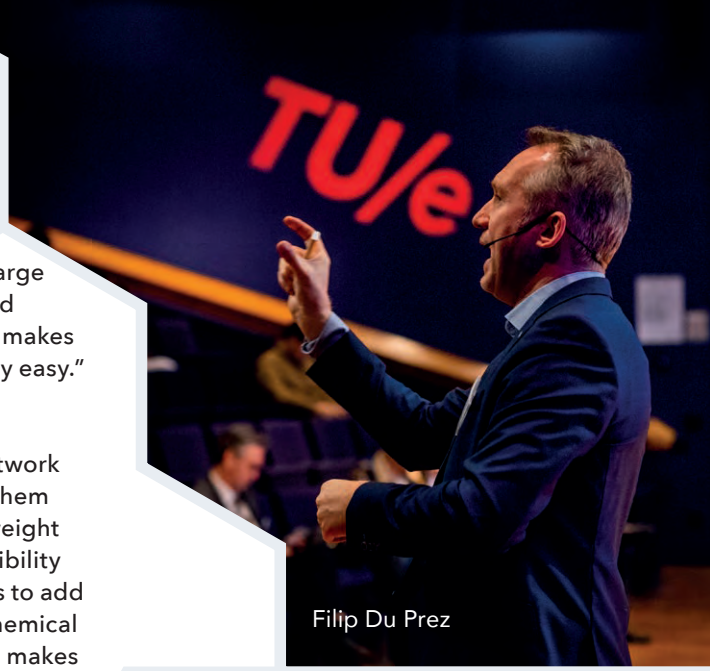
SHARING EXPERIENCES

But it's not only about having fun. In April a mini symposium featured former ICMS PhD students in their next career stage. Sharing their experiences in academia or industry can be very valuable for current PhD students, Janssen and Zarin-Bal say. And last but not least, there's the annual ICMS PhD Paper Award. "It enables sharing the science done in ICMS, and finding overlapping research topics," Zarin-Bal says. Last November, Mert Astam received the award as can be read elsewhere in this magazine. As first-year PhD students, Janssen and Zarin-Bal both experience the weight of pulling off such a large scientific project for the first time. Do they even have time for organizing and attending social events? "Yes, it's actually not that time-consuming," Janssen says. "And I like organizing these things. It's definitely worth it, I'm having a lot of fun."

Stay updated on upcoming events of the PhD Outreach Committee

Pulling the trigger on thermosets

At present, producing fully reusable yet functional thermoset polymers might sound as difficult as turning back time. It is not. The technical challenge is still huge, but thanks to scientific progress dynamic sustainable materials are becoming a serious option. One of the leading powerhouses to develop such materials is Filip Du Prez's Polymer Chemistry Research Group at Ghent University. He welcomes ICMS as a contender to the field, bringing its own specialized knowledge.



Filip Du Prez

"About 400 million tons of polymers are produced per year worldwide," says Filip Du Prez. "Of those, 65 million tons are thermoset materials – wind turbine blades, high-end cycling frames, automotive parts and other high-performance applications. Where plastics such as PET can be fully recycled, presently there are at best only downcycling solutions for thermosets." Du Prez and his group (see box) are working on dynamic sustainable materials to change that. The key lies in a built-in sensitivity to a trigger – temperature or light – that turns the crosslinking points in covalent networks dynamic again. Following this trigger, molecular structures once again come into motion. This means that an object consisting of such dynamic covalent networks can be recycled into its original starting material, and that new objects can be made from thermoset and composite recyclate. Same materials, same process, same objects, same characteristics – potentially endlessly.

EXTRUDED THERMOSETS

To Du Prez, this functional reuse is the future. "It goes far beyond the present best practice of recovering fibers from composites for example through hydrolysis. In that process, of which the economic feasibility is doubtful, the organic components which comprise half of the volume still cannot be recovered. And what's more, this production and recycling process still involves chemicals such as specific epoxy compounds that industry and government wish to abolish over time."
Dynamic covalent networks – or circular thermoset materials – wouldn't need the low viscosity production processes of present thermoset materials, but could ideally be used in the same extrusion and injection molding processes as thermoplastic materials are used in today. That would bring down production costs considerably – and thanks to that, enlarge the field of application. Du Prez: "As a bonus, thermosets are used mainly for quite large objects in a rather clear and concise supply chain. That makes recycling logistics relatively easy."

PUSH PERFORMANCE

The highly cross-linked network nodes in thermosets give them an unrivaled strength-to-weight ratio. "The secret to reversibility of the thermoset process is to add weaker bonds or loosen chemical groups deliberately, which makes the network dynamic. This can trigger the materials above a certain temperature to become plastic again. The American spin-off Mallinda already brings this into practice with its polyimine-based Vitrimer resin VITRIMAX™." In 2020, the Du Prez research group managed to produce fully recyclable crosslinked materials in an extruder. "They are sufficiently plastic to enable flow. It's a good proof of concept, but the resulting material has a rather high creep," Du Prez says.

To stretch scientific boundaries further, his group received an ERC advanced grant. "We go for the use of cheap, ideally biobased bulk chemicals as the starting point for dynamic sustainable materials," he states. "The high technical requirements for thermosets and corresponding composites make that a hard thing to achieve.
The required creep resistance, for instance, should at least mimic that of non-recyclable analogues.
Most of the patents and literature for dynamic covalent networks show much lower performance than classic thermosets. That's not good enough for industry. That will still demand a lot of research, but we soldier on. We are now at the stage of first in-company application testing. We expect the first practical applications in three to five years. But, as ever, success depends on a lot of different parameters."

KNOWLEDGE SHARING

ICMS has been involved in developing dynamic materials for years on end. "I regard it as one of the world leaders in dynamic materials based on non-covalent bonds," Du Prez states. Gradually, the focus within ICMS shifts to dynamic materials with covalent bonds as well, which is the field of the Du Prez group at Ghent University. He considers it a great development: "It places ICMS in a very strong position when it comes to possible combinations of non-covalent and covalent bonds in the same dynamic material.
Our fields of expertise are therefore very complementary, which makes it highly worthwhile to collaborate and to share knowledge."

Professor Filip Du Prez
is the head of the Polymer Chemistry Research Group within the Centre of Macromolecular Chemistry (CMaC) at Ghent University in Belgium. He is a member of the Scientific Advisory Board of the Interactive Polymer Materials Research Centre within ICMS. As such, he is involved in a new gravitation program that aims "to develop a new generation of intelligent, dynamic polymer materials."

Jan van Hest and Monique Bruining

Full speed ahead on a crystal clear course

ICMS thrives. The combination really works: multidisciplinary talent, excellence in scientific knowledge, strong partnerships, a vibrant community, and an outstanding equipment infrastructure. It was assessed that external branding of the ICMS organization could be further improved – and that's what will happen. The course for the future is crystal clear.

"Our third lustrum offers an excellent opportunity for evaluation," says professor Jan van Hest, scientific director of ICMS. "We are proud of fifteen years of scientific excellence in molecular systems for advanced, interactive materials, and for engineering life. This has for instance already led to seventeen spin-off companies – a number that will further increase."
Apart from the two fields of application, ICMS is also organized in seven thematic domains. Van Hest: "We noticed that these domains made our profile somewhat confusing to the outside world." Monique Bruining, managing director of ICMS adds: "Internally, we actively work together in a highly multidisciplinary and interdisciplinary way. No problem there. But for our partners and customers we wish to make things also crystal clear. We therefore adjusted the ICMS vision and established that we are basically active in three domains."

A CLEAR PROFILE

Van Hest: "Our basis is fundamental knowledge development. We establish what molecules there are, or can be designed, and we theorize what can be done with them. We describe these molecules ever better and predict their behavior. We utilize new technologies to characterize them for more thorough understanding and we test them in new practical applications. This way, we span the entire knowledge chain from theory to application."
Bruining summarizes: "That is a nicely integral approach with a clear profile. In practice it boils down to smart processing of ever larger amounts of data: Big Data, high throughput analysis, and Artificial Intelligence (AI)." ICMS invests heavily in these Big Chemistry capabilities, in collaboration with Radboud University Nijmegen and the University of Groningen. There will be also a proprietary robot laboratory where companies get the opportunity to tap into drug discovery capabilities supported by machine learning.
Bruining: "Next to drug discovery, AI is also used to improve formulation and to develop novel drug release systems, apart from the standard lipid globule-based approach. Our platform for a combined chemical and biological approach really makes us stand out in the world." Van Hest adds: "We already have strong ties with major chemical companies in relation to our advanced (interactive) materials research. As to engineering life, the fact that Big Pharma research is no longer present in the Netherlands has its influence. But by providing a unique combination of talent, knowledge, a community, and an equipment infrastructure, we are raising a growing interest from major pharma companies."

