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"POLYMER SELF-ASSEMBLY CAN CONTRIBUTE TO SOLVING BIG SOCIETAL PROBLEMS"

AIMING FOR AN E-SKIN: VERY INTERDISCIPLINARY, TARGETED RESEARCH

RESEARCH ON SOFT ROBOTIC HEART IS GRANTED 10 MILLION

ICMS

INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS



ICMS Highlights



The ICMS community celebrated its 15th anniversary over the past year, making it a memorable period filled with reflections and accomplishments. Various segments of our community came together to celebrate science. Also in 2023, ICMS fellows hosted a series of events focused on career choices, and the Grip on Complexity community released a special edition of the ICMS Highlights magazine. And 2023 saw a great deal of personal grants, prizes, and team accomplishments. Our PhD community organized its third paper competition, where Harm van der Veer was honored for best overall performance and Changlin Wang won the audience award.

As we look to the year ahead, our primary focus will be on the integration into our community of substantial research proposals that were recently granted. While securing research funding is a significant step, it's equally important to ensure that acquired funds are used effectively to advance science and bring about meaningful changes in academia and industry. The approved proposals aim to provide a deeper understanding of molecular systems and will potentially create opportunities for, e.g., new value chains to support the material transition. We will team up with our sister TU/e Institutes to make our science count!

We would like to welcome Samir Vinchurkar to the ICMS community as Business Engagement & Research Development Manager. He will focus on building a thriving interplay between industrial and academic researchers. In this issue of ICMS Highlights, we showcase the scientific journey of our members and friends. 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.

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ADVANCED MATERIALS

Craig Hawker: "Polymer self-assembly can contribute to solving big societal problems"

Craig Hawker

Professor Craig Hawker, chairman of the ICMS Scientific Advisory Board, is a regular guest in Eindhoven. The professor of Chemistry and Materials at UC Santa Barbara (USA) is "very pleased with the rapid and successful development of ICMS," he says. "What has already been achieved is impressive and lays the foundation for long-term impact."

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"I'm very excited to be associated with ICMS," says Hawker, who has been closely involved in ICMS right from the start. "It was modelled on the multidisciplinary environment of our Materials Research Laboratory (MRL) at UCSB, but ICMS has taken this collaborative concept to a whole new level." Hawker is enthused by the true entrepreneurial spirit in the ICMS organization. "It brings together a lot of young researchers with great ideas. I regularly visit Eindhoven and I am surprised at how engaged researchers at all levels are. They not only know how to do research very well, but they also show a high level of dedication and partnership. One of the great aspects of seeing this new initiative blossom, is that it in turn inspires our own work."

Hawker is especially glad with the new ICMS program in (active) polymers and soft matter. His own research group is also very active in this field. "Together we focus on new applications in polymer chemistry and polymer self-assembly. We build on the foundation laid by multiple Nobel Prize winners over the last twenty years. They have discovered the tools for mimicking Nature in the construction of functional materials. These advances make polymer selfassembly the right topic at the right time. With more international groups focusing on this field and bringing their own competences, societally important problems can now be addressed and hopefully solutions developed."

"THAT'S HOW IT SHOULD WORK"

Santa Barbara and Eindhoven each have their own emphasis in the polymer self-assembly field, in part resulting from a different mix of knowledge inputs from different disciplines. Hawker: "While at Santa Barbara a major focus of our work is bulk self-assembly, Eindhoven has driven multiple advances in solution-state self-assembly, with key discoveries impacting both disciplines. So, we develop in different complementary areas, all to the benefit of the field as a whole. That's how it should work when addressing significant scientific challenges."

This multidisciplinary research into new functional materials allows major societal problems to be addressed. This includes sustainability, energy production, water purification and biomedical research, all of which are impacted by polymer self-assembly. "Through understanding of complex molecular systems at the most fundamental level," savs Hawker, "we are able to shape the future of materials, energy, mobility, health, and life itself. Synthetic organs or tissues, high capacity batteries derived from abundant materials and fully recyclable plastics are all achievable."

"ICMS has been able to establish an impressive infrastructure to support these challenging goals. Their long term investments in world class characterization and imaging equipment, coupled with outstanding support staff, guarantee sustained impact. Overall, this creates an optimistic picture about what can be achieved in polymer selfassembly over the next decade. I'm really looking forward to seeing this evolve."

A TWO-WAY STREET

The beauty of collaboration in science is that all involved benefit, Hawker remarks. "The ICMS knowledge position makes it an ideal place for international exchange. It's a two-way street - that's why I'm involved. It's a great experience for researchers to spend six months abroad to pick up new knowledge, new methods and new thinking. Before Covid, we had multiple researchers from Eindhoven and Santa Barbara spending extended periods at each institution and I am excited to get this level of exchange happening again. It is great for the professional development of individual researchers and significantly strengthens both the host and guest institutions. It is key to building a world-class organization such as the MRL or ICMS."

TU/e Honorary Doctorate for polymer genius with a commercial spirit





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"WE ARE ABLE TO SHAPE THE FUTURE OF MATERIALS, ENERGY, MOBILITY, HEALTH, AND LIFE ITSELF."

Mutual involvement as the key to successful collaboration

Remco Tuinier (left) and Max Martens (right)

With the PhD work of Max Martens, the TU/e Laboratory of Physical Chemistry and Unilever together dive deep into fundamental phase separation modeling. The cliche has it that such collaboration between academia and industry will at some point lead to friction. After all, academic groups strive for publication and industry aims for application. To Jo Janssen from Unilever, however, there's no problem. "When you are genuinely involved," he assures, "both sides benefit."

The origin of the collaboration lies with Remco Tuinier, professor of Physical Chemistry at TU/e, who in 2015 started a group around predicting the stability of complex mixtures. "Food and coatings have always been important application areas of phase stability research," he says. "I had conversations with Unilever researchers at several conferences, one thing led to another and eventually I came into contact with Jo Janssen. We decided that it would be beneficial for both parties to have Max Martens, a talented student, on a PhD assignment for modeling phase behavior. That is how this research field was opened."

A JOINT JOURNEY

Jo Janssen is a senior researcher at Unilever R&D in Wageningen. "Phase separation has always been an interesting topic for us," he says. As an example he mentions the relevance to mixtures of proteins and polysaccharides, such as the continuous phase of emulsions like dressings and mayonnaise. "Lately it has become even more important, due to the focus on low fat and plant-based food. It is also essential for meat-like structures. A sound, fundamental science-based phase separation model provides fundamental insight and will save a lot of lab time. It will reveal where and why things go wrong."

There are several types of corporateacademic collaborations, Janssen explains. "There is contract research where a company has a good picture of what it wants but lacks the time or the specialists to carry it out. An opposite type involves broad explorative consortium research such as EU-funded projects to stay on top of the latest developments in a field. Our present collaboration lies somewhere in between. It's a joint journey where the academic researcher dives deep into matters that are of real long-term importance to us as a company." Martens explains: "My model is all about the physics; Unilever has the opportunity to build software to implement it later. I describe the model generically for my thesis, but Unilever applies it in specific cases."

EXCITING RELEVANCE

The research is partly funded by Unilever and partly by the Top consortium for Knowledge and Innovation (TKI) Chemistry. Since the research will lead to a publicly available PhD thesis, isn't there a risk that vital aspects for Unilever become common knowledge? Janssen: "The beauty of our collaboration is that specific applications to our products are not included in the scientific publications. We will develop most of the applications within our company." Martens adds: "The scientific value lies in the theory and the new physics. My challenge is to describe the complex systems with a large degree of abstraction. From there, I work my way towards the details that are relevant to Unilever. For me it's very valuable and challenging to know the real use cases of the models, and to implement them optimally. Real operational conditions are never as ideal as model conditions." Tuinier comments that this challenge of catering to the needs of actual applications makes working with large companies so exciting: "We regularly collaborate with large companies. A big plus is that we get to know how newly developed knowledge is used in practice. That adds to the relevance. Of course, as Max says, it also adds to the complications when the counterpart responds with problems from



o ounssen

practice that you didn't see coming from your theory. But that broadens your view of your own field. It prevents that you dig deeper and deeper into details, forgetting about the big picture. That far outweighs possible complications."

INVESTING IN COMMITMENT

"Success in collaboration is all about investing in commitment," Janssen knows. "As a company you cannot say: here's the budget, we are looking forward to the publication in four years, success! Corporate researchers have to be involved and should internalize results in real time, so you can act as a sparring partner for academia. Max and I share details frequently and also have videocalls outside formal progress meetings. This builds real insight."

This close collaboration will also help both parties in fruitful conversations on what can be published and how. "Always keep communications lines open," Janssen concludes. For his part, says Martens, "It's a relief that everyone I talk to at Unilever is a researcher, who understands what it's about and is just as excited about the research. People may think there is a culture difference between academy and industry; in our case, there really isn't."

ADVANCED MATERIALS

"THE GOAL IS NOT JUST A SCIENTIFIC PAPER IN WHICH WE DESCRIBE A NEW PHENOMENON. WE SHOULD WORK TOWARDS AN END-PRODUCT THAT IS MANUFACTURABLE."

