ICMS Highlights

Edition 12
May 2019

MOLECULAR GLUES
For new drug development

NEXT-GENERATION MATERIALS FACE DIVERGING DRIVERS

THREE FELLOWS,
three continents, three disciplines

A NEW PATHWAY TO VESICLE FORMATION

ICMS
INSTITUTE FOR COMPLEX MOLECULAR SYSTEMS

TU/e

INTRODUCTION

ICMS Highlights

In this era, scientific expertise develops at an unprecedented pace and allows us to exploit our technical capabilities in uncharted territories. The continuous flow of knowledge and know-how serves not only as a cornerstone for academic scientists to build upon, but also as a unique source of new principles and concepts for the industry.

In this edition of ICMS highlights, we present a plethora of possible connections between academia and industry, reflecting the ever dynamic and symbiotic environment at ICMS. Eline Sijbesma en Madita Wolter will outline the potential industrial impact of chemical biology, and a group of excellent materials scientists with whom we have warm connections will give their expert view on the next generation polymeric materials. In a similar context of connecting industry and academia, at our latest Outreach Symposium companies pitched their research challenges to researchers, inspiring, guiding and stimulating them to come up with out-of-the-box solutions for these challenges.

We are very happy to welcome Elizabeth McKenzie and Nicholas Tito to ICMS. Elisabeth's main focus will be on utilising TU/e expertise to the benefit of the ICMS Industrial Partners, and on expanding our industrial network. Nicholas has recently been appointed as ICMS fellow. Within the program for ICMS fellows, ICMS supports young, talented scientists to start their academic career. Together with the two other fellows, Danqing Liu and Ghislaine Vantomme, he will contribute to strengthening and opening up research domains in the field of complex molecular systems.

Our doors are always open for new ideas for the benefit of research and researchers.

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

Jan van Hest
Scientific director

Monique Bruining
Managing director

Calendar

June 11th, 2019, 14:00 hrs
Prof.Dr. O. Kranenburg
UMC Utrecht
NOVEL TREATMENT CONCEPTS IN COLORECTAL CANCER
Translational approaches
Ceres 0.31

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

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COVER Artist impression of fragment-based drug design. Small molecules are explored as possible stabilizers for protein-protein interactions.

FUNCTIONAL SUPRA-MOLECULAR SYSTEMS

Dynamic droplets lead the way

INTERVIEW WITH FMS RESEARCHERS PETER KOREVAAR AND EVAN SPRUIJT

Evan Spruijt (left) and Peter Korevaar

Korevaar and Spruijt are assistant professors in the department of Physical Organic Chemistry at Radboud University in Nijmegen. Both participate in the Research Center for Functional Molecular Systems (FMS), both are interested in using out-of-equilibrium self-assembly to create dynamic synthetic systems that exhibit functional behavior, and both see nature as a source of ideas. But within that shared context, Peter Korevaar and Evan Spruijt each focus on different questions and possibilities. For ICMS Highlights, they offer a brief introduction to their respective research topics.

"INSPIRED BY NATURE'S WAY OF BUILDING STRUCTURES AND SYSTEMS, PETER KOREVAAR AND EVAN SPRUIJT ARE PUSHING SELF-ASSEMBLY APPROACHES TO NEW LEVELS OF COMPLEXITY AND FUNCTIONALITY."