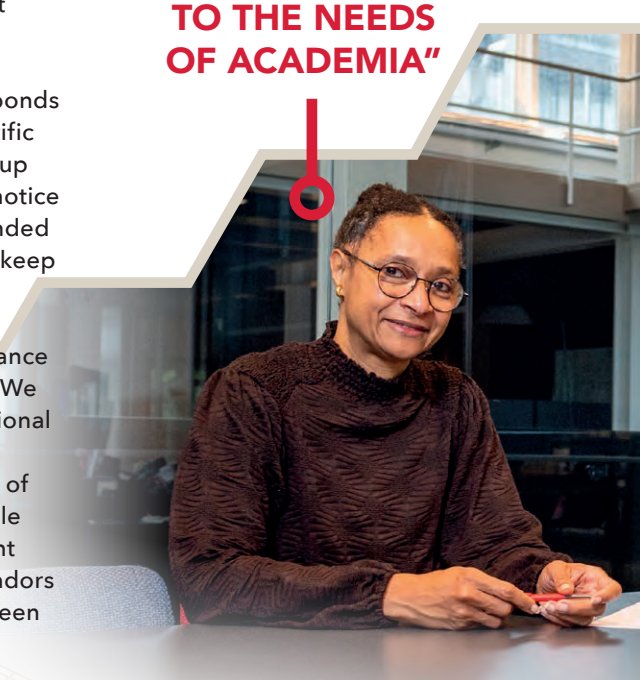
EXCELLENCE AND FUN

Existing strengths will of course be maintained. "Our strong, vibrant expert community is one of our main assets," says Bruining. "We organize a lot of networking events for our PhD students with their widely varying international backgrounds, encouraging strong informal connections and knowledge exchange. We have our own paper competition with a thorough assessment by a postdoc jury on the basis of scientific merits and 'sexiness' of the topic. During our November event the latest winner was announced during a buoyant gathering. Sparks did fly! Cross linking is not only a molecular phenomenon, it also makes the bonds between people stronger. Scientific excellence is stimulated bottom-up by sheer fun. And top-down we notice that the ideas we've launched landed well within the community. We'll keep on training the 'scientific muscle' within the ICMS Community."
Van Hest emphasizes the importance of informal ICMS ambassadors. "We have a strong appeal on international PhD students and post-docs. For instance, the enthusiastic writing of a Turkish blogger had a noticeable impact on the arrival of new talent from his native country. Ambassadors strengthening connections between talent, academic partners and businesses are very important to the growth of our community."

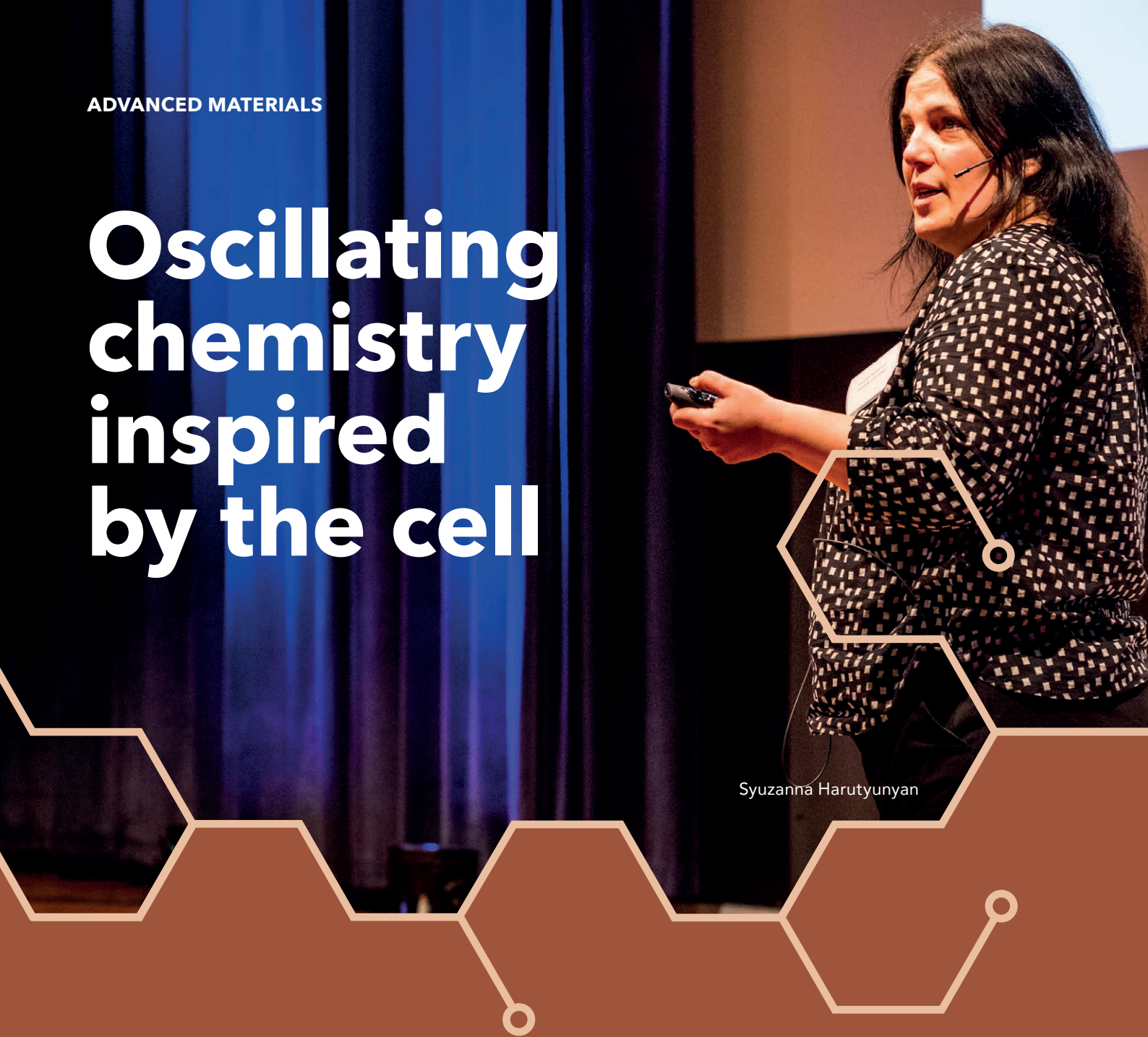
GROWING INTERACTION

"ICMS was the first institute at TU/e to enter a multidisciplinary itinerary," Van Hest remarks. "Since then, exchanging knowledge between disciplines and taking away barriers has become ever more important in science. The same goes for the exchange between universities, like we for instance have with Nijmegen, Groningen and IBEC in Barcelona. We also maintain ties with Utrecht, Wageningen and Leiden. We are strongly engaged in a partnership with the Max-Planck-Institute for Polymer research in Mainz. We choose our partners very carefully – and make sure ICMS stands for a great complementary fit."

"THE PASSION AND DEDICATION WITH WHICH THE ICMS STAFF HAS ACTED IN RECENT YEARS HAS BEEN KEY TO REACH OUR GOALS. IT IS A COHESIVE AND OPINIONATED TEAM THAT UNDERSTANDS AND RESPONDS WELL TO THE NEEDS OF ACADEMIA"



Oscillating chemistry inspired by the cell



Syuzanna Harutyunyan

A chemical reaction can be quite straightforward. Add one or several reactants to a flask, maybe use a catalyst and under the right conditions you can expect chemical products. In one of her research lines, Syuzanna Harutyunyan of the University of Groningen focuses on a different kind of chemistry. As a professor of Homogeneous Catalysis she performs synthesis based upon chemical reaction networks that are able to autonomously and periodically generate and inhibit a catalyst. These so-called oscillating reactions could one day lead to more efficient chemical processes. Harutyunyan was a guest speaker at the ICMS symposium last March.

The biological cell is a chemical marvel. Chemists can still only dream of performing hundreds or even thousands of parallel chemical reactions in a single reactor. Moreover, cell reactions barely have unwanted by-products and often provide "feedback" to other reactions, triggering, catalyzing or inhibiting them. This can create so-called oscillating behavior which underlies many important physiological functions such as respiration, heartbeat and ovulation.

Syuzanna Harutyunyan is impressed by what Nature does, even more since she started her research in this field four years ago. "It's amazing when you realize what is happening in the body. We often take that for granted, but in fact we have a lot to learn from the biological cell." She refers to the quite restricted set of organic molecules used by the cell. "It's mainly sugars, amino acids, nucleotides and fatty acids. With such a simple set of compounds Nature is able to do extremely complex chemistry." Harutyunyan is trying to design her own chemical reaction networks that exhibit oscillating behavior. This could allow for well-regulated and efficient chemical synthesis of various molecules within one flask. "Multi-step synthesis can be labor-intensive. It often involves activation and deactivation of catalysts, separation steps, product purification, and so on," she says. "We are trying to design multi-step synthesis that can regulate itself autonomously, without interventions."

CREATING A RYTHM

Probably the most well-known non-biological example of an oscillating reaction is the Belousov-Zhabotinsky (BZ) reaction. It can lead to a constantly moving pattern of bright colors in a petri dish – an almost psychedelic spectacle – or a solution in a flash that changes color continuously. These and many other oscillating reactions are inorganic and often require highly acid conditions, which prevents their diversification and application. Creating an organic equivalent would overcome these problems. But this is where it gets complicated. Whereas the BZ reaction was discovered serendipitously, designing an oscillating organic reaction from scratch is highly challenging. Harutyunyan explains that if you combine many chemicals in one reactor, a lot of chemical reactions are possible. Most of the reactions are unwanted. "It is like an orchestra without a conductor that creates a lot of noise," she says. "But with the right combinations and concentration of compounds that we can find through calculations and modeling we can start to control the chemical system and create a rhythm."