Zhenan Bao

Aiming for an e-skin: Very interdisciplinary, targeted research

What will it take to make a functioning e-skin in the next twenty years? This question is the starting point for the highly interdisciplinary scientific research of professor Zhenan Bao of Stanford University. She identifies the fundamental hurdles that need to be overcome in materials research, electronics, bioengineering and mechanical engineering, to make this application a reality. Bao visited ICMS early November and presented a lecture on her work.

As an organics and polymer chemist, Zhenan Bao designs polymer molecules capable of transporting electrical charges. This is a rather fundamental research topic. But her starting point is a real application, be it for a quite remote future: e-skin, an artificial, functioning skin. Bao: "Think of giving back the sense of touch to patients who have lost a limb." With her colleagues she wants to make the necessary molecules to enable electrical signal transport to nerves, in a substrate that looks, feels and functions like human skin. "It will be hard," Bao says. "For instance, for a hand, you need a high density of touch receptors over a large area of skin. Also, the sense of touch of human skin necessitates signal processing and signal transfer to the brain, and back from the brain to steer body functions." This asks for a bio-interface that can also be applied to wearable electronics, monitoring mental health and to neural probes and implants in the brain and gut. And that in turn asks for various types of high-resolution sensors.

MAPPING FUNDAMENTAL CHALLENGES

The e-skin concept contains many ingredients that cannot be made at this point in time. Bao: "These functional organics and polymers for electronic and bio-engineering applications demand a highly interdisciplinary effort. It involves a coordinated approach, joining polymer chemistry, physics, biomedical science, materials science, mechanical engineering and electrical engineering." She explains the multiple steps in developing suitable molecules: determine what they need to do; draft a hypothesis of their design; then synthesize them, test them and fit them into an actual setting. The latter will probably be a crude one, but should be the closest to the design of the remote application you have in mind. Bao underpins that the goal of her research is to break down what missing knowledge currently prohibits achieving the far-away target. "We're in the game of applied science, but not for the sake of it," she says. "You have to understand how each step influences the molecules in the integrated circuits and sensors in order to constantly refine the molecular design. It's all about the feedback we get in the process: what fundamental bottlenecks are there in all relevant fields? What further steps have to be taken? We have to map the remaining fundamental challenges."

A MULTIFACETED CHALLENGE

It is a multifaceted challenge, with lots of problems to solve. Interdisciplinarity is therefore simply the only way to go. "There are three basic elements involved in the e-skin concept," Bao explains. "First, you need a design platform, for the sensors that are capable of sensing touch, and the neuro chemicals to transmit their signals to a soft integrated circuit (IC). That is the second element: organic, stretchable, self-healing and biodegradable ICs. From there it goes to the third element: signal communication to the brain, through a bio-interface that doesn't damage bio-organic tissue." For each element fundamental chemistry is needed, Bao argues.

Zhenan Bao, skin-like electronics pioneer

Zhenan Bao is K. K. Lee professor in the School of Engineering and professor (by courtesy) of Materials Science & Engineering and Chemistry at Stanford University in Stanford, California, USA. She is a pioneer in the field of skin-like electronics and co-founded two Silicon Valley start-ups: PyrAmes, which is developing non-invasive blood pressure monitors, and flexible electronic material company C3 Nano.

"To design the right conductive, semiconductive and dielectric materials, and to process them into a thin film – from tens of nanometers to tens of micrometers thick."

She describes how it all works. It starts with a solution of newly designed molecules with an expected performance. Then a deposition technology is chosen for application of the solution on the thin film substrate. "There it will for instance form ordered clusters together with amorphous disordered domains," she says. "You have to see to it that molecules align in the right way to get the electronic and mechanical properties that are required for the intended functionality." This means: analyze, test, improve, and repeat, until at last the right pattern emerges. Bao: "And that is just the first step in the process. Additional chemistry knowledge comes in for making layers in a way that is scalable towards an industrial setting. Remember, the goal is not just a scientific paper in which we describe a new phenomenon. We should work towards an end-product that is manufacturable and can be integrated in practical devices." >>

Greatest breakthrough: Solving stretchability issues

A bottleneck in the polymer electronics field is that the somewhat brittle, rigid macromolecular wires for electric conductivity get bent and twisted in a stretchable matrix. This poses a problem for transferring electric charges at high speeds. Zhenan Bao managed to mix these rigid wires with elastic or self-healing polymers with particular molecular characteristics that make them assemble into bundles of nanoconfined structures. This forces the macromolecules to pack more straight. Bao: "Compare it with hair; one hair will easily bend. But when vou bundle it, it will become more straight. This enables the wires to better conduct electricity."

PROOF OF CONCEPT

Recently Bao achieved a milestone with the design of a Genetically **Targeted Chemical Assembly** (GTCA) that is capable of sending an electronic signal from e-skin to the brain. Together with professor of Bioengineering Karl Deisseroth at Stanford University she demonstrated that it is indeed possible to transfer a signal to nerves. "It means you have to selectively target a specific type of cell, to label certain nerve fibers. Selecting the right pathway to do that proved quite challenging." The proof of concept of GTCA nerve stimulation in a living organism was delivered using the one millimeter long worm C. elegans. Bao: "We showed that the muscle movement pattern of the worm was changed successfully using our GTCA. This was an important first step. However, we have a long road

ahead of us before we have actual applications in humans. There are still so many questions to address: How to do it in a subtle and controllable way? How will the novel chemistry impact humans?"

TEAM ATMOSPHERE

In her work, Boa is not just motivated by science itself, but also by the research environment. Science is teamwork and therefore the atmosphere within the team is highly determinant of the results. The influence of interdisciplinarity in a team goes beyond mere functionality, she says. "I get inspired when I work in an interdisciplinary team, when I get the opportunity to learn from researchers from different disciplines. Interdisciplinarity results in a creative environment." People in interdisciplinary teams are aware that they don't understand the finesses of other fields. Bao: "Everybody therefore feels comfortable asking questions - even basic ones that people in the field themselves have never thought about or take for granted. Such guestions are important. They lead to new, original ideas." Adding to this, trust is essential according to Bao. "In a team vou have to be able to work without reservation for the collaboration to thrive. Therefore, as a team lead you have to start by trusting others instead of being cynical and holding back knowledge. We are not stupid or naive. We know that at some point you will come across someone that misuses that trust. The point is, it's not worth missing the good opportunity to do great work for a rare rotten apple. That destroys the opportunity for all to benefit. Most people are worth trusting, and like to contribute to winning together."

"INTERDISCIPLINARITY IS THE WAY TO GO IF YOU WANT TO DESIGN SOLUTIONS THAT MAKE A REAL IMPACT."

AN ECOSYSTEM WHERE EVERYONE THRIVES

Bao is glad to see that even when people leave the team to start their own independent careers, they retain that philosophy and culture. "In academia, they take their collaborative attitude elsewhere and continue to share with each other. And even when they go to industry, the collaboration remains; they become customers or suppliers to each other. That helps to build an ecosystem where everyone thrives. The returns are there." Bao feels that science in general is becoming more collaborative and interdisciplinary. "Problems such as climate change, human health and energy transformation are extremely complex and cannot be solved from a single area of expertise. You need to understand a problem with all its separate aspects, from all angles and all disciplines, to contribute to solving the issue. Interdisciplinarity is the way to go if you want to design solutions that make a real impact."



Bao: "New polymers must be sustainable"

"The way we look at polymers has changed. We know that for new materials, sustainability is a necessity. It is important to incorporate sustainability into their design, which is much easier than to figure out how to recycle or degrade them afterwards."

ADVANCED MATERIALS

Increasing lifetime and recyclability of plastics

Stan Looijmans

Despite the bad reputation of plastics these days, synthetic polymers play an irreplaceable role in our daily lives. To make them more sustainable, assistant professor Stan Looijmans seeks total control over their microstructure.

It was during an internship in Genova, Italy when Stan Looijmans first learned about process-induced structure formation, in particular polymer crystallization. "The interplay between material processing and subsequent structure formation fascinated me. During my masters project and my PhD project I continued working on this topic. And I will continue to do so in my future research." According to Looijmans, if we wish to develop new plastic solutions or extend a product's lifetime and recyclability, we need to understand the influence of processing on the microstructure, and how this microstructure will deform and fail under a certain applied load. "If we have this fully under control, we might be able to achieve circularity of all products."

TODAY'S AND TOMORROW'S STANDARDS

Plastics production will continue to grow exponentially, towards an estimated annual production of 600 million ton in 2050. This growth results from the many advantages of plastics, including their durability, lightweight, versatility, and cost-effectiveness. They are simply superior to other materials, says Looijmans. "It is just a matter of time before the public and politicians will realize this. I seek to further develop my research in such a way that plastics will meet today's and tomorrow's standards." Name Stan Looijmans

Position

Assistant professor, Processing & Performance of Materials group (since July 2023).

Previously PhD at TU/e, Processing & Performance of Materials group.

Studies

MSc Mechanical Engineering TU/e, internship at University of Genova.

Motivation

Resist against "green-washing," see the sense in nonsense.

Dream Creating mono-material product solutions thanks to absolute control over the desired microstructure.