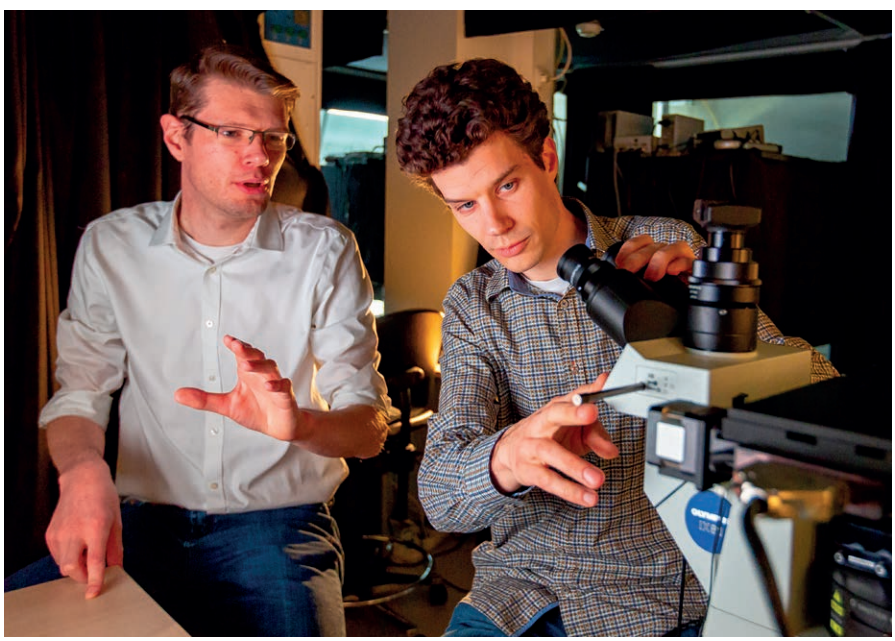
SLIME MOLD

"I am interested in coupling self-assembly processes to chemical networks and feedback mechanisms, as well as to physical chemistry phenomena such as surface tension, osmosis, and diffusion", says Korevaar. "That way, we can achieve more than by applying classical, equilibrium-based self-assembly strategies."
He takes inspiration from nature, currently in particular from a rather unassuming little creature called *Dictyostelium discoideum*. This is a slime mold that is well-known for its quorum sensing ability which allows unicellular individuals to come together and form a temporary multicellular organism that can move over larger distances to search for food. "It does so by spreading as a network of slime threads over a surface. We are mimicking these principles in a system based on chemical self-assembly, and that results in interesting behavior. When we apply a drop of our material to a thin layer of water, filaments start growing in all directions. It just happens right before our eyes."
The material is just a simple surfactant, according to Korevaar. "It assembles into a bilayer, and by altering the surface tension filaments get 'pulled out' of the central droplet. They follow the gradient in the surface tension, and we are now very interested to find out if we can use that to control filament growth and couple the growth to chemical reactions, signal transduction, or feedback mechanisms." Or even to adaptive behavior and self-learning abilities? "I think this offers a very nice toolbox to connect molecular interactions to functional behavior on a much large scale, for example in adaptive materials."

MICRO REACTORS

Droplets also play a central role in Spruijt's research. But here they function as a minimal representation of cells. "My main source of inspiration is the living cell itself. To me, it is the most fascinating and complex functional molecular system that you can think of. We try to design and build an extremely simple version of a cell, which turns out to be a complex challenge." Spruijt employs coacervates; self-assembling membraneless droplets that exhibit dynamic behavior. "A major advantage of coacervates compared to commonly used vesicles is that only coacervates can (self-)assemble spontaneously, and they can dissolve and reassemble again." One of the applications of coacervates is to use them as compartments to accommodate specific chemical reactions or to concentrate (parts of) chemical networks to enhance their efficiency. "We want to be able to control the formation of these compartments in space and time. They can be viewed as microreactors that offer different conditions compared to the bulk solutions, where reagents or catalysts preferentially accumulate, and where specific reactions are stimulated. Just as it happens in the organelles of living cells."

Korevaar and Spruijt definitely see links between their research and the topics studied within ICMS. "We are all interested in complex systems and the nice thing about ICMS is that it attracts people from a wide variety of research fields", says Korevaar. "I spent ten years in Eindhoven and I still have fond memories of my time working within ICMS." But complexity in itself is not the goal, they both agree. Spruijt: "In the end, it is about generating functionality. It is very hard to predict whether your complex system will be of use. But when you work in an environment where many researchers share your interest, chances increase that someone recognizes a possibility."



MATERIALS FOR REGENERATIVE MEDICINE

Believe in your cells

THE RESEARCH OF MICHAEL RAGHUNATH ON MACROMOLECULAR CROWDING

Michael Raghunath

In January this year, Michael Raghunath from Zurich University of Applied Sciences visited ICMS to give a lecture on 'macromolecular crowding' and how to recreate the complex extracellular environment in the laboratory. It is part of the 'Great Debate on Extracellular Matrix', a series of lectures organized by ICMS to encourage young scientists and world-renowned experts to connect and explore new strategies to drive research forward. This initiative was kicked off in 2018 with a lecture of Tony Weiss from the University of Sydney.