LIKE A CLOCK

She mentions a chemical reaction network her group designed. It consists of nine molecules in one flask and displays four different reactions happening at the same time. The concentrations of various molecules increase and decrease periodically at specific time intervals. It is like a clock, she explains. "One of these oscillating molecules is a catalyst. Therefore, in addition to keeping track of time, it can promote other chemical reactions. If we add new compounds to the same flask, this oscillating catalyst can allow them to react when its concentration is high. It's quite remarkable that we then have six reactions and twelve different molecules in one reactor, regulating each other autonomously through feedback loops."
The system consists of very simple molecules available in every lab. "For example for our oscillator we use Fmoc-protected piperidine, N-methylpiperidine, phenylacetate and nitrophenylacetate. And we showed that if we add other reagents, such as malonate and salicyl aldehyde we could catalytically and periodically synthesize coumarin derivatives, which are at the core of some drugs," Harutyunyan says.

A SMALL CHEMICAL FACTORY

Harutyunyan is clear about her scientific drive: "Most importantly, it is a cool thing to be able to do chemical synthesis in this way," she says. "To be able to carry out chemistry the way our body does it. For now, this is purely fundamental research. And to be honest, to produce simple commodity chemicals you don't need this kind of chemistry." Harutyunyan works together with scientists from ICMS. "My experience is that in institutes like ICMS you can really use each other's expertise. More people around you means that there are more potential solutions available to the problems you are facing. Such a 'family feeling' is a great advantage," she says. In the end the chemical networks could lead to more efficient chemical synthesis. "You could design multi-step parallel chemical synthesis in one flask. This small chemical factory wouldn't generate byproducts and doesn't require isolation and purification steps," she says. "But this chemistry is still very new. We know we can do it but the systems we are using are still far from that point."

Sofia Calero

Inventing materials for a green future

Bridging the gaps, in every possible direction. That is one of Sofia Calero's scientific challenges. As a professor, she leads the Materials Simulation & Modelling group at the Department of Applied Physics and Science Education and is involved in the TU/e research institutes EIRES (Sustainable Energy) and EAISI (Artificial Intelligence). Recently, she joined ICMS to establish new collaborations.

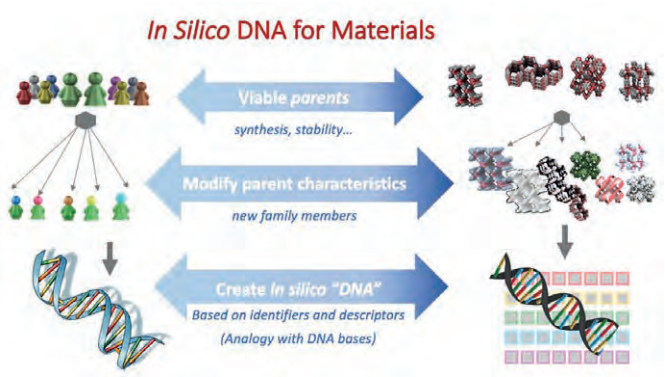
Sofia Calero is at the center of numerous new, often multidisciplinary collaborations that are somehow related to molecular simulation. Her field of research is very broad, Calero explains. "We can deal with all modes of simulation, especially molecular simulation in materials. An important goal is our search for new materials used in the implementation of new green technologies." Enthusiastically gesticulating, she lists diverse examples: "Green hydrogen technology, developing materials for efficient carbon capture, optimizing perovskite solar cells, and methods to produce ammonia, urea, and formic acid."

The work of Calero's group can be roughly divided into two lines of research, where both applicability and fundamental research have their place. And where necessary, Calero is there to connect the two. "In the first line, we try to optimize existing materials and processes, to design how certain materials could perform better after some modifications. These studies are often in collaboration with industrial partners. They want to improve their materials and products and our simulations help investigate whether those modifications are beneficial." This is often in the field of green materials, but Calero also works on the development of carriers for drug delivery or the design of unique liquids for smart (mobile phone) screens. "One of the advantages of simulations is that you can easily adapt to a given problem," Calero clarifies the diversity.

THE DNA OF MATERIALS

In the second research line, Calero is developing a completely new way to design materials. She enthusiastically explains: "To make industrial processes more sustainable, we want to design new materials with a stable structure and a high performance. To do so, we are trying to 'crack the DNA code' of materials. We are building a multilayer Machine Learning architecture that is based on how DNA contains our genetic code. Just as each species has a distinct DNA that determines its key traits, we aim to build an in silico DNA for materials. Whenever you need a material with specific characteristics, you can have a look at this databank. To get an idea which material could be useful, or which material can be used as 'father' in the design of a new material."

For the simulations, the group of Calero developed their own software. In fact, several times Calero was at the cradle of internationally recognized modeling software. She is one of the originators of the open-access software RASPA – used in molecular simulation of adsorption and diffusion in flexible nanoporous materials – and iRASPA, which is GPU-accelerated visualization software for materials scientists. Due to the expertise with this state-of-the-art software, researchers worldwide are increasingly finding the Materials Simulation & Modelling group.



METHODOLOGY IS THE CORE

Calero enjoys performing research under the wings of TU/e's leading research institutes EIRES (Engineering for Renewable Energy Systems) and EAISI (Eindhoven Artificial Intelligence Systems Institute). Her latest project also involves ICMS. "Never stop building bridges," she says with a wink. "Recently, a PhD student started a joined project optimizing materials used in the production and storage of hydrogen. He will work in between these institutes. Hopefully, this states the beginning of more intense contacts and the formation of new collaborations in this triangle."

"Methodology is the core of our research. With modeling you can do anything, you just need a good project. Researchers often have a wrong image of simulation, they think we are far away from reality. But the opposite is true. So there are still plenty of bridges to build. Because precisely multidisciplinary projects are very valuable. My group is very good at simulation and modeling. But we need close interaction with experimentalists and industry, to see whether the results we find with our models are also correct in practice. And I am looking forward to strengthening these interactions within the framework of my new collaboration with ICMS. ICMS has an extensive network of researchers with expertise in many disciplines. This is very helpful in generating new ideas, forming new collaborations, and doing real science. If we all work together, science will move in the direction I envision."

PHOTO IMPRESSION ICMS ANNUAL SYMPOSIUM 2023


TU/e
multidisciplinary research

Early-stage drug discovery with AI

How to make AI work without Big Data

From left to the right:
Derek van Tilborg,
Francesca Grisoni,
Rıza Özçelik

Deep learning typically enables finding patterns in large amounts of data, patterns that humans cannot detect. But can the benefits of this methodology also be exploited when the large amounts of data are taken out of this equation? That is the all-important question for methodology development in AI-based early-stage drug discovery. Francesca Grisoni, Derek van Tilborg and Rıza Özçelik tell how they eventually hope to replace the "educated guesses" that often dominate early-stage drug discovery.

"Finding good starting molecular cores with high chances of success, that is what early-stage drug discovery is all about," Francesca Grisoni states. She is an assistant professor in the department of Biomedical Engineering at TU/e, where she leads the Molecular Machine Learning team. "But how do you find those among an estimated 10^{60} drug-like molecules?" That is the million dollar question. Grisoni: "The search is after non-toxic molecules that bind to and modulate disease-related proteins in the body."

THE CHALLENGE

Already methods such as similarity search, QSAR modelling or virtual screening are deployed to help find therapeutic needles in the giant molecular haystack. "These consist mainly of trial and error based on human intuition," Grisoni summarizes. But then neutral networks appeared. "In no time these neural networks gave a powerful boost to progress in many fields. The combination of Big Data with AI enables researchers to find meaningful information that humans cannot find." Grisoni explains where the challenge lies when it comes to AI and early stage drug discovery: "We don't have Big Data to work with. That is why the results don't match those in other fields." The idea of designing chemicals with AI has been around for some years, PhD student Rıza Özçelik says, but progress has not been impressive lately. "Results seem to have reached a plateau. This means we have to rethink all steps and ingredients to revitalize AI for molecular design. From molecular representation to more data-efficient models. That is what we do now."

WORKAROUNDS

There are several ways to work around the lack of data. Grisoni: "A promising approach is transfer learning. When you only have a tiny dataset, you can feed the algorithm with knowledge from neighboring fields and transfer this 'partly meaningful' knowledge to your model." She reveals what she personally thinks will work: "Introducing knowledge from chemistry into neural networks will have a beneficial effect. Teaching the system general chemistry knowledge might alleviate the need for big data sets." Another important direction, she hypothesizes, is to represent molecules differently than has been done so far, specifically aimed at deep learning. "We have represented molecules in the same way for decades, leaving out a lot of what we know about the underlying 'chemical reality'," Grisoni says. "Humans have built abstract representations over time. For AI this abstract and missing knowledge has to be specified and introduced to the architecture. We must provide the models with the ingredients that enable them to learn in small data regimes. I recently received an ERC starting Grant to explore this path."

MOLECULAR REPRESENTATION

PhD Student Derek van Tilborg researches how to apply graph neural networks to screen molecule libraries for their bioactivity with respect to relevant drug targets. Van Tilborg: "You could phrase this as 'how to predict molecular properties with deep learning, by learning from molecular data.' Part of this is the translation of molecules into numbers that can be used in combination with an AI model. At present, the high throughput screening of molecules for their bioactivity is horribly expensive." Van Tilborg: "It would therefore be very attractive to optimize the 'hit rate' by performing an AI driven pre-selection process. You want a pretty good indication beforehand of which molecules will and will not work." Two theoretically possible workarounds – adding more data and coping with uncertainty through Bayesian methods – only seem able to replace high costs with equally high cost. This is the reason why Van Tilborg investigates a graph approach instead of representing molecules with "classical" molecular descriptors. "Although we are still pondering the best method," he says.