Spare time Travel and enjoy nature with my family.

Towards this ultimate goal, Looijmans now co-supervises a postdoc-project where he and his colleagues are considering the melting behavior in polymer extrusion, in particular for recycled materials. "This is a challenging work since until now people were merely interested in polymer crystallization to understand product performance. Little is known about the inverse process. With the increasing demand for recycling of materials it is becoming more and more important to focus on the sorting, melting and re-crystallization process."

ADVANCED MATERIALS

Clint van Hoesel (left) and Hiroki Tomita (right)

SEQUOIA: Suppressing Exciton Quenching in OLEDs: an Integrated Approach

Unravelling quantum mechanics for brighter OLEDs

Organic LEDs can be cheaper and easier to produce than the more traditional, inorganic LEDs. However, OLED efficiency and life span are limited due to exciton quenching. PhD students Hiroki Tomita and Clint van Hoesel unravel the underlying quantum chemical processes. "For physicists, there is still a lot to discover in the OLED field."

Today, LEDs are used widely in lightning and TV-screens. Their organic counterparts, the OLEDs, you find in mobile phones or tablets and in some high-end, large TV-screens. Break-through to the mass TV-display market is going slowly. PhD student Hiroki Tomita grabs his own mobile phone to explain why. "When I move the slider for brightness to twice the current level, the light intensity of my OLED screen doesn't double. The efficiency of OLEDs drops at higher light intensities." Tomita is trying to tackle this problem at ICMS, together with physicist and PhD student Clint van Hoesel.

Why does this problem interest the two PhDs? "It's an interesting and complex problem," says Van Hoesel. "The quantum mechanical processes behind exciton quenching are still not fully understood. As physicists, we have a lot to learn in this field; OLEDs have mainly been developed by chemists. This leaves a large open space for the development of new physical and mathematical models. I love working on that." Tomita: "I think of OLEDs as reversed solar cells. I've always been fascinated by the energy conversion between electricity and light, by optoelectronics. It has a touch of magic."

TWO POSSIBLE PATHWAYS

In an OLED device, Van Hoesel explains, exciton quenching occurs when an excited phosphorescent molecule (an exciton) encounters a polaron, a charged quasiparticle that runs through the OLED because of the applied voltage. The "collision" results in molecular vibrations instead of the emission of light, as an exciton is supposed to do. Tomita: "Quenching not only reduces the energy-to-light efficiency, but also the lifespan of OLEDs." The energy released in exciton guenching is sufficient to break up carbon-carbon bonds, so that an OLED device may degrade and irreversibly lose its light-emitting capacity. In the literature, two possible pathways have been suggested for exciton guenching: so-called "Förster resonance energy transfer" and "Dexter electron transfer." Van Hoesel: "Both mechanisms are named after the scientists who proposed them. An important difference is that Dexter happens between nearest neighbors while Förster works over a longer distance. And Förster is well defined, whereas Dexter can be caused by various mechanisms." Förster interactions are generally assumed to dominate. In the two years that Tomita and Van Hoesel have studied exciton guenching, they surprisingly found signs of both Förster and Dexter interactions. Van Hoesel: "If we can further substantiate these preliminary results, it would be remarkable. It could be a break-through in the design of OLED molecules."

MODEL AND EXPERIMENT

Tomita is the experimentalist of the duo. He fabricates OLEDs with varying compositions, to get a grip on what exactly affects exciton quenching: "There are many parameters that influence quenching and they often have non-linear effects, which makes the experiments quite a puzzle." Van Hoesel catches the exciton quenching process in computer models. "When we work on the same materials we compare the outcomes and try to explain what's happening."

Their joint research is part of the SEQUOIA-project: "Suppressing Exciton Quenching in OLEDs: an Integrated "PREVENTING EXCITON QUENCHING COULD GIVE OLEDS A REAL PUSH FORWARD."



Approach." It is a cooperation with VU Amsterdam, the company Merck that manufactures OLED materials, and the simulation software companies SCM and Simbeyond. Van Hoesel: "In Amsterdam, novel quantum molecular models are developed to describe exciton quenching. I use those for my models at both molecular and device level. The two software companies provide state-of-theart models that we adjust for our research. In this way, we can relate the experimental exciton quenching rates to the most fundamental quantum chemical processes."

LONG LIFESPAN

What if the researchers succeed in unravelling the quantum mechanisms behind OLED exciton quenching? Van Hoesel: "When we know the details of why and how quenching occurs, chemists may design alternative phosphorescent molecules. That could give the OLED field a real push forward." Tomita: "Currently, many eyes are on the development of microLEDs, a new generation of inorganic LEDs composed of tiny emitting pixels, just like OLEDs. If the quenching problem can be resolved, OLEDs will be far ahead in price and performance."

News, awards & grants

Scan the QR codes to read the full articles





SEVEN EARLY-STAGE TU/E RESEARCHERS HAVE BEEN AWARDED A VENI GRANT FROM THE DUTCH RESEARCH COUNCIL (NWO), WHICH IS AIMED AT RESEARCHERS WHO HAVE RECENTLY OBTAINED THEIR PHDS. PEPIJN MOERMAN, KATHRIN HÖVELMANNS, MIRUNALINI THIRUGNANASAMBANDAM, ROB WOLFS, RIANNE CONIJN, DINESH KRISHNAMOORTHY, AND CLEMENS DUBSLAFF WILL EACH RECEIVE A GRANT WORTH 280,000 EUROS TO CONDUCT RESEARCH OVER THE COMING THREE YEARS.



With light into the nanoworld

THE FIRST RESULTS OF THE SUPERCOL PROJECT WAS PRESENTED AT AN EVENT OF THE EUROPEAN MATERIALS RESEARCH SOCIETY ON JUNE 1ST IN STRASBOURG.



Six TU/e researchers appointed fellows of the new Netherlands Academy of Engineering

THE ACADEMY WANTS TO ENSURE THAT NEW TECHNOLOGICAL DEVELOPMENTS ARE EMPLOYED TO ADDRESS CRITICAL SOCIETAL ISSUES SUCH AS SUSTAINABILITY, ACCESS TO HEALTHCARE, AND ENERGY PRODUCTION.

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Therapy targeting specific immune cells appears promising for sepsis

NANOPARTICLES CONSISTING OF A DESIGNER PROTEIN THAT COUNTERACT AN OVERREACTION OF THE IMMUNE SYSTEM, WHILE SIMULTANEOUSLY BOOSTING THAT SYSTEM.

Photo: Shutterstock

2023 ICMS Publication Award for Harm van der Veer



Digitally designed protein works like an anti-freeze for biological material Frank Baaijens awarded the Huiskes Medal for Biomechanics



Biotrip: Revolutionizing nanotechnology for immune therapy

Bio: Willem Mulder

Willem Mulder studied chemistry at Utrecht University. He worked for a long time in the USA at Mount Sinai's Biomedical Engineering and Imaging Institute (BMEII, Icahn School of Medicine, New York, USA), as professor of Radiology and Oncological Sciences.

His research focuses on precision imaging and targeted therapy in cardiovascular disease, cancer and transplantation. He is currently professor of Precision Medicine at the department of Biomedical Engineering at the TU/e and also at Radboud University, where he closely collaborates with immunology professor Mihai Netea. Merge the latest knowledge of immunology with nanotechnology and thus create a bridge between internal medicine and biomedical engineering. Next, replace papers as scientific end products with working therapies in patients. With that, you have some of the main ingredients of the biotech incubator Biotrip. But there's a lot more to it, explains co-founder Willem Mulder, professor of Precision Medicine at the department of Biomedical Engineering.

Mulder founded Biotrip together with Nijmegen immunology professor Mihai Netea. "I met him in 2016 in the United States, where I worked at the time," Mulder recalls. His meeting with this visionary medical scientist contributed to Mulder's decision to return to The Netherlands in 2020. As a bio-engineer, he decided to team up with the "softer" science of immunology. "Mihai and I are very complementary," says Mulder. "He is a true intellectual, a walking encyclopedia and a clinician. I am an entrepreneurial scientist. That goes together well."

ENORMOUS OPPORTUNITIES

The knowledge of the immune system and its role in human health and disease has grown immensely over the last decades. Contrary to the common understanding, Mihai found that the innate part of the immune system has some kind of memory. Mulder: "It's a fascinating framework that creates enormous immune system-directed treatment opportunities for developing sophisticated immunepharmaceutical strategies. >>

INNATE IMMUNE MEMORY

- Innate Immunity

 Rapid

 Effective

 Nonspecific, inducrimin

 Lacks immunological m
- Trained immunity

 A de facto innate immune memory of myeloid

Willem Mulder (right) and Mihai Netea (left)

Think of vaccination, immune regulation and innate immune programming. Targeting the innate memory could result in decisive changes in the immune balance."