Since the first decade of the 20th century and the very first techniques of cell culture, scientists have been struggling to recreate the natural environment of human cells in the laboratory. In our body, cells are surrounded by a complex microenvironment, the extracellular matrix, which is richly decorated with growth factors, vesicles, and proteins, to name a few. "When abruptly removed from their natural microenvironment and cultured in the laboratory", explains Raghunath, "cells have to scrape a living while trying to adhere on stiff plastic covered with adsorbed proteins from animal-based serum, the ultimate voodoo component for cell survival". Also, the amount of salt water used for cell culture is such that cells are literally 'drowned in seawater'. Last but not least, cells are stressed by too much oxygen and kept constantly in darkness. None of these environmental settings resembles the scenario occurring in nature.

ARTIFICIAL MICROENVIRONMENTS FOR CELLS: ARE WE DOING IT ALL WRONG?

Scientists have been rushing to the aid of struggling cells in culture, propping them up with scaffolding structures which differ in fabrication processes and

geometries. Coated, extruded, fusion-deposition printed, nano-textured, electrospun, laser-sculpted, plotted, spotted, and nanofiber-reinforced materials - the list is long. Ironically, in all the excitement of searching for the holy grail of biomaterials, the spontaneous ability of cells to recreate their own microenvironment has been long overlooked. "It became", says Raghunath, "the forgotten 'Sauron's ring' of this research field".

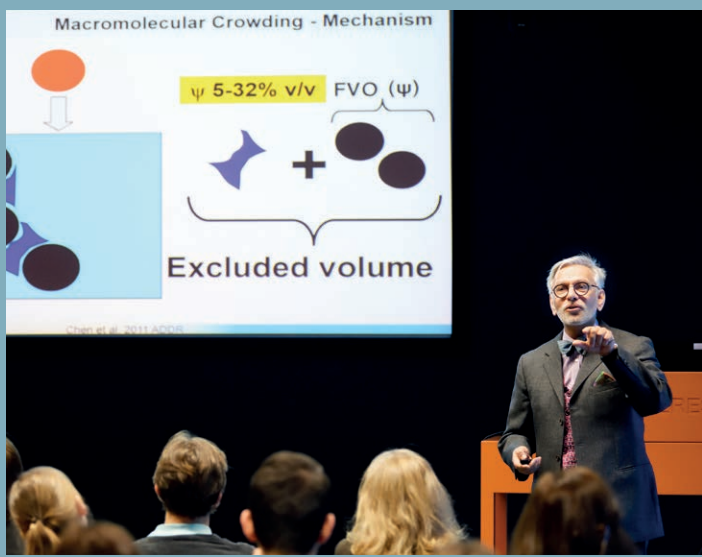
When it comes to recreating the cellular microenvironment in vitro, the question thus arises: are we doing it all wrong? Raghunath: "As humble practitioners of matrix biology, we often witnessed concerted attempts to supersede nature and its 700 million years of most rigorously materials testing". Raghunath has been trying to revert the trend, bringing back into cell culture the physiological interior and exterior of cells. It might sound complicated, yet it all comes down to one magic ingredient: Macromolecules. Raghunath: "If we look at the interior of a cell, we see crowdedness. It is crammed with macromolecules. Also, in multicellular organisms cells are surrounded by macromolecules which are immobilized within the so-called extracellular matrix. Both these observations tell us that these macromolecules originate from cells." So, if cells already have all it takes to recreate their own natural microenvironment, why not let them do the job?

MACROMOLECULAR CROWDING: HOW TO?

Raghunath's research focuses on empowering cells to make their own microenvironments because they can actually do so - as nature teaches us. Specifically, the macromolecular crowding is recreated by using powders of sugar-derived polymers, which are dissolved in the culture medium, filtered and mashed together. At the end of this process, the resulting culture medium contains a specific concentration of macromolecules which start occupying their own space and create, indeed, crowdedness.

While it holds true that we should all "believe more in our cells", it still takes nine months to make a human. And who would like to continuously culture cells for nine months? "With macromolecular crowding", explains Raghunath, "we offer a tool to speed up the formation of extracellular matrix", which is a necessary step towards the formation of human tissue in vitro. "For example", he continues, "we could create a better microenvironment for cells on top of synthetic materials, especially on top of those materials that are notoriously challenging in terms of cellular adhesion. We could do so in a sort of beehive fashion, with bees - our cells - depositing the wax - the extracellular matrix - on top of a man-made artificial structure." Along this line, Raghunath is already thinking of possible collaborations within ICMS and Carlijn Bouten of the group of Soft Tissue Engineering and Mechanobiology of the Biomedical Engineering Department.

"SO, IF CELLS ALREADY HAVE ALL IT TAKES TO RECREATE THEIR OWN NATURAL MICROENVIRONMENT, WHY NOT LET THEM DO THE JOB?"