MOLECULES AS GRAPHS

Van Tilborg further explains: "As useful data in the public domain are scarce, the challenge is to creatively make the models more effective on the basis of small data sets. I therefore investigate the effects of graph representation on model uncertainty, and a model's ability to deal with new data that are very different from the data it has used to learn from in the past. But first of all, the quality and information content of the data we do have are vital. If a candidate molecule is too different from the molecules used for training, the model predictions will be less reliable."

Van Tilborg mostly looks at direct molecular representation, meaning the structure itself, without calculating properties of the molecule. "My approach is to represent the molecule as a graph, where atoms are nodes and bonds are edges, and to use AI to learn from the corresponding graph topology and chemistry." The representation of a molecule as a graph seems to work well for quantum chemistry and atom-level predictions. However, for more complex situations like bioactivity, older methods still outperform graph-based models. Predicting bioactivity is extra challenging due to the complex molecular interactions involved. Especially when using only the structure of the ligand, as Van Tilborg does. "This makes it very complex to achieve predictive deep learning models."

So how can dynamic characteristics of a molecule be included in a numerical representation? "If we indeed find a way to get the dynamics into the picture, it might make a difference. It's too early to assess how much of a difference it will make."

CHEMICAL LANGUAGE APPROACH

"I work at the same challenge as Derek, but we both work from a different perspective," PhD Student Rıza Özçelik indicates. "AI has the potential to accelerate early stage drug discovery. And – at least equally important – to reduce the number of false candidates that now consume lots of testing capacity and budget." Özçelik is exploring that path by designing molecules from scratch. "So molecules that would be bioactive for a disease-related protein." He does that by feeding millions of molecules with a known structure into a model that should "learn the language of the molecule." Özçelik: "You can take that quite literally, as that model has the same architecture as a model for learning natural language. Model-wise, it hardly makes a difference whether you want to learn English, Turkish or 'chemical language'." By showing millions of arbitrary examples of molecules in the chemical language and a handful of bioactive molecules, the model learns to spit out sentences that hopefully contain drug candidates. Özçelik: "This means: bioactive molecules that would strongly bind to the target protein." In due time the molecules he designed will be tested in a wet lab, but for now that is still too early.

AMBITIOUS MOLECULES

Özçelik emphasizes that the promise of AI early-stage drug discovery actually goes beyond beating the present approach of educated guesses. "The limitation of what we do now, is that humans always build on what they already know. The molecules that this delivers will always resemble those we already worked with. As humans we have an inescapable tunnel vision." In contrast, AI is not hindered by experience. "The molecules that we are looking for don't have to be close to the ones we already know," Özçelik states. "The important thing is that they can bind to disease-related proteins and affect their function. We can even encourage the models to design molecules that are ambitious, diverse, and remote from what we already know. We need candidates that bind specifically and that bind strongly. That is especially needed with disease-related proteins without any known binders."

Grisoni, van Tilborg and Özçelik are discovering uncharted territory. Özçelik: "AI for drug discovery is still in its infancy, but it is plausible that it will eventually help us find better drug candidates more easily." Grisoni adds: "We have only explored the tip of the iceberg so far. We have only started to witness what this new technology can achieve."

Key publications

NOVEMBER 2022 – APRIL 2023

01. BIOLUMINESCENCE GOES DARK: BOOSTING THE PERFORMANCE OF BIOLUMINESCENT SENSOR PROTEINS USING COMPLEMENTATION INHIBITORS
A. Grawe, M. Merkx
ACS Sens. 7, 3800–3808 (2022)

02. ENGINEERED HYDROGELS FOR MECHANOBIOLOGY
U. Blache, E.M. Ford, B. Ha, L. Rijns, O. Chaudhuri, P.Y.W. Dankers, A.M. Kloxin, J.G. Snedeker, E. Gentleman
Nat. Rev. Methods Primers 2, 98 (2022)

03. FUNCTIONAL MAPPING OF THE 14-3-3 HUB PROTEIN AS A GUIDE TO DESIGN 14-3-3 MOLECULAR GLUES
B.A. Somsen, F.W.B. Craenmehr, W.W. Liu, A.A. Koops, M.A.M. Pennings, E.J. Visser, C. Ottmann, P.J. Cossar, L. Brunsveld
Chem. Sci. 13, 13122–13131 (2022)

04. HIGH EFFICIENCY QUASI-2D RUDDLESDEN-POPPER PEROVSKITE SOLAR CELLS
A. Caiazzo, R.A.J. Janssen
Adv. Energy Mater. 12, 2202830 (2022)

05. POLYMER DISPERSED CHOLESTERIC LIQUID CRYSTAL MIXTURES FOR OPTICAL TIME-TEMPERATURE INTEGRATORS
A.A.F. Froyen, M.G. Debije, A.P.H.J. Schenning
Adv. Opt. Mater. 10, 2201648 (2022)

06. ROBOTIC PICK-AND-PLACE OPERATIONS IN MULTIFUNCTIONAL LIQUID CRYSTAL ELASTOMERS
P. Lyu, M.O. Astam, C. Sanchez-Somolinos, D. Liu
Adv. Intell. Syst. 4, 2200280 (2022)

07. SPECTRALLY PAINTING A SINGLE CHAIN POLYMERIC NANOPARTICLE AT SUPER-RESOLUTION
E. Archontakis, L. Deng, P. Zijlstra, A.R.A. Palmans, L. Albertazzi
J. Am. Chem. Soc. 144, 23698–23707 (2022)

08. THE ONGOING QUEST FOR THE FIRST TOTAL ARTIFICIAL HEART AS DESTINATION THERAPY
A. Vis, M. Arfaee, H. Khambati, M.S. Slaughter, J.F. Gummert, J.T.B. Overvelde, J. Kluin
Nat. Rev. Cardiol. 19, 813–828 (2022)

09. THERMAL PAPER AND TIME TEMPERATURE INTEGRATORS MADE FROM A STRUCTURAL COLORED POLYMER CROSSLINKED WITH HYDROGEN BONDED CYCLOHEXANOIC ACID DERIVATIVES
Y. Foelen, D.A.C. van der Heijden, A.M.J. Verdurmen, D.J. Mulder, J. Lub, A.P.H.J. Schenning
Adv. Opt. Mater. 10, 2201462 (2022)

10. CIRCULARLY POLARIZED LIGHT PROBES EXCITED-STATE DELOCALIZATION IN RECTANGULAR LADDER-TYPE PENTAPHENYL HELICES
R. Ammenhäuser, P. Klein, E. Schmid, S. Streicher, J. Vogelsang, C.W. Lehmann, J.M. Lupton, S.C.J. Meskers, U. Scherf
Angew. Chem. Int. Ed. 62, e202211946 (2023)

11. CLOSED-LOOP RECYCLABLE HIGH-PERFORMANCE POLYIMINE AEROGELS DERIVED FROM BIO-BASED RESOURCES
C. Wang, F. Eisenreich, Z. Tomovic
Adv. Mater. 35, 2209003 (2023)

12. COMPLEX COACERVATE MATERIALS AS ARTIFICIAL CELLS
A.B. Cook, S. Novosedlik, J.C.M. van Hest
Acc. Mater. Res. 4, 287–298 (2023)

13. COVALENT PROTEIN IMMOBILIZATION ON 3D-PRINTED MICROFIBER MESHES FOR GUIDED CARTILAGE REGENERATION
M.J. Ainsworth, O. Lotz, A. Gilmour, A. Zhang, M.J. Chen, D.R. McKenzie, M.M.M. Bilek, J. Malda, B. Akhavan, M. Castilho
Adv. Funct. Mater. 33, 2206583 (2023)

14. DETERMINANT ROLE OF SOLUTION-STATE SUPRAMOLECULAR ASSEMBLY IN MOLECULAR ORIENTATION OF CONJUGATED POLYMER FILMS
J. Deng, L. Zheng, C. Ding, Y. Guo, Y. Xie, J. Wang, Y. Ke, M. Li, L. Li, R.A.J. Janssen
Adv. Funct. Mater. 33, 2209195 (2023)

15. LEVERAGING MOLECULAR STRUCTURE AND BIOACTIVITY WITH CHEMICAL LANGUAGE MODELS FOR DE NOVO DRUG DESIGN
M. Moret, I. Pachon Angona, L. Cotos, S. Yan, K. Atz, C. Brunner, M. Baumgartner, F. Grisoni, G. Schneider
Nat. Commun. 14, 114 (2023)

16. MICRO-TOPOGRAPHIES INDUCE EPIGENETIC REPROGRAMMING AND QUIESCENCE IN HUMAN MESENCHYMAL STEM CELLS
S. Vermeulen, B. Van Puyvelde, L. Bengtsson del Barrio, R. Almey, B.K. van der Veer, D. Deforce, M. Dhaenens, J. de Boer
Adv. Sci. 10, 2203880 (2023)

17. NONLINEAR TRANSIENT PERMEABILITY IN PH-RESPONSIVE BICONTINUOUS NANOSPHERES
W.P. van den Akker, H. Wu, P.L.W. Welzen, H. Friedrich, L.K.E.A. Abdelmohsen, R.A.T.M. van Benthem, I.K. Voets, J.C.M. van Hest
J. Am. Chem. Soc. 145, 8600–8608 (2023)