Mulder and Netea initiated Biotrip as a platform that brings together medical scientists and biomedical engineers to work with entrepreneurs with the common goal to restore "immune health" in important immunemediated diseases. These include cancer, infections such as COVID-19, cardiovascular disease, sepsis, and organ transplantation. Mulder: "For instance in cancer, the tumor 'hijacks' innate immunity to mislead the adaptive immune system, a status known as immunosuppression. This is co-orchestrated by stem and progenitor cells in the bone marrow. As a result, for many cancers the current immunotherapy with so-called checkpoint inhibitor drugs is relatively ineffective. Overcoming immunosuppression by targeting stem and progenitor cells can make checkpoint inhibition much more effective. Many more opportunities like this exist."

ONE GROUP WITH A SHARED GOAL

Mulder set up two teams, a technology team in Eindhoven and an immunology group for in vivo research as part of Netea's research program in Nijmegen. Currently the combined efforts involve twelve PhD students and ten master students that together function as one multidisciplinary research group with a shared goal. Mulder underpins that the focus goes beyond writing scientific papers as a final result. "We also engage in entrepreneurial activities to help make our technologies available to patients, in a bottom-up approach."

The technology platform encompasses nanomaterials derived from natural lipoproteins, which allows meticulously designing nano-immunotherapies. These promote or inhibit an immune response by polarizing macrophage function or by targeting myeloid cell dynamics. As an example, in the journal "Immunity" Mulder and co-workers recently presented data of their nano-immunotherapy in a mouse transplantation model, reporting spectacular results in organ acceptance without the need for chronic immunosuppression. Concurrently, the team develops methods that allow non-invasive and high-precision imaging of immune responses.

MIMICKING A BACTERIAL CELL WALL

In another line, the researchers mimic bacterial cell walls for the purpose of triggering an immune reaction. This follows an idea that goes back to American surgeon William Coly, who at the end of the nineteenth century experimented in New York Hospital with intravenously injecting bacteria to cancer patients. "The idea was to have the infection trigger a severe immune reaction, which then would also work against cancer," Mulder explains. "While some patients did indeed recover from cancer, others died due to sepsis."

At present, the team is able to replicate a bacterial cell wall by templating certain molecular features onto nanoparticles. "This cell wall replica is indeed recognized by immune cells. But since it in itself is harmless, it comes into action without the risk of an overwhelming bacterial infection." The concept was developed at Mount Sinai Hospital in New York City and is further worked out in the company Trained Therapeutix Discovery.

AN IP POWERHOUSE

In Mulder's view, to promote the translation of such developments to the clinic requires an "IP powerhouse." And that is precisely what Biotrip is. "Our organization model is guite unique and we work very result-oriented. We do this along the lines of the American system of the National Institutes of Health (NIH), which is not obvious in Europe. We aim for the long term with the intention that some of our current PhD students will remain involved after graduation, all the way to the patient's bedside." According to Mulder, much has already been accomplished and many decisions have been taken within a short timeframe and with a relatively small team, for which he acknowledges the support of TU/e and Radboudumc. "With our IP specialist, we have developed a comprehensive IP portfolio and we are working with renowned biotech-specialized investors on plans for new biotech start-ups," he concludes.

Key publications

MAY 2023 - OCTOBER 2023

01. A RETRAINABLE NEUROMORPHIC BIOSENSOR FOR ON-CHIP LEARNING AND CLASSIFICATION

E.R.W. van Doremaele, X. Ji, J. Rivnay, Y. van de Burgt Nat. Electron. 6, 765-770 (2023) DOI: 10.1038/s41928-023-01020-z

02. CONTROLLING HELICAL ASYMMETRY IN SUPRAMOLECULAR COPOLYMERS BY IN SITU CHEMICAL MODIFICATION F.V. de Graaf, S.A.H. Jansen, T. Schnitzer,

E.W. Meijer, G. Vantomme J. Am. Chem. Soc. 145, 14379-14386 (2023) DOI: 10.1021/jacs.3c03411

03. DE NOVO DESIGNED ICE-BINDING PROTEINS FROM TWIST- CONSTRAINED HELICES

R.J. de Haas, R.P. Tas, D. van den Broek, C. Zheng, H. Nguyen, A. Kang, A.K. Bera, N.P. King, I.K. Voets, R. de Vries Proc. Natl. Acad. Sci. U. S. A. 120, e2220380120 (2023) DOI: 10.1073/pnas.2220380120

04. DNA STORAGE IN THERMORESPONSIVE MICROCAPSULES FOR REPEATED RANDOM MULTIPLEXED DATA ACCESS

B.W.A. Bögels, B.H. Nguyen, D. Ward, L. Gascoigne, D.P. Schrijver, A. Makri Pistikou, A. Joesaar, S. Yang, I.K. Voets, W.J.M. Mulder, A. Phillips, S. Mann, G. Seelig, K. Strauss, Y. Chen, T.F.A. de Greef Nat. Nanotechnol. 18, 912-921 (2023) DOI: 10.1038/s41565-023-01377-4

05. ENZYMATIC REGULATION OF PROTEIN-PROTEIN INTERACTIONS IN ARTIFICIAL CELLS

T.W. van Veldhuisen, W.J. Altenburg, M.A.M. Verwiel, L.J.M. Lemmens, A.F. Mason, M. Merkx, L. Brunsveld, J.C.M. van Hest Adv. Mater. 35, 2300947 (2023) DOI: 10.1002/adma.202300947

06. FROM TETHERED TO FREESTANDING STABILIZERS OF 14-3-3 PROTEIN-PROTEIN INTERACTIONS THROUGH FRAGMENT LINKING

E.J. Visser, P. Jaishankar, E. Sijbesma, M.A.M. Pennings, E.M.F. Vandenboorn, X. Guillory, R.J. Neitz, J. Morrow, S. Dutta, A.R. Renslo, L. Brunsveld, M.R. Arkin, C. Ottmann

Angew. Chem. Int. Ed. 62, e202308004 (2023)

DOI: 10.1002/anie.202308004

07. FULLY (RE)CONFIGURABLE INTERACTIVE MATERIAL THROUGH A SWITCHABLE PHOTOTHERMAL CHARGE TRANSFER COMPLEX GATED BY A SUPRAMOLECULAR LIQUID CRYSTAL ELASTOMER ACTUATOR

S. Tian, S.J.D. Lugger, C. Lee, M.G. Debije, A.P.H.J. Schenning J. Am. Chem. Soc. 145, 19347-19353 (2023) DOI: 10.1021/jacs.3c05905

08. HAPTEN/MYRISTOYL FUNCTIONALIZED POLY(PROPYLENEIMINE) DENDRIMERS AS POTENT CELL SURFACE RECRUITERS OF ANTIBODIES FOR MEDIATING INNATE IMMUNE KILLING

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17. SOLVENT-INDUCED PATHWAY COMPLEXITY OF SUPRAMOLECULAR POLYMERIZATION UNVEILED USING THE HANSEN SOLUBILITY PARAMETERS

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20. TWO-PHOTON NANOPROBES BASED ON BIOORGANIC NANOARCHITECTONICS WITH A PHOTO-OXIDATION ENHANCED EMISSION MECHANISM

S. Li, R. Chang, L. Zhao, R. Xing, J.C.M. van Hest, X. Yan Nat. Commun. 14, 5227 (2023) DOI: 10.1038/s41467-023-40897-4

Coupling knowledge to improve organic solar cells

Make electrons move faster and farther

There is increasing research into the development of organic solar cells. These have many advantages over conventional cells: they are flexible and have a more cost-effective production process. However, their efficiency still lags behind. Master student Lian de Jong (Applied Physics) tried to improve that through the physical phenomenon of "strong coupling." She combined knowledge from her research group Photonics and Semiconductor Nanophysics with that of the Molecular Materials and Nanosystems group. Her first steps on this pioneering path have proven quite successful.

Solar energy is an important renewable resource in the energy transition. New technologies emerge to improve the efficiency and lower the cost of conventional silicon solar cells. At the same time, the market for organic solar cells is growing. These have several important advantages over their conventional counterparts. They are thin, flexible and lightweight, making them ideal for incorporation into facades and other specific surfaces. In addition, they are easier and cheaper to produce. Still, large-scale rollout has yet to occur. And that has everything to do with the inferior efficiency of organic solar cells.

"The generation and conduction of electricity in an organic solar cell is somewhat different from silicon solar cells," says Lian de Jong, a former Applied Physics master student. In March she graduated cum laude on a new method to improve the efficiency of organic solar cells. She is currently busy with her new job at ASML, but can still be found at TU/e from time to time - a paper needs to be completed. "When light falls on an organic solar cell, it is converted into so-called excitons by the organic semiconductor material inside," De Jong continues her explanation. "These excitons consist of an excited electron and its remaining cavity,

which cannot move independently of each other. Current starts flowing only when the excitons disintegrate at the interface of two different organic solar cell layers. Electrons then move in one direction, and the cavities in the opposite direction." She says the organic solar cell industry has a strong focus on developing new materials to improve exciton mobility and ultimately enhance efficiency. Work is also underway to develop UVresistant and air-tight coatings that prevent degradation of the organic semiconductor layers. "This is all from a chemistry perspective," De Jong adds. "We chose a physical approach to improve the organic solar cell."