Michael Raghunath is a physician scientist heading the Center for Cell Biology and Tissue Engineering at the Institute for Chemistry and Biotechnology, Zurich University of Applied Sciences. Raghunath is also director of the Competence Center TEDD (Tissue Engineering for Drug Development). He is an internationally distinguished scientist in the field of matrix biology and skin biology, with more than 30 years of experience in basic and translational research. His research on macromolecular crowding in cell biology led to the development of a novel field in tissue engineering, to build cell-specific and lineage-directing microenvironments.

CHEMICAL BIOLOGY

Molecular glues for new drug development

COMBATTING THE COMPLEX MOLECULAR INTERACTION NETWORK OF DISEASE PROTEINS

Eline Sijbesma (left) and Madita Wolter

Eline Sijbesma and Madita Wolter, PhD students with Christian Ottmann and Luc Brunsveld in the Chemical Biology group at the TU/e Department of Biomedical Engineering, are at the forefront of a promising novel approach in early drug development. By exploring small molecules that can stabilize protein-protein interactions (PPIs), they hope to find more subtle yet more effective drugs to target a range of diseases. A first result related to a protein involved in breast cancer was recently featured on the cover of the Journal of the American Chemical Society.

Next to cancer, the list of disorders that can benefit from the new approach is long: neurodegenerative diseases such as Alzheimer's and Parkinson's, pulmonary diseases, inflammation, metabolic diseases such as diabetes. Not surprisingly so, since the focus is on PPIs which are crucial to all cellular processes. What is surprising, though, is that the approach differs in a fundamental way from established drug development.

Put bluntly, in drug development the focus since many decades has been on molecules that bind to the active site of enzymes or receptor proteins. Many drugs combat disease by replacing or competing with these natural ligands, thus changing signal cascades in the cell or altering biocatalytic molecular conversions. Although this has led to successful therapies, simply competing with a natural ligand turns out to be a somewhat rude procedure that often evokes troublesome side effects. What's more, evolving pathological cells often develop workarounds, slightly changing the protein and thus frustrating the binding of the drug molecule. As a result, the drug becomes less effective over time.

The new approach now advocated by Sijbesma, Wolter and many others was developed in the last two decades and focuses not on protein-ligand interaction but on PPIs. This is because in many cellular processes - thus including >>

pathological processes - proteins, in addition to ligands, bind to other proteins to alter their function. Within this new approach of targeting PPIs, Sijbesma and Wolter propose an even newer route for drug development.

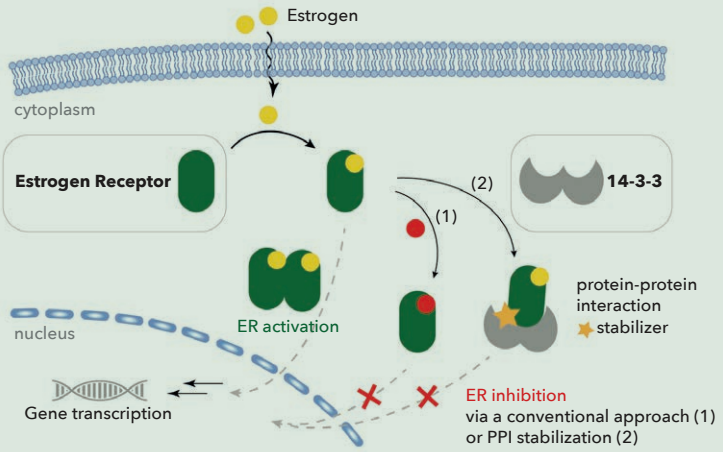
SHIFTING EQUILIBRIA

"Most researchers in this field try to disrupt PPIs", says Sijbesma. "This, in fact, is relatively straightforward. If you know how the proteins bind to each other, you can use that information to find a molecule that binds to one of the two proteins at exactly that same spot. Often such a molecule is identified by means of massive screening procedures. When it binds strongly at the interaction site of the two proteins, it inhibits the interaction. As a result, it disturbs the pathological pathways involving the targeted proteins." The alternative advocated by Sijbesma and Wolter involves stabilizing rather than disrupting PPIs. "In fact, nature itself makes extensive use of stabilization", says Wolter. "It has the effect of shifting the chemical equilibria in the cell". In many diseases, proteins are too active, or just not active enough. Stabilizing PPIs, thus enhancing or decreasing activity, is a subtle way of interfering with the cellular pathways. "We expect that this will open up new avenues for therapy. What's more, since PPI stabilizing drug molecules are designed to only bind a specific protein complex and not the individual proteins, they probably will have less off-target side effects."