18. ON-DEMAND MICROFLUIDIC MIXING BY ACTUATING INTEGRATED MAGNETIC MICROWALLS
S. Broeren, I.F. Pereira, T. Wang, J. den Toonder, Y. Wang
Lab Chip 23, 1524–1530 (2023)

19. POLARITONS IN A POLYCRYSTALLINE LAYER OF NON-FULLERENE ACCEPTOR
L. Liu, Z. Wei, S.C.J. Meskers
J. Am. Chem. Soc. 145, 2040–2044 (2023)

20. POLYDOPAMINE-BASED ALL SOLID-STATE FLEXIBLE ORGANIC NEUROMORPHIC DEVICES FOR ACCESS DEVICE-FREE ARTIFICIAL NEURAL NETWORKS
S. Kazemzadeh, L. Dodsworth, I.F. Pereira, Y. van de Burgt
Adv. Electron. Mater. 9, 2200427 (2023)

21. REVERSIBLE DUAL-COVALENT MOLECULAR LOCKING OF THE 14-3-3/ERRY PROTEIN-PROTEIN INTERACTION AS A MOLECULAR GLUE DRUG DISCOVERY APPROACH
B.A. Somsen, R.J.C. Schellekens, C.J.A. Verhoef, M.R. Arkin, C. Ottmann, P.J. Cossar, L. Brunsveld
J. Am. Chem. Soc. 145, 6741–6752 (2023)

22. SIMULATING ASSEMBLY LANDSCAPES FOR COMPREHENSIVE UNDERSTANDING OF SUPRAMOLECULAR POLYMER-SOLVENT SYSTEMS
S.A.H. Jansen, E. Weyandt, T. Aoki, T. Akiyama, Y. Itoh, G. Vantomme, T. Aida, E.W. Meijer
J. Am. Chem. Soc. 145, 4231–4237 (2023)

23. TRAINED IMMUNITY – BASIC CONCEPTS AND CONTRIBUTIONS TO IMMUNOPATHOLOGY
J. Ochando, W.J.M. Mulder, J.C. Madsen, M.G. Netea, R. Duivenvoorden
Nat. Rev. Nephrol. 19, 23–37 (2023)

24. TRANSIENTLY HERITABLE FATES AND QUORUM SENSING DRIVE EARLY IFN-I RESPONSE DYNAMICS
L.C. Van Eyndhoven, V.P.G. Verberne, C.V.C. Bouten, A. Singh, J. Tel
eLife 12, e83055 (2023)

25. VALENCY AND AFFINITY CONTROL OF APTAMER-CONJUGATED NANOPARTICLES FOR SELECTIVE CANCER CELL TARGETING
L. Woythe, D. Porciani, T. Harzing, S. van Veen, D.H. Burke, L. Albertazzi
J. Controlled Release 355, 228–237 (2023)

Finding the clues to inflammatory or healing cells

Livia Angeloni

Biomedical engineer Livia Angeloni is the newest ICMS fellow. She uses advanced atomic force microscopy to unravel how living cells respond to biomaterials.

"Sometimes, I wonder where the original idea for a particular experiment came from," says Livia Angeloni. "From curiosity about atomic force microscopy techniques, or from a fascination for biological principles. I think it's often both."

Angeloni is an expert in advanced atomic force microscopy, but also in cell mechanics. She wants to elucidate how immune cells mechanically respond to the physical properties of implants such as heart valves or cartilage replacements. In particular, she is interested in the responses of macrophages, the immune cells that are best known for their ability to engulf and disarm microbes or cancer cells. Her interest stems from the fact that macrophages also orchestrate the body's immune response to biomaterials. Angeloni: "In contact with an implant, macrophages can develop into different phenotypes, assuming, for example, pro-inflammatory or pro-healing functions. Thereby, they may determine the failure or success of an implant."

UNIQUE TOOLS

To unravel possible fundamental relationships between physical cues and cell response, Angeloni studies cell-surface interactions quantitatively. How do visco(elastic) properties of a biomaterial, a particular topography, curvatures, or an external load influence the development of macrophages? "Establishing such relationships could help bioengineers in the design of innovative biomaterials." Angeloni uses atomic force microscopy techniques such as single-cell force spectroscopy and fluidic force microscopy. These unique tools are able to measure physical interactions at the nanoscale. Over the years, she has also become an expert in technology development. She is, for example, combining fluorescence and atomic force microscopy to study mechanical properties of a single, live cell or, even smaller, cellular structures such as the cytoskeleton.

Name
Livia Angeloni

Position
ICMS Fellow, Soft Tissue Biomechanics & Tissue Engineering group (since 2023).

Previously
Postdoc (Eindhoven University of Technology), postdoc and Marie Curie-fellow (Delft University of Technology).

Studies
MSc Nanotechnology engineering (Sapienza University of Rome, Italy), PhD Material engineering (Sapienza University and Université Laval, Canada).

Motivation
I love it when you prove a hypothesis.

Dream
Building up my own research group.

Spare time
Playing with my children.

“It’s cool to pitch your ideas to the minister”

In Februari Robbert Dijkgraaf, the Dutch Minister of Education, Culture and Science, visited Eindhoven. He discussed some educational “valuables” with ICMS students.

“The setting was quite impressive,” says master student Claudia Hanegraaf. “I expected a small circle of people, but the minister arrived with a large delegation. And several members of ICMS staff came to listen too.” Former PhD student Richard Post was happily surprised. “The more listeners, the better. You don’t get the chance to speak about your ideas before such an audience every day.”

TWENTY MINUTES

On Monday February 13, nine ICMS students got exactly twenty minutes to speak with the minister of Education, Culture and Science during his work visit to Eindhoven University of Technology. Hanegraaf: “Twenty minutes is too short to give poster presentations. Therefore, we chose to discuss some aspects of the educational system that we treasure.” In groups of three, the students had prepared pitches. The first focused on the TU/e-system of challenge based learning – learning in small groups along actual societal problems. The second was on the rather easy-going, direct manner in which students and teachers interact on campus. The third pitch highlighted the large efforts students put into team projects such as building a solar car or a health care robot. After that pitch, PhD-student Maritza Rovers asked the minister for more support for such extracurricular activities, for example through scholarships or educational credits. “I’ve been part of such a student team myself, and it was an excellent training in soft skills such as communication and teamwork.”

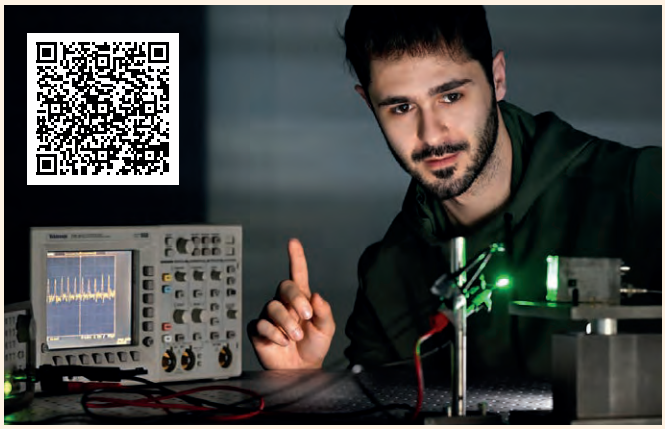
FRIENDLY AND HIGHLY INTERESTED

Hanegraaf expressed her concerns to Dijkgraaf that student-teacher relations may become less personal due to the increasing numbers of students, and Post pointed out the consequences for postdocs. Post: “I’ve just finished my PhD TA. The TA stands for teaching assistant, which means I got the opportunity to give lectures during my PhD studies. I really enjoy teaching. However, the fast growth causes an increasing pressure on PhDs to pass up research time for teaching.”
The ICMS students all agree that Dijkgraaf was friendly and highly interested, and that he replied very politically. “He expressed his confidence that our university would come up with innovative solutions,” says Hanegraaf. Rovers: “I understand that a minister can’t make immediate promises. But it’s a pity that there wasn’t more time for in depth discussion.” Post: “It was a really cool experience to pitch our ideas directly to the minister. I hope we’ve planted some tiny seeds for improvements.”

News, awards & grants

This "Harry Potter" light sensor achieves magically high efficiency of 200 percent

USING GREEN LIGHT AND A DOUBLE-LAYERED CELL, PHD RESEARCHER RICCARDO OLLEARO HAS COME UP WITH A PHOTODIODE THAT HAS SENSITIVITY THAT MANY CAN ONLY DREAM OF.



Researcher Riccardo Ollearo shows how the photodiode (right) picks up the signal from his finger, allowing him to see how fast his heart is beating on the screen (left).
Photo: Bart van Overbeeke

The future of data storage lies in DNA microcapsules

DNA ARCHIVAL STORAGE WITHIN REACH THANKS TO NEW PCR TECHNIQUE.

Tom de Greef.
Photo: Bart van Overbeeke.

Photo: Hans Dirksen.

Vici grant to help Patricia Dankers turn dreams into reality

PATRICIA DANKERS HAS BEEN AWARDED THE GRANT WORTH 1.5 MILLION EUROS TO REALIZE HER DREAM OF MAKING A SYNTHETIC EXTRACELLULAR MATRIX THAT DISPLAYS INTERACTIVE BEHAVIOR.