Lian de Jong

COUPLING LIGHT AND MATTER

De Jong focused on the physical phenomenon of "strong coupling" which is an important research topic at the Photonics and Semiconductor Nanophysics group of professor Jaime Gomez Rivas (department of Applied Physics). It is an extreme form of light-matter interaction in which molecules exchange energy with an optical cavity. Using strong coupling in organic solar cells is a new exciting field, says de Jong. She explains how it could improve the solar cell: "Light can travel fast and far. By giving an exciton these properties, more excitons could reach the organic semiconductor interface in the solar cell, and thus generate more current. In short, we want to couple light and matter, creating a quasiparticle with the interacting properties of matter as well as the fastness of light."

To induce strong coupling, you need a cavity in the material, a place to store light. De Jong used a simple cavity to study whether the coupling phenomenon would also work in solar cells, going about it with mirrors and lenses. "When you shine (laser) light against a mirror it reflects. When you place a mirror opposite to it, the light keeps going back and forth between the mirrors and you have 'captured' it. By placing two mirrors at nanometer intervals, you can interfere with the selection of light waves that will fit - the resonance wavelengths."

SUCCESSFUL COLLABORATION

For more knowledge in the field of organic solar cells and their production, de Jong knocked on the door of the Molecular Materials and Nanosystems group of professor René Janssen (both at the departments of Applied Physics and the department of Chemical Engineering and Chemistry). "To test our strong coupling hypothesis in practice, we needed a working solar cell." Thanks to the successful collaboration, de Jong was able to make solar cells equipped with a reflective thin metal layer, and tested them extensively. She is enthusiastic

THESIS PRIZE The pioneering work of Lian de Jong was unanimously awarded the Master thesis prize of the Netherlands' Physical Society (NNV), division Atom, Molecular and Optical Physics (AMO) during its annual conference held last October. Due to work commitments abroad, De Jong participated by means of a video connection.

about the first results: "We show that strong coupling in a solar cell is indeed possible, and the efficiency seems higher. The main challenge is that by introducing a mirror the amount of light entering the solar cell is reduced, due to reflection. We are able to correct for this in the test system, using a mathematical model." Thus her pilot study successfully showed that the physical coupling phenomenon can potentially contribute to the improvement of organic solar cells. "But the coupling between the two departments also proves essential," De Jong says. "The combined expertise really helped to get this far, and still helps in taking the necessary follow-up steps."

Bas Overvelde In his hands a soft robot.

Research on soft robotic heart is granted 10 million

A soft implantable robotic heart for people with severe heart failure. To develop it further, the Holland Hybrid Heart consortium – in which TU/e scientists Carlijn Bouten, Frans van de Vosse and Bas Overvelde are involved – has received 10 million euros from the Dutch Research Agenda. The soft robotic heart can be placed in the chest of patients with severe heart failure and takes over the function of the real heart. The team hopes to realize this within 10 years. In the consortium Holland Hybrid Heart (HHH), universities, higher vocational education, companies, and patient organizations collaborate. Cardiothoracic surgeon Jolanda Kluin of the Erasmus MC Thorax Center leads the collaboration. Kluin: "We want to offer patients a good and viable alternative to transplantation with a natural heart." Worldwide, there are over 23 million people with heart failure, for whom the best treatment is getting a donor heart. There is a serious shortage of these. In the Netherlands, there are 250,000 heart failure patients, half of whom die within five years.



Cardiothoracic surgeon **Jolanda Kluin** of the Erasmus MC Thorax Center leads the research on the soft robotic heart. *Photo: HHH*

Kluin got the idea of a soft robotic heart when she saw the work of TU/e researcher Bas Overvelde in the media. He works with robots made of soft and flexible materials that can respond themselves to changes in their environment. Think of a robot that resembles an octopus or a starfish. Inspiration by soft robotic octopus. Kluin: "When I saw such a soft-robot moving octopus, I thought: surely we should be able to make a heart with this, too," "These kinds of artificial muscles, made of soft materials, are ideal for building an artificial heart that mimics the functioning of a natural heart," says Overvelde, associate professor at the department of Mechanical Engineering. Because the inner lining of the Hybrid Heart consists of cells from the patient himself, it is going to look even more like a real heart.

Frans van de Vosse *Photo: Bart van Overbeeke*

"This inner lining prevents the formation of blood clots and rejection of the robotic heart," says Carlijn Bouten, professor of Cell-Matrix Interactions in Cardiovascular Regeneration at the Biomedical Engineering department. The addition of this "living" layer will give the artificial heart its hybrid function. Professor of Cardiovascular Biomechanics Frans van de Vosse adds: "We are going to calculate the interplay between the deformation of the artificial heart muscle and the functioning of the inner lining in preventing blood clots with computer models. In this way, we can arrive at a good design of the Hybrid Heart in a short period of time."

Carlijn Bouten Photo: Vincent van den Hoogen

ABOUT THE DUTCH RESEARCH AGENDA

This project is receiving funding in the fourth round of the Dutch Research Agenda: Research along Routes by Consortia (NWA-ORC). A total of over 131 million euros is available for the consortia. Holland Hybrid Heart is made possible in part by the Heart Foundation with a grant of 700,000 euros. In addition, several organizations/companies are jointly providing 700,000 euros worth of services: SBMC, TrailBlazers, evos GmbH, DCVA and EE Labels. This project builds on previous work by the aforementioned researchers in a European consortium.

FOUNDATIONS OF COMPLEX MOLECULAR SYSTEMS

The Visualization group of the department of Mathematics and Computer Science is internationally recognized as one of the top groups in the field. In August 2022, Fernando Paulovich became a member of this team, bringing his own well-known tools and expertise. And now also as a member of ICMS, the associate professor in Visual Analytics for Data Science sets out to help researchers in various fields, from design materials to analytical chemistry and even medicine, to visualize their data and be part of the entire data analysis process.

Fernando Paulovich PLOS lization of Protein Folding Funnels in Lattice ihe power visual anal

"THROUGH VISUALIZATIONS, USERS ARE NOT MERE CONSUMERS BUT ESSENTIAL COMPONENTS OF THE ANALYTICAL PROCESS, ENTERING KNOWLEDGE AND JUDGING THE GENERATED OUTCOME."

Visual analytics is the integration of machine learning and data mining with visualization as the output. Many people know charts and graphs, but Paulovich is doing much more than that. "The idea is to open the black box and see what the computer is doing," he explains. "I want to allow final users to be part of the data analysis loop as active participants, instead of just as consumers of the results. One good example is the process of classification. In the usual approach, users enter data into a model and get a prediction. Visualization tools allow us to go a step further, letting users understand the reasoning behind a prediction model, enter additional data to improve it, and audit the final results. This will make the model more accurate, and the results it generates more trustworthy."

Paulovich studied computer technology at the Federal University of São Carlos in Brazil. His fascination with visualization began in 2000, when he left his job at a big tech company and decided to return to academia for a PhD. "A colleague mentioned a sister working at the University of São Paulo, Brazil, on this particular subject. Arriving there, she showed me the powerful idea of visual representations. I was astonished that this was even possible at that time! Shortly after, I began working with her and I learned even more about the strength and various possibilities of visualization, and later visual analytics."

FROM BIOSENSORS TO PROTEIN FOLDING

After completing his PhD in 2009, Paulovich started working at the University of São Paulo. In 2017 he moved to Canada as the Canada **Research Chair in Visual Analytics** at Dalhousie University. Then, after five years in Canada, he applied for a position at TU/e. For several reasons, he says. "I had been here before and I really like the culture of using bicycles to get everywhere. But more importantly, I wanted to be part of the team of professor Jack van Wijk. In 2007, still during my PhD, he won the IEEE Visualization Technical Achievement Award, the highest recognition in the field. I remember his speech, and I was really impressed by what he had achieved in his career."

In the twenty years of his career, Paulovich has accomplished a lot himself. For example, he was one of the pioneers in dimensionality reduction (DR). "This is the process of combining or selecting data features (or attributes) to reduce their number, usually to two or three, so that a visual representation can be created. I have applied DR to different domains, from sensor and biosensor data to protein folding processes."

SETTING A COMMON LANGUAGE

Applying visualization to a variety of research fields has some challenges, according to Paulovich. "Especially within ICMS we have to work towards a common language. For example, what I call a classification model may be called differently by other scientists. The same goes for the term 'bias.' Adding to this, working from the perspective of the final users is challenging. All have their own expertise and I need to adjust my tools to suit them best."

Since he arrived at TU/e a year ago, Paulovich is creating new connections. "Back in Brazil and Canada I have been collaborating with researchers from multiple universities and also non-profit organizations, for instance to analyze data from quality-of-life surveys. But now I hope to build new partnerships in the Netherlands. I think ICMS can help me with this in the years to come." He expects the use of visualization will increase in the near future, as more people start working together, sharing knowledge and developments. "We want to show everybody the value of what we are doing; that we need to understand what the machine is doing since we cannot go blind while making decisions. I think our main purpose is making the power of visual analytics being part of almost every field of natural science."

News, awards & grants

Scan the QR codes to read the full articles

Talented postdoc Fabian Sobotta received Walter -Benjamin stipendium

FABIAN SOBOTTA, POSTDOC AT THE SELF-ORGANIZING SOFT MATTER GROUP, RECEIVED THE WALTER - BENJAMIN STIPENDIUM.