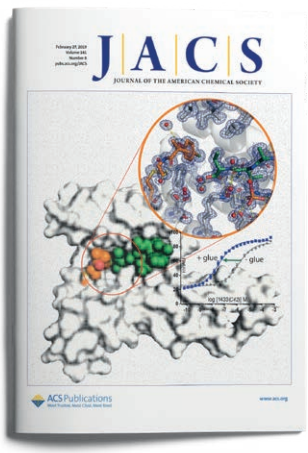
DRUG THE UNDRUGGABLE

As far as developing ideas, so far so good. But when it comes to bringing these to reality, it surely is a matter of 'easier said than done'. Sijbesma: "Finding molecules that stabilize PPIs is far less obvious than finding molecules that disrupt them. We want to build molecular bridges, find molecular glues that can tie two proteins together. That implies we first have to look for binding sites adjacent to the site of the PPI, and subsequently develop molecules that are capable of making interactions to not one but two proteins." All this entails detailed structural studies of the PPI using X-ray crystallography and NMR and the development of intelligent strategies for molecular discovery. Wolter: "The research challenge of focusing on these targets that are hitherto seen as 'undruggable' is huge. That's the academic challenge of our work: can we do this, at all?"

The recent paper in the Journal of the American Chemical Society provides a first, tentative, positive answer. It concerns the interaction between the so-called 14-3-3 'hub' protein and the Estrogen Receptor alpha (ERα). Certain types of breast cancer display an over-active Estrogen Receptor, which can be targeted with drugs blocking its active site. However, current drugs doing just that have a tendency to result in resistance over time. As an alternative, Sijbesma and co-workers investigated stabilizing the interaction of the receptor with the 14-3-3 hub protein (see image).



The Estrogen Receptor becomes activated by binding of its natural hormone ligand (Estrogen). It dimerizes and translocates to the nucleus, where it turns on gene expression. This activity can be inhibited by a drug molecule that blocks the Estrogen-binding site (1). The problem is that this can lead to mutations of the protein, which causes therapy resistance. An alternative approach is to regulate Estrogen Receptor activity via its PPI with 14-3-3 (2). A small molecule stabilizer could further enhance this regulatory function of the 14-3-3 protein.



Front cover of the JACS issue highlighting Eline Sijbesma's research on a molecular glue for the stabilization of the interaction between the 14-3-3 adaptor protein and a phosphopeptide derived from the C-terminus of an Estrogen Receptor.

“WE ENVISIONED TO APPLY A COVALENT FRAGMENT-BASED STRATEGY KNOWN AS ‘DISULFIDE TRAPPING’.”

40-FOLD INCREASE

Sijbesma first explored the concept during her master’s study in Biomedical Engineering at TU/e, when she was a research intern at the group of Michelle Arkin, Professor of Pharmaceutical Chemistry at the University of California at San Francisco. The collaboration continued into her current PhD research, also involving the pharmaceutical company Novartis in a purely academic partnership - the company does not fund the research.

The inspiration for developing the molecular glues reported in the JACS paper was the natural molecule Fusicoccin-A, a known stabilizer of the 14-3-3/ERα interaction. “Since it is not selective and structurally complex, we wanted to know if we can find new, smaller and more effective stabilizing molecules that bind at the same site”, explains Sijbesma. “For this, we envisioned to apply a covalent fragment-based strategy known as ‘disulfide trapping’. This has been used before to find very selective modulators of oncogenic proteins. We were the first to show that this strategy is indeed also very suitable for finding stabilizers of PPI’s!” The most effective of these molecular glues led to a 40-fold stabilization of the 14-3-3/ERα interaction. “The next step in this research would be to elaborate the hits into a series of non-covalent binders that are able to modulate ER biology.”