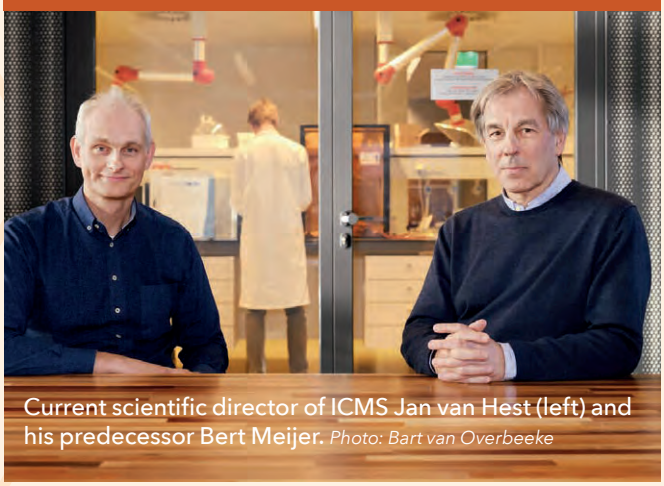
Education minister Robbert Dijkgraaf to visit Summa College, Fontys and TU/e

THE THREE ORGANISATIONS CALL FOR ATTENTION TO RAPIDLY GROWING DEMAND FOR TALENT IN BRAINPORT

Minister Robbert Dijkgraaf. *Photo: Martijn Beekman.*

ICMS: the institute that revolves around people

THE PLACE WHERE INTERDISCIPLINARY COLLABORATION HAS BEEN STIMULATED FOR 15 YEARS.



Current scientific director of ICMS Jan van Hest (left) and his predecessor Bert Meijer. *Photo: Bart van Overbeeke*

From left to right: Francesca Grisoni, Ruud van Sloun and Maarten Schoukens. *Photo: Loraine Schoukens*

Embarking on a new adventure with a huge European grant

FRANCESCA GRISONI, MAARTEN SCHOUKENS AND RUUD VAN SLOUN ARE ALL ASSISTANT PROFESSORS AT TU/E AND THE MOST RECENT RECIPIENTS OF AN ERC STARTING GRANT.

Monica Zakhari

Name
Monica Zakhari

Position
Assistant professor, Processing and Performance of Materials group (since 2021).

Previously
Postdoc (Stanford University and University of Texas, USA).

Studies
BSc Engineering and Material Science (German University in Cairo, Egypt), MSc Computational Mechanics (Polytechnic University of Catalonia, Spain & Swansea University, UK), PhD (TU/e).

Motivation
Making the world a tiny bit better.

Dream
Cleaning up microplastics with films of porous particles.

Spare time
Painting, calligraphy.

Understanding the behaviour of "mini-sponges"

Assistant professor Monica Zakhari models liquids containing porous particle. Her computational studies improve food products, paints, and diagnostics.

"My models can be applied in a lot of fields," says Monica Zakhari. "My research may look abstract to many, but for me it's very tangible because of all these applications. Although I enjoy the mathematics, I'm not in computational mechanics for the numerics. I use them to understand the physics of actual products."
Zakhari's models mathematically describe the physical behaviour of suspensions containing porous particles: How they flow, and if the particles stick to a surface, or roll or slip over it. Such particles can be the virtual counterparts of living cells, but also of food or paint ingredients. "Any particle that behaves like a kind of mini-sponge," Zakhari says.
The dynamic behaviour of her suspensions is surprisingly different from suspensions containing solid or soft non-porous particles. Processing such suspensions thus requires a different approach. Zakhari: "The flow dynamics are for example important to tune the optimal speed or pressure of the equipment, for example a 3D-printer."

INCREASING COMPLEXITY AND ACCURACY

By incorporating different particle shapes, particle interactions and chemical interactions, Zakhari's models gradually gain complexity and accuracy. Yet, a crucial aspect is continuously comparing calculated and experimental results "ICMS is an ideal environment to do so," emphasizes Zakhari. "I describe the behaviour of materials under development, but I can also provide clues to design materials tailored to achieve desired properties."
Does she have a favourite field of application? "It's impossible to choose, I like many. It's highly interesting and important to contribute to advanced diagnostic tools for metastatic cancer, but being a calligraphy hobbyist myself, I find paints also fascinating." For Zakhari, teaching and coaching on the job are the most rewarding aspects of being an assistant professor. "It feels very special when someone confides in you for personal or professional struggles, big or small."

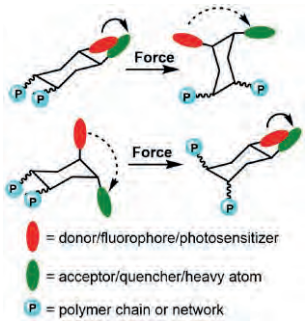
Introducing four EuroTech postdocs within ICMS

EUROTECH POSTDOC: **KHALID NAIM**

Khalid Naim obtained his PhD at the Institute of Nano Science and Technology (INST) in Mohali, India. While working on small boron-containing organic molecules, he found an interesting crystalline material that was not brittle, as most crystals are, but flexible. The finding sparked his interest in mechanical properties of materials. It motivated him to apply for a EuroTech postdoc with Rint Sijbesma, a pioneer in mechanochemistry, as his host at TU/e, and Charles Diesendruck at Technion Israel Institute of Technology as co-host.

Naim started last October at TU/e and is currently working on so-called mechanophores, molecules that change their chemical and physical properties under mechanical stress. The goal is to design mechanophores based on cyclohexane, with polymer chains and optically active groups attached, so that when stress is applied, they adjust their optical, mechanical or photosensitization properties. These new mechanophores could, for example, be used as stress and damage sensors. They might also enable mechanically tuning the photosensitization in a photosensitizer-heavy atom combination, which could be used in photodynamic cancer therapy.

Khalid Naim



Ansgar Oberheide

EUROTECH POSTDOC: **ANSGAR OBERHEIDE**

Ansgar Oberheide started as a postdoc in Luc Brunsveld's Chemical Biology group at the TU/e in September and has been an EuroTech postdoc since October. Oberheide obtained his PhD in organic chemistry at the University of Jena, Germany, where he worked on the synthesis of natural products with bio-activity that needed further elucidation.

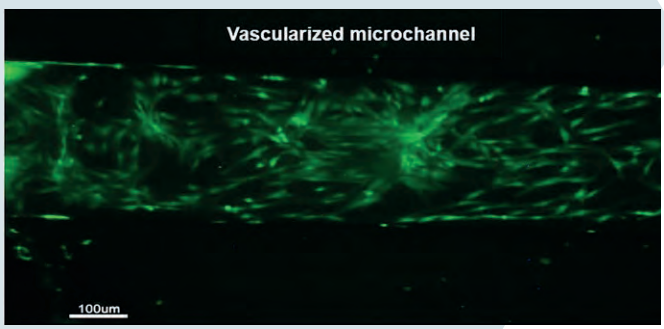
In Brunsvelds group he works on protein-protein interactions (PPIs) and studies small molecules that could be used to inhibit or stabilize those interactions.
The stabilizing molecules are called molecular glues.
The group focuses on a protein called 14-3-3 which binds to many different proteins. This includes proteins that are important in cancer, Alzheimer's disease and cystic fibrosis. The long-term goal is to develop drugs that can target those diseases by inhibiting or stabilizing the protein-protein interactions. But before anyone can start drug development, a fundamental understanding of PPI stabilization is needed. Oberheide now works on the development and synthesis of new molecular glues, and he studies how they work. That is already a big challenge.

EUROTECH POSTDOC: **ANA CARINA MANJUA**

Ana Carina Manjua fell in love with biomedical research during her masters at the New University of Lisbon, when studying electroconductive materials as biobatteries for pacemakers. During her PhD at the Instituto Superior Técnico in the same city, she worked on building a microchip to regenerate blood vessels. After that, she worked 1.5 years in a biomaterials company.

Manjua returned to research last March as a EuroTech postdoc at the TU/e Biosensors and Devices Lab. She will again work on microchips, this time in the context of cardiovascular diseases. The goal is to remodel cardiac tissue on a chip and recreate its micro-environment in order to simulate the disease and find ways to regenerate the tissue. Manjua's research will include the microchip design, developing a hydrogel for electromagnetic stimulation to regenerate cells, building a stretchable platform – at the Swiss University EPFL – to simulate cardiac rhythm, and arranging a computational interface, before she can actually study the cardiac tissue.

Ana Carina Manjua

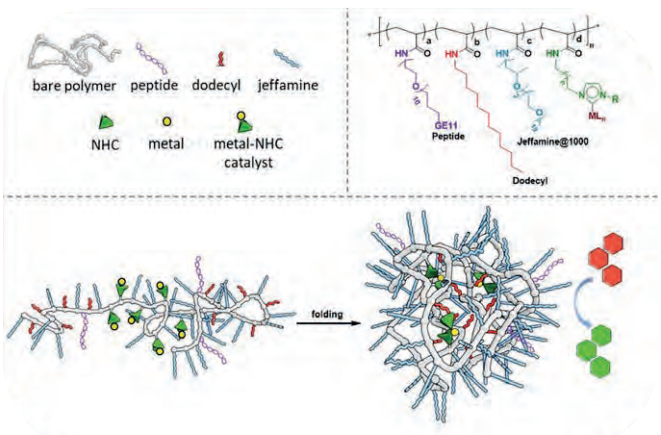


Prakasham Ayyampudur Palanisamy

EUROTECH POSTDOC: **PRAKASHAM A.P.**

Prakasham A. P. received his PhD in Chemistry from the Indian Institute of Technology Bombay, for research involving N-heterocyclic carbene complexes as catalysts for organic transformations. After his PhD, he moved to Tel Aviv University, Israel, to work as a postdoc. He studied pincer palladium phosphine complexes for metal-ligand cooperative catalysis, and high-valent platinum phosphine complexes for modification of small, biological molecules like nucleotides and peptides.