ERC Advanced Grant for René Janssen and his research on more efficient solar cells

HE AIMS TO MAKE SOLAR CELLS WITH THIS MATERIAL THAT ARE UP TO TWICE AS EFFICIENT AS CURRENT SOLAR PANELS WHICH ARE MADE OF SILICON.

Scan the QR codes to read the full articles

DSM Biomedical joins hands with the Institute for Complex Molecular Systems (ICMS)

DR. MATILDE PUTTI (LEFT) FROM DSM BIOMEDICAL AND DR. MONIQUE BRUINING (RIGHT) FROM THE ICMS AGREE TO STRENGTHEN THEIR RENEWED COLLABORATION.



Breakthrough way to train neuromorphic chips

NEUROMORPHIC COMPUTERS – WHICH ARE BASED ON THE STRUCTURE OF THE HUMAN BRAIN – COULD REVOLUTIONIZE OUR FUTURE HEALTHCARE DEVICES.





New model to help valorize lignin for bio-based applications

WOODY BIOMASS AND WHEAT STRAW ARE ALL SOURCES OF THE NATURAL POLYMER LIGNIN WITH MORE THAN 50 MEGATONS OF LIGNIN PRODUCED ANNUALLY AT COMMERCIAL SCALE. FOUNDATIONS OF COMPLEX MOLECULAR SYSTEMS

From left to right: Pim van der Hoorn, Federica Eduati and Mike van Santvoort

Mathematically mapping the way tumor cells comunicate

TU/e researchers Federica Eduati (Biomedical Engineering, Computational Biology) and Pim van der Hoorn (Mathematics and Computer Science, Probability) met each other at an ICMS meeting on immunoengineering. Now, three years later, with their joint PhD student Mike van Santvoort they have developed a surprisingly successful mathematical model to map the network of cells within the tumor microenvironment. Based on random graphs, the new model is able to pinpoint differences in cellcell interactions between cancer patients belonging to four characteristic immune profiles. This mechanistic understanding of the tumor could pave the way towards a more rational design of personalized anti-cancer therapies. In a corner of the open meeting room in ICMS building Ceres, Federica Eduati and Pim van der Hoorn are bent over the laptop screen of joined PhD student Mike van Santvoort. He is updating them on the results of a new set of experiments. Besides unraveling how cells around a tumor communicate with each other, Van Santvoort also had to learn a new language himself, he explains with a laugh. "As a mathematician, I think and work in a very different way than immunobiologists do. I have learned a lot over the past few years. Now when I sometimes hear Federica and Pim talking past each other, I can more easily help out." "The student becomes a teacher," Van der Hoorn winks.

A SYSTEMIC APPROACH

The first fruits of their collaborative research will soon be published. For some time, Eduati has been trying to use a systemic approach to find out why cancer patients respond differently to the same therapy. Van der Hoorn became interested in this issue during a brief presentation by Eduati at an ICMS meeting, he says. "Using limited data, Eduati wanted to investigate whether she could distinguish patients based on the presence of certain cell types and how these cells communicate with each other. From a mathematical perspective, I could contribute to that."

After a brief search, van Santvoort - strong mathematical background, broad biological interest - joined them. Together they started using algorithms on patient data to determine the quantity of certain cell types. Van Santvoort briefly summarizes the idea behind their model. "We can see how often a protein and the receptor it binds to occur; the algorithm can match these ligand-receptor pairs to cells. That is where the randomness comes in, we have to generate many different networks for a given patient, get an average overview, and subsequently extract properties from this overview. These could then be used as a kind of biomarkers indicating the status of a patient."

AN UNBIASED MODEL

According to van der Hoorn, the challenge is to use bulk RNA sequencing data - the average expression level of individual genes in pooled cell populations from a patient biopsy - to gather information on the communication network of all the cells around the tumor of the patient in question. Another aim is to establish how the individual cells communicate with each other. "Because we cannot measure this cellular communication for all cells simultaneously, we need a model," he explains. "This model has to be unbiased, using only the input data. With a random graph model, no additional assumptions are made in advance."

Mapping the network of cellular communications is important to understand the tumor, Eduati emphasizes. "We want to understand what makes a person's cancer unique, and which parts of the communication network contribute to this. In a next step, we could use this model as a predictive tool for the effectiveness of certain anticancer therapies, such as immunotherapy." Although the step toward personalized medicine is still large, Eduati shows that the first version of their mathematical model looks very promising. "In a pilot study, we were able to distinguish four different immune phenotypes, which are independent of the type of cancer. Each phenotype has its own characteristics of cellular communication, which indicate whether a therapy is more or less likely to succeed."

INTERESTING CHALLENGES

Not only is their mathematical model "Random Cell-Cell Interaction Generator" (RaCInG) still producing relevant information by using bulk data, it is also theoretically trackable, Van Santvoort explains. "Our aim is to develop models that we understand. In this way we can face new interesting challenges more easily and then adapt the model accordingly."

To the three enthusiastic researchers it is obvious that the project will be continued. At its onset, however, it was mostly a big gamble, van der Hoorn agrees. "Multidisciplinary research initially does take a lot of effort and time. And it is not always clear what the outcome will be. But sometimes you just have to take the gamble. Fortunately, we all are not afraid to take a chance. And with ICMS we have a supportive institute behind us to fund these exploratory projects." GENERAL

"We are an educational institution"

Bert Meijer has handed out his hundredth PhD degree.

Marle Vleugels (left) and Bert Meijer (right)

On September 14, 2023, Marle Vleugels successfully defended her PhD thesis entitled "Bioactive supramolecular assemblies." This defense was special for her PhD advisor professor Bert Meijer, because Vleugels was his hundredth PhD student. Since Meijer awarded his first doctoral degree almost thirty years ago, he has seen his former PhD students move on to a wide variety of jobs, ranging from professor, industrial researcher or teacher to manager in a hospital. "Although we perform research, we are not a research institution. We are an educational institution. We don't hire people to do a job. We give young people the opportunity to develop themselves." The Meijer Research Group designs, synthesizes, characterizes and sometimes applies complex molecular systems. Although he loves research, it is not his main focus, says Bert Meijer, professor of Organic Chemistry and co-founder of the Institute for Complex Molecular Systems (ICMS). "Being a university professor means being a teacher," he says, and he takes that role very seriously. "The researchers in our group are not my people, implementing my ideas. What we do is all about them and their education. My goal has always been to give them everything they need to develop for their future careers, obviously by doing cutting-edge science."

Meijer shares this ideology with his former supervisor and role model professor Hans Wijnberg. Many of Wijnberg's PhD students have had admirable scientific careers, including Nobel laureate Ben Feringa. The Meijer Research Group also shows that this ideology can be very successful. Out of those hundred PhD students, eleven are now professors. The first was Jan van Hest, the current scientific director of ICMS. He also received the 2020 Spinoza Prize, 19 years after Meijer himself received this prestigious recognition.

SCIENTIFIC THINKER

A significant number of the former PhD students have ended up in research. Marle Vleugels, for instance, is currently at Linköping University (Sweden). Others chose to work in teaching, as clinical chemists, or as managers in hospitals. Take Eva Wisse, who is now Director of Care and Operations at Catharina Hospital Eindhoven. But most of Meijer's PhDs found jobs in industry, varying from plant manager to researcher, at companies like Philips, DSM, Covestro, Shell or Agfa. Meijer: "In November we will have a group outing to the Brightlands research and innovation campuses in Limburg. This is hosted by six former PhD students of our group." Meijer really cares about what could be called his scientific "offspring": "When I retire, my international colleagues will no longer matter, as will most of our publications. But the people I educated will still matter. I am proud to see that our education has provided all hundred PhD's, but also hundreds of master students and postdocs, the opportunity to develop in these different directions. In our group you learn to become an independent scientific thinker by diving deep into the many challenges of scientific research. This knowledge serves you well in any future role."

THESIS REPRINT

We have asked former PhD students to reflect on their time with the Meijer Research Group. They answered positively, telling that the atmosphere in the group and Meijer's supervision are a pleasant experience. They agree that doing a PhD in the group comes with opportunities such as conferences abroad, collaborations with other groups and access to good equipment.

But it's up to you to seize these opportunities. You also get a lot of freedom, which requires independence and taking initiatives. You are the lead in your own PhD with Meijer as a supportive mentor. Meijer: "We demand a lot from our PhD students. I do not want to interfere too much, especially in the beginning. Who knows, there might be a new Oppenheimer walking around, who is much smarter than me."

Meijer tries to assist when needed. "Years ago, while traveling by train to a conference, a Japanese colleague asked what Brigitte Folmer - then a PhD student - was working on," says Meijer. "As she tried to explain, I realized that the research topic was too vague. Even I couldn't explain what we were doing. When we got back to Eindhoven I proposed to switch to something different. She made that into a complete success. Her thesis on supramolecular polymers was so popular that it got a reprint."