He joined Anja Palmans' group of Supramolecular Chemistry and Catalysis at TU/e last November. As an EuroTech postdoc he is currently working on bio-orthogonal catalysis. The goal is to develop catalysts which can be used for drug delivery, in cancer treatment. To reduce side effects and enhance efficacy it is important to activate anticancer drugs only at the cancer site. The bio-orthogonal catalytic approach aims to demask an anticancer drug selectively at the cancer site by using a metal-based catalyst. Prakasham A. P. and colleagues are now working on developing an enzyme-like catalyst which is protected from biological environment by encapsulation of single-chain polymeric nanoparticles. The main challenge is to stabilize the catalyst in complex biological media.



Theses

NOVEMBER 2022 – APRIL 2023

Advancing tissue engineering of in vitro human bone models
BREGJE DE WILDT
November 4, 2022
PhD advisors:
S. Hofmann
K. Ito

High-throughput computational screening of organic molecules for organic ion battery cathodes
XUAN ZHOU
November 9, 2022
PhD advisors:
R.A.J. Janssen
S. Er

The optoelectronic characterization of organic and perovskite thin-film semiconductors and photovoltaic devices
TOM VAN DER POL
November 9, 2022
PhD advisors:
R.A.J. Janssen
M.M. Wienk

Thermodynamics and kinetics of halide segregation in perovskite solar cells under operation
ZEHUA CHEN
November 16, 2022
PhD advisors:
P.A. Bobbert
G.H.L.A. Brocks
S. Tao

Foods inside out: super-resolved imaging of biomacromolecules in dairy gels and emulsions
SANAM FOROUTANPARSA
November 24, 2022
PhD advisors:
I.K. Voets
J. Hohlbein

Particle flow analysis for multi-material 3D food printing
DOLF KLOMP
December 6, 2022
PhD advisors:
P.D. Anderson
M.A. Hulsen

Motility in structured liquid crystal polymers
ROEL VAN RAAK
December 7, 2022
PhD advisors:
D.J. Broer
A.P.H.J. Schenning

Electronic structural colored devices
ARNE FROYEN
December 9, 2022
PhD advisors:
A.P.H.J. Schenning
M.G. Debije

Simulations of excitonic processes in thermally activated delayed fluorescence organic light-emitting diodes
CHRISTOPH HAUENSTEIN
December 15, 2022
PhD advisors:
R. Coehoorn
P.A. Bobbert
H. van Eersel

Taking time into the equation: potential and pitfalls of using real-world longitudinal data in developing clinical prediction models
RUBEN DENEER
December 21, 2022
PhD advisors:
V. Scharnhorst
N.A.W. van Riel
A. Boer

A first-principles theory of the complex dynamics of glass-forming liquids: a generalized mode-coupling theory
CHENGJIE LUO
January 17, 2023
PhD advisors:
L.M.C. Janssen
C. Storm

Modeling mechanobiology in guided kidney morphogenesis: a combined experimental and computational study
MARJAN HAGELAARS
January 20, 2023
PhD advisors:
C.V.C. Bouten
S. Loerakker

Real-time monitoring of low-concentration pollen in the air
JIAJING YANG
January 20, 2023
PhD advisors:
H.M. Wyss
J.M.J. den Toonder

Waterborne barrier coatings on paperboard
STERRE BAKKER
January 27, 2023
PhD advisors:
A.P.H.J. Schenning
A.C.C. Esteves
G.A. Metselaar

Reconstructing living tissue organization: a bottom-up bio-engineering approach with a focus on the corneal stroma
CAS VAN DER PUTTEN
February 16, 2023
PhD advisors:
C.V.C. Bouten
N.A. Kurniawan

Functional block molecules with nanoscale order
MARTIN VAN SON
February 24, 2023
PhD advisors:
E.W. Meijer
G.M.E. Vantomme

Decoding type I interferon response dynamics using microfluidics and modeling
LAURA VAN EYNDHOVEN
March 3, 2023
PhD advisors:
J. Tel
C.V.C. Bouten

Causal effect heterogeneity: statistical formalization and analysis of the individual causal effect
RICHARD POST
March 7, 2023
PhD advisors:
E.R. van den Heuvel
H. Putter

Strawberry supracolloids for water-borne coating applications
SIYU LI
March 8, 2023
PhD advisors:
A.C.C. Esteves
R. Tuinier

PAINTing receptors: a quantitative single-molecule view on cell membrane receptors
ROGER RIERA BRILLAS
March 10, 2023
PhD advisors:
L. Albertazzi
P. Zijlstra

The amazing osteoclast: towards an in vitro 3D co-culture model of bone
STEFAN REMMERS
March 14, 2023
PhD advisors:
K. Ito
S. Hofmann

Cardiovascular in situ tissue engineering: unraveling heterogeneity and variability
BENTE DE KORT
March 16, 2023
PhD advisors:
C.V.C. Bouten
A.I.P.M. Smits

Quantification of nanomaterials with spectrally-resolved super-resolution microscopy
EMMANOUIL ARCHONTAKIS
March 22, 2023
PhD advisors:
L. Albertazzi
P. Zijlstra

Understanding the divergence of prostate cancer genomics among patients: the multifaceted face of prostate cancer
JEROEN KNEPPERS
March 23, 2023
PhD advisors:
W.T. Zwart
A.M. Bergman

Highly sensitive photocurrent spectroscopy on hybrid perovskite solar cells
BAS VAN GORKOM
April 3, 2023
PhD advisors:
R.A.J. Janssen
M.M. Wienk

From data to patient prognosis: novel applications of prognostic markers in clinical care
JONNA VAN DER STAM
April 18, 2023
PhD advisors:
V. Scharnhorst
N.A.W. van Riel
A. Boer

A biomimetic artificial cervical disc replacement: biomaterial and biomechanical design characterization
CELIEN JACOBS
April 19, 2023
PhD advisors:
K. Ito
S. Hofmann

Exploring perovskite photodiodes: device physics and applications
RICCARDO OLLEARO
April 21, 2023
PhD advisors:
G.H. Gelinck
R.A.J. Janssen
A.J.J.M. van Breemen

Opening up new avenues in green chemistry

Fabian Eisenreich

Name
Fabian Eisenreich

Position
Assistant professor, Polymer Performance Materials group (since 2022).

Previously
Visiting scientist (University of California, USA), postdoc (TU/e).

Studies
MSc Chemistry, PhD summa cum laude (Humboldt University, Berlin).

Motivation
Being creative.

Dream
Turning fossil plastics into useful, easily

Spare time
Climbing, drawing: scientific illustrations & art.

Future chemistry is "green." Products are made and recycled in water, using biobased compounds and light. Assistant professor Fabian Eisenreich invents new concepts that are needed to get there.

Fabian Eisenreich worked on biodegradable polymers, studied redox-photochemistry, and came to Eindhoven to add supramolecular chemistry to his toolbox. Currently, he combines all this knowledge to develop new concepts in sustainable chemistry. For example, Eisenreich designs and synthesizes tiny "nanoreactors" that perform chemistry under natural, "green" conditions: at room temperature, in water, and using light as the sole, renewable energy source. He has proved that such nanoreactors can break down halogenated compounds, a class of chemicals which includes many pesticides and "forever chemicals" such as PFAS. "We designed a polymer that in water folds itself into a spherical nanoparticle. Within its hydrophobic interior, a built-in photocatalyst can break up halogenated compounds as soon as we switch on a UV-light."

RECYCLING AND UPCYCLING

Another green challenge that Eisenreich has taken up is minimizing energy use and waste production when recycling and upcycling plastics. "We want to recycle conventional fossil polymers in water using light. That's indeed very challenging, but I have a lot of ideas." A first result is a method for recycling polycarbonate, a hard plastic found for example in safety glasses. Eisenreich was able to retrieve the original molecular building blocks using biobased chemicals, a catalyst and water. During the reaction another polymer is produced that can easily be recycled by only adding an acid. He has not investigated if this type of polymer could be commercially attractive. "Our focus is primarily on developing new concepts for recycling. Hopefully, some of these concepts will eventually find their way to application."
What Eisenreich enjoys most in his work is that it requires a fair amount of creativity. "I like the puzzle of how to achieve a particular goal: Which molecules do we need and how can we synthesize them? And of course, a fascinating aspect of chemistry is that most of these molecules have never been made before."

Smart, dynamic, sustainable: designing a new generation of polymers

Loai Abdelmohsen

During a festive kick-off meeting last January, the new Interactive Polymeric Materials (IPM) Research Center presented its innovative research program. ICMS researcher Loai Abdelmohsen has been appointed as the IPM Center Manager. He aims to take the research of a new generation of interactive polymeric materials to the next level.