ETCHINGS AND SCREEN PRINTS

That Marle Vleugels is the hundredth came not as a surprise to Meijer. "I give everyone a numbered artwork titled 'Chemistry,' he explains. The artwork shows a fume hood and the process of synthesizing molecules, with some structural formulas in the background. The first forty PhD students got a black-and-white etching, made by an acquaintance some thirty years ago. "After forty prints, the etching plate was worn out," Meijer says. "Then my wife lektje Meijer-Oosterbeek, who is an artist, designed a colored silkscreen print. That covered the numbers forty to ninety. When that screen worn out, she made a more modern but similar silkscreen. That has been my gift to PhD students ninety and beyond. Hopefully a few more will follow in the years to come."

The reason Meijer gives all PhD students the same artwork is twofold. "It means I never have to think about what to give. And for the PhDs it's a way for to recognize each other later in their careers. When you see the etching or silkscreen in someone's office, you know you share a history with the same research group." GENERAL

Visual artists Benjamin Simmers, Milan van Wezel and Koen Pieterse **Balancing science**

The ICMS Animation Studio operates at the intersection of science, art and education. It has been four years since Milan van Wezel and Benjamin Simmers joined the Studio. They create graphical illustrations and animations that support new scientific publications, or help to communicate science to the public. It's unique for an institute to have an animation studio within the organization, and this greatly stimulates fruitful collaboration with researchers. Scientists set the bar high, Simmers and Van Wezel know. If they agree with your work, you know it's good.





What does the formation of yogurt look like, on a molecular level? "In a scientific publication, the global process could perhaps be explained in a few sentences," says Milan van Wezel. Bacteria in milk produce acidic compounds, lowering the pH of the fluid, causing casein proteins to form clusters. As acidity further increases, the casein clusters organize into large three-dimensional structures, partly solidifying the milk.

But does the written word completely capture the complexity and threedimensionality of the molecular process that lies underneath? Probably not, says Van Wezel, who works as an animator at ICMS. He points to his current work-inprogress: an animated video on the molecular dynamics behind the formation of yogurt. The video shows an incredible mess of somewhat round and pointy white balls, moving all over the place. The balls represent the casein proteins, some 80 thousand of them. As the balls are moving, blue wormlike creatures appear: bacteria. As the acidity increases, a caseinbased skeleton forms around them. Slowly but surely, some pink-colored compounds are secreted from the blue bacteria, stabilizing the skeleton. The incredible mess of moving balls turns into a well-organized, solid-like structure, accurately depicting the formation process of yogurt.

To Van Wezel the video is his most challenging project. "It required a lot of research," he says. "I had little to work with, as my inspiration mostly came from structural images in scientific publications. After that, it was a lot of trial-and-error to learn how these proteins should actually be moving. I'm finally getting to the point where it starts to resemble reality."

ENTERING THE WORLD OF CHEMISTRY

Van Wezel was educated at an art school in Breda, focusing on contemporary arts. It wasn't until after graduation that animation truly piqued his interests. His colleague Benjamin Simmers, who started at ICMS at the same time in 2018. has known since high school that he wanted to do graphical design. Neither was trained with complex chemistry in mind, though. "In high school, I dropped chemistry as soon as I had the chance," Simmers laughingly admits. "Looking back, I regret that. Everything here is fascinating. Every day I learn something new."

From a graphical design perspective, atoms and molecules are awesome to work with, he continues. "They can usually be represented with lines, balls and other simple shapes. And as they arrange in the most energy-efficient way, a variety of interesting patterns emerges. The molecular world is completely different from our everyday reality, like in a science fiction movie."

A BALANCING ACT

Having a background in visual arts, both designers notice a certain tension when working in an academic environment. "A scientific audience demands a very realistic image," Van Wezel says. "Most of the time that is not entirely possible, as the size of molecules is just too small. And of course, an illustration should also look nice. Design is always a puzzle, balancing esthetics, function and realism."

This tension is strongly present in a recent animation by Simmers that to him characterizes the work of the animation studio.

It's a video explaining the technical process behind the Smart*Light, a very compact "tabletop" particle accelerator developed by TU/e



professor Jom Luiten. It stretches a ten-nanosecond process into a four-minute animation with a concise but in-depth commentary.

GLOWING DOTS

The main character of the movie is a small beam of 100 million electrons. Once again, there is a strong interplay between scientific validity, esthetics and the educational purpose of the video. Some aspects are clearly fictional: the beam is reduced to a hundred glowing dots, representing the electrons. As they travel through the accelerator, the dots leave a blue "trail", resembling that of a falling star. At the same time, the video incorporates real scientific data provided by Luiten, Simmers emphasizes. And there is more: the beam subtly rotates as the electrons accelerate, just like it does in the actual machine. Probably inconspicuous to a layman, this is a meaningful detail to the scientific eye. For Simmers the video thus represents the fruitful collaboration that is typical for ICMS.

The video ends with an exciting surprise, fulfilling the video's educational purpose. Some X-rays leave the machine, directly followed by the "camera." The "Girl with a Pearl Earring" emerges, painted by Johannes Vermeer in his beloved masterpiece. She looks over her shoulder, right at the viewer. As the final X-ray beam hits the painting, the narrator explains how it allows scientists to obtain highly detailed chemical analysis of materials - including the famous artworks of Dutch masters.

"Founding fathers" reflect on 15 years of ICMS

How it started, and how it's going

From left to right: Bert Meijer, Hans van Duijn, Arno Peels and Sagitta Peters at the opening of the Ceres building

How did ICMS become what it is today? The answers to this question brings us back to a basement where "founding fathers" Bert Meijer, Rutger van Santen, Mark Peletier, Jaap Schouten, Amandus Lundqvist and Hans van Duijn met almost two decades ago. Now, they share their memories of those early days of ICMS. A tale of how it all started, and how the institute came to thrive. The space felt like a large living room. The atmosphere was informal, the interior cozy. When you entered, you walked past some large couches. Scattered over the table were scientific journals like Nature and Science. The coffee was decent. The basement of the main building at Eindhoven University of Technology was cleverly furnished to look much more sunlit than it actually was. Walls were purposefully painted in light colors, to reflect as much light as possible.

For about three years, a small group of scientists gathered here every Friday. It was instigated by Bert Meijer, professor of organic chemistry, aiming to organize scientific collaboration throughout TU/e. Over time the group grew larger, but at first Meijer was joined by a small scientific core: Rutger van Santen, Mark Peletier and Jaap Schouten. Their weekly conversation topics were as diverse as their scientific backgrounds, with all participants bringing different expertise to the table. Van Santen, who had been the first to join Meijer, had built a strong career as professor of inorganic chemistry and catalysis. Schouten was a chemical engineer, particularly interested in microfluidics. Peletier's expertise was in mathematics. From a short distance they were supported by Hans van Duijn, the university's rector at the time, and Amandus Lundqvist, chairman of the executive board. Six people with different backgrounds, but a shared goal: to shape what would become the Institute for Complex Molecular Systems. Interdisciplinarity was to be at the core of the institute, combining biochemistry, theoretical physics and engineering. "We noticed how those disciplines are often combined, but never all at once," Meijer reminisces. "That is what we wanted to realize."

INCEPTION

In fact, the journey of ICMS originated even before those basement meetings. Meijer had been approached by Lundqvist and Van Duijn with a remarkable proposition: the opportunity to establish a new institute entirely on his own. "We noticed a trend among universities like Groningen and Nijmegen, which were establishing institutes around their most esteemed professors," Lundqvist recollects. "These institutes aimed to provide optimal support for these professors and foster international networks. For us, it was about Bert Meijer - and ensuring his future in Eindhoven."

"It took me completely by surprise," Meijer reflects on the effort, admitting he wasn't immediately enthused. It took some time and some advice from colleagues to really get behind the idea. Meijer approached Henk de Wilt, former chairman of the TU/e executive board, with whom he had always had a great connection. De Wilt advised him: "Bert, you're going to write down everything you want. Ask for your own building and a lot of research money, until you retire. Then, if they still say yes, you do it."

DEFINING THE INSTITUTE

But what should be the focus of the institute? What name should it carry? What pressing scientific challenges should it address, and how? In a first attempt to answer these questions, Meijer turned to his friend and colleague Van Santen. The new institute was all theirs to make; Meijer had received zero requirements or even recommendations from the TU/e board. Together they began their first brainstorm. "We were envisioning the future of chemistry," Van Santen recalls, "and we agreed that the focus needed to be shifted - that chemists started thinking in terms of systems rather than molecules.

However, science tends to be inherently conservative. Scientists embrace innovation, but personal reinvention can be challenging. Bert and I were well aware of this. We needed fresh perspectives and additional collaborators." So in the following brainstorming sessions in the basement, the two chemists were joined by two new "partners in crime" as Schouten puts it: an engineer and a mathematician.

CREATING UNITY

Was it difficult to unite scientists from diverse backgrounds in the creation of this new institute? According to the "partners in crime," not so much. Their primary challenge was learning to "speak each other's language." They recall delving into questions such as: Why is a chemist interested in a particular signal frequency spectrum when researching Alzheimer's disease? What instrumentation does the chemist employ? How is the data interpreted, and what insights does it yield? And given current limitations of chemical machinery in measuring interactions within molecular systems, could a mathematician maybe attempt to compute them?

"Honestly, my best memories of ICMS are from our time in that basement," Peletier recounts. "We were genuinely exploring our opportunities and investigating new ways to collaborate. Our plans were incredibly ambitious, all rooted in an idea I strongly support: the most exciting science unfolds at the edges of scientific disciplines." It's worth noting that the most significant uniting factor wasn't necessarily a scientific one. Everyone involved in the basement sessions holds Sagitta Peters in high regard. She became the first managing director of the institute and played a pivotal role in creating a harmonious environment where everyone could get along.



ICMS TAKES FORM

After countless meetings, how did the six scientists ultimately define their institute? ICMS remains an embodiment of multidisciplinarity to this day, bringing together five participating departments that encompass theoretical and applied physics, engineering, biochemistry, and more. Their work was deemed "new science," focusing on complex molecular systems in a manner pursued by relatively few scientists worldwide. The institute's most fundamental quest became to investigate the natural emergence of molecular complexity: the origin of life.

Inevitably, the institute outgrew its basement, relocating to the beautiful new Ceres building. Peters again played a substantial role in the designing process of ICMS's new study center, transforming a rather antiquated boiler house into their modern home, an achievement that garnered the Dutch prize for "Building of the Year."

ICMS STRATEGY

Perhaps the most important aspect of the ICMS strategy was to attract new people, in particular people with interests and qualities that go beyond a single TU/e department. Van Santen: "I've always considered that to be among the institute's most remarkable achievements: the ability to draw in brilliant individuals from diverse backgrounds, not only excelling scientifically but also as executives." Meijer describes "his" institute as a "hotspot" for scientists to come together, inspiring boundary-crossing work. Typical for ICMS is that it not directly employs researchers: these are hired by the contributing faculties. The role of the institute merely is to lower the barriers. "The purpose has always been to unify people and disciplines," he says. "We have money to fund projects, but you can't come to us for money - only for ideas."

The absence of direct employment at ICMS has a significant consequence: every scientific practice within the institute arises from an intrinsic willingness to collaborate, to create interdisciplinary crossovers, to follow one's curiosity beyond the confines of one's own department. Once your fascination extends department limits, your work may seamlessly

continue through ICMS. If the science is good, people within ICMS will be there for you. The principle that nothing is obligatory lies at the core of ICMS. This philosophy even stems back from the institute's early days. Meijer: "No one was obligated to be there. Ideally, you want to attract people because they are genuinely interested, not because they have to be there. That was a significant advantage of starting in that basement: no substantial investment had been made into a new building, so everyone could have dropped out at any time. The fact that no one did, says it all."

SHAPED FROM THE START

In many ways, the course of the institute over the past fifteen years has undeniably been shaped by its design at the start. "My wife always says how incredibly conservative I am," Meijer laughs. "I tend to think very long about everything I'm going to do. And once I commit to it, I stay on course. It's almost a strategy. And if it's up to me, ICMS will last like this forever."

After a span of fifteen years, the original core of ICMS is no longer involved with the institute on a day-to-day basis. Some members have redirected their scientific focus within their departments already at an early stage, refraining from intensive collaboration within the institute. Others have since retired or ventured into entirely new career paths. Meijer also passed on the torch as scientific director, succeeded by Jan van Hest. With a fresh cohort of individuals who have come on board over the years, the institute is here to stay. As new executives bring their own unique perspectives and expertise, ICMS is likely to embark on new directions while maintaining the institute's original purpose: to stimulate interdisciplinary collaboration and perform boundary-pushing research. After all, as long as the science is good, the people will be there.

Interview:

"Broaden the horizon and retain long term value of ICMS research"

Samir Vinchurkar

Samir Vinchurkar joined the ICMS community as Business Engagement and Research Development Manager back in July this year. After a few months, we took the time to sit down over coffee to chat about his adventurous career path that has ultimately lead him to ICMS. What are his plans now that he is here, and what keeps him occupied in his free time?

Originally from India, Vinchurkar's career took him to the USA for his masters and PhD, after which he moved around the world for a variety of jobs. He has held academic positions in India and Ireland and gained business experience in Belgium, India, South Africa and Ireland. These range from being the first employee of a company, to board positions and directorships. With such an extensive history in academia and industry, Vinchurkar is well placed to look at research from both sides. Combined with his intercontinental experience, he has a unique perspective on what can work within the right environment, and more importantly what it takes to make it work.



That being said, experiences can make us take a second look at what we have and what we shouldn't take for granted. Here in the Netherlands, what are some things that you won't be taking for granted? "Unlike my Dutch colleagues who were born here, I realize how lucky I am to be in the world's most livable country. I think freedom in all its forms is something that cannot be taken for granted universally."

TU/e's attitude towards business engagement and commercialization is very positive, with a number of ICMS projects on that path. What sort of endeavors are you looking forward to?

"I hope to broaden the horizon to additional multidisciplinary domains and strengthen the industry network beyond our waters. And I want to assist ICMS members in retaining long term value of their research within various partnerships and commercialization initiatives."

Do you see any particular development that will be worthwhile in the coming years?

"Looking at our initiatives such as the upcoming high throughput robot lab, I feel that in the near future companies will start outsourcing some of their research pipelines to ICMS."

Finally, when your feet and mind are pointing home, what do you look forward to?

"Tennis with fluitjes, the occasional frikandel, and long walks in the Veluwezoom."

Predicting the behavior of complex fluids

Alexandra Alicke

Complex fluids are present in many different areas, from the food industry to tissue engineering. Assistant professor Alexandra Alicke studies studies the rheological behavior of these kinds of fluids to make better use of them.

Rheoloav is the science of deformation and flow of matter. Alexandra Alicke wants to understand how the "building blocks" of soft materials affect their overall deformation and flow behavior. "If we understand this, we can predict how a certain material will behave in a given situation." Take mayonnaise - ideally with French fries it should stay in a blob on top, but when making a sandwich it should be easily "spreadable." So, its consistency, or rheology, is different in these cases. Alicke is interested in explaining such rheological behavior via the microstructure of the material. In the case of mayonnaise, the structure arises from the way many tiny liquid droplets are dispersed in another liquid.

MAKING A DIFFERENCE

At TU/e, Alicke is looking how to impart structure to such liquidliquid interfaces by using small solid particles, and which are the most efficient stabilizing strategies. "I also want to explore whether it is possible to use these interfaces as 2D-model-systems to predict the behavior of other bulk (3D) materials where experiments are more challenging to carry out." On the more applied side, she is working on a few 3D printing problems, especially within the food industry food inks are typically complex fluids. On the long term Alicke would like to apply her knowhow to biomedical applications. There, many complex fluids and fluid-fluid interactions have not yet been explored much. "Think about hydrogels used in tissue engineering, or microbubbles for drug delivery and as contrast agents. I think investigating rheology can surely make a difference there."

NAME:

Alexandra Alicke

POSITION:

Assistant professor, Processing and Performance of Materials group (since September 2022).

PREVIOUSLY:

PhD in Materials Science at ETH Zürich.

STUDIES:

MSc Mechanical Engineering at Pontifical Catholic University of Rio de Janeiro.

MOTIVATION:

Do the best science I can.

DREAM:

Help solving big problems with my knowledge in rheology and interfacial sciences.

SPARE TIME:

Hiking and photography.



Glenn Weber

EUROTECH PhD: Glenn Weber

Glenn Weber has an educational background in Biomedical Sciences (BSc) and Systems Biology (MSc), respectively from Amsterdam University College and Maastricht University. Throughout his study, he has been interested in complex diseases such as neurodegenerative disorders and cancer. During his master studies he focused on obtaining the programming skills that would enable him to model the biological systems affected in these diseases. In July this year, he started his EuroTech PhD at TU/e.

A key reason that Weber decided to apply is the interdisciplinary component of the group, Systems Biology for Oncology. Under the supervision of Federica Eduati he now studies how to improve mathematical modelling for personalized treatment of cancer, by mining large datasets of the responses of different cell lines to drug treatment. Towards the end of the project, Weber hopes to be able to predict how certain tumor cells respond to immunotherapy. He also expects that the introduction of Artificial Intelligence (AI) in the modelling process can improve predictive powers whilst maintaining interpretability.

EUROTECH POSTDOC: Xue Wan

Xue Wan received her bachelor degree in Materials Science and Engineering from Jilin University, China, in 2016. She continued her studies at Harbin Institute of Technology, China, where she obtained her doctoral degree just last year. During her PhD studies, she spent a year at EPFL in Lausanne, Switzerland as a visiting student. There she learned about the EuroTech program and decided to apply. In June of this year she joined the research group Stimuli-responsive Functional Materials & Devices at the department of Chemical Engineering and Chemistry.

Xue's current research is about liquid crystal elastomers. These are fully reversible polymers that can be actuated by external stimuli such as heat and light. Their stimuli-responsiveness and reversible, large deformation are highly desired for soft robotics applications. For now, Xue is trying to use different processing techniques to fabricate these intelligent polymers with more intricate geometries. There are still many challenges ahead, but through discussion with her supervisors and literature investigations she hopes to solve the problems and contribute to this fascinating research field.

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