Last year, an ICMS-led consortium received a prestigious NWO Gravitation grant of over 15 million euros, resulting in the new polymer research center IPM. It is quite remarkable that the multidisciplinary project involves only TU/e researchers – usually the Gravitation scheme awards cross-university research programs. This is a recognition of Eindhoven's polymer expertise, according to Abdelmohsen. "We are going to focus on the development of intelligent, dynamic polymers. These can react with their environment and change their properties in response to that environment. Dynamics and sustainability are key concepts in this."

FIVE RESEARCH THEMES

Whereas today's polymer materials are designed for a single application, the new multifunctional materials should provide a broader applicability and less waste.
To accomplish this, the IPM has five different research themes. Both fundamental research and societal issues are addressed, Abdelmohsen explains. "Together with our Industrial Board, we look at how to bring new technology to an industrial context. Our industrial partners often have a better view of societal needs, so we can adapt our research where necessary."

ATTRACT TALENTED RESEARCHERS

In addition to innovative technology, the research center will also train a new generation of scientists, Abdelmohsen emphasizes. "They will soon be able to tackle academic, industrial, and societal issues. The first PhD students have already started and thanks to the Gravitation funding, we can attract other talented researchers. We are now organizing a monthly colloquium with invited speakers so that everyone can get to know each other; an annual IPM symposium is also in the planning. IPM means interaction in all forms."

The five research themes of the new Interactive Polymeric Materials Research Center

A brand new "button" to control molecules

So called light-matter states were already known by physicists when Thomas Ebbesen started to use them in chemistry. Now chemistry and material properties like (super)conductivity and magnetism can be adjusted with the flip of a switch, as can transport of charge and energy. This holds the potential for more efficient industrial processes. In March, Ebbesen was a guest speaker at the annual ICMS symposium.

Sometimes an entire new research field can emerge from someone just browsing a magazine. Thomas Ebbesen remembers it was a copy of Physics Today. It was 1989 and he was working for the Japanese NEC Corporation, at that time the world's largest chip producer. An article on quantum electrodynamics in optical cavities fascinated him. Physicists described how they were studying fundamental aspects of light-matter interactions, more specific of hybrid light-matter states. Interestingly, these also form in total darkness, when matter interacts with the so-called vacuum field consisting of electromagnetic background fluctuations.

"Because of my chemistry background I wondered what this would do to the properties of molecules in that cavity," Ebbesen says. "I realized that this had to be tested. So that we could use the principles put forward in the article for chemistry and material science." Today, as a professor of physical chemistry at the University of Strasbourg, Ebbesen specializes in exploiting light-matter interactions to induce significant changes in material properties. "We create cavities that are resonant to frequencies that match electronic or vibrational transitions in molecules. This can alter their ground state and thereby their chemical properties," Ebbesen explains. He adds that his lab uses the same approach to modify solid state properties of matter, like conductivity and energy transport.

IMPROVED CONDUCTIVITY AND TRANSPORT

After reading the Physics Today article, Ebbesen set out to discover what properties of matter could be altered by light-matter states. He found there are many, of which conductivity is one. "In the cavity, the molecules are basically forming collective states," he says. "Typically conduction should improve, and indeed, in 2015 we found that organic semiconductor conductivity can be enhanced by an order of magnitude." Ebbesen also mentions a remarkable result obtained by one of his former postdocs, Anoop Thomas, now at the Indian Institute of Science in Bengaluru. "He and his colleagues found that by coupling a molecular vibration of polystyrene to the vacuum field its conduction goes up a million times." In essence, this common polymer then turns from an insulator to a semiconductor. Another former post-doc, Tal Schwartz at Tel Aviv University, recently reported a similar huge increase in exciton diffusion in organic dyes. "Using a cavity in the visible range, he and his colleagues found that the exciton diffusion coefficient went up by six orders of magnitude, to two-thirds of the speed of light," Ebbesen says. The list goes on, for instance the ferromagnetism of YBaCuO nanoparticles could be boosted by a factor of 700 through coupling of a vacancy phonon mode.

FROM SOLID STATE TO SOLUTION

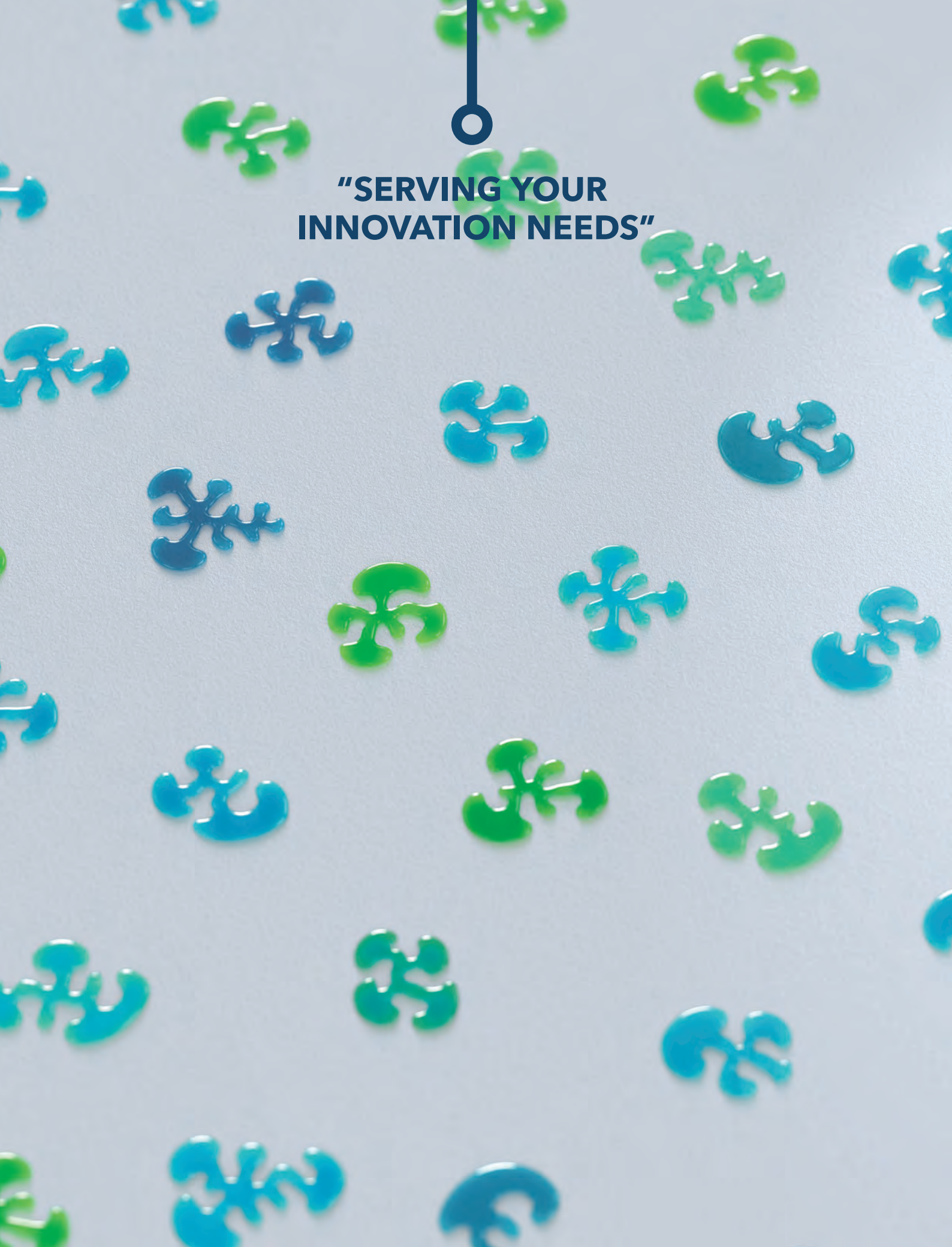
Many of the transitions between ground states in molecules correspond to energies of photons in the optical range. This means that the cavities used to alter these ground states need to be in the range of that wavelength. Many of Ebbesen's initial experiments were done in submicrometer cavities, which only allowed for chemistry in the solid phase. In 2014 the Ebbesen lab developed a microfluidic cavity with an optical pathway in the 10 micrometer range that corresponds to the infrared spectrum. This paved the way to couple vibrational transitions of molecules in solution, or the solution itself. In water, for instance, this can enhance the activity of (bio)catalysts.

A NEW "BUTTON" FOR TUNING CHEMISTRY

There is no known limit for altering molecular properties with light-matter states. Ebbesen and others have so far altered the rate, the thermodynamics and the site selectivity of chemical reactions, leading amongst others to different product ratios. Eventually, if the chemical landscape is altered enough, maybe even new products could be formed. And controlling the amount of unwanted side products would be very valuable for industry. Ebbesen: "Normally, it is hard to get a 100% pure product from a reaction. It would be phenomenal if we can use our technology to improve the yields and purity of industrially relevant reactions." He reports great interest from large chemical companies, where people are excited about his research. "They already have a lot of 'buttons' they can use to optimize chemical reactions, adjusting temperature, pressure, and use specific solvents. They were quite surprised when I showed up with a brand-new button they didn't even know existed," Ebbesen says.

BEYOND BORDERS

Ebbesen's research shows that when you look beyond the borders of your field, new science can be within reach. "You have to keep an open mind at all times," he says. He is very much interested in exploring collaboration between his groups and that of ICMS. "There's lots of knowledge and know-how in both places," he says. "When we combine that, new things can emerge."


"SERVING YOUR
INNOVATION NEEDS"