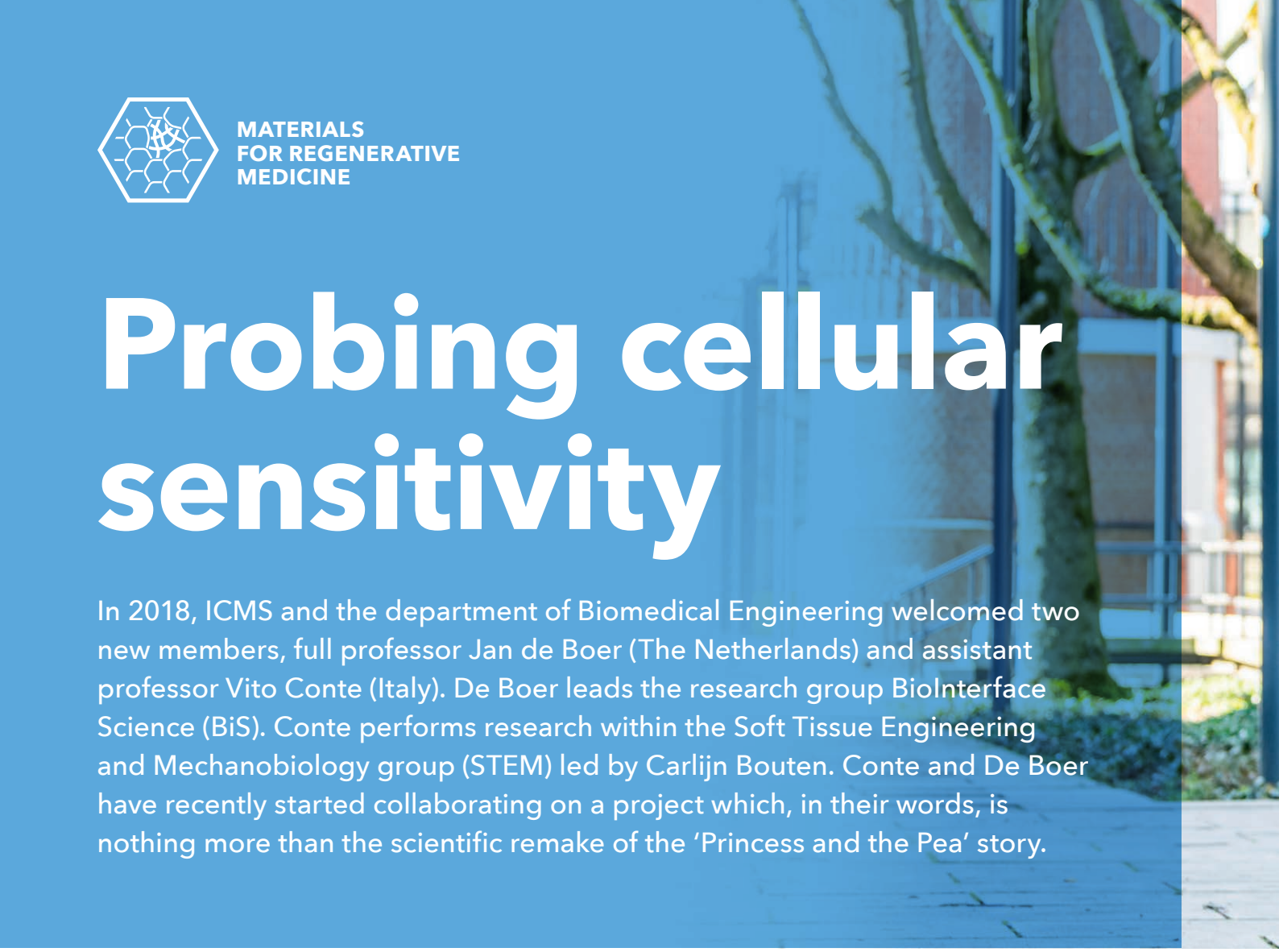
ON THE RIGHT TRACK

To Wolter, these first explorations of the concept, establishing the stabilization of the 14-3-3/ERα interaction, provides a validation of the approach. “It proves we are on the right track.” In her research she also focuses on the 14-3-3 adapter protein since it acts as a ‘hub’, interacting with several hundred partner proteins in human cells. “These proteins are involved in a huge variety of diseases, from small infections to severe metabolic diseases or cancer. So it makes a lot of sense to explore the interface of 14-3-3 proteins and their interaction partners.”

Wolter’s work is part of the European Innovative Training Network TASPPI (Targeted Stabilization of PPIs) supported by the EU H2020 Marie Curie Actions. The project involves 6 European universities and 5 companies. She is one of 13 TASPPI PhD students working to identify and optimize small-molecule 14-3-3 PPI stabilizers as novel tools for basic research and starting points for drug development. Wolter pursues just like Sijbesma the concept of fragment based drug discovery where she identifies the binding potential of small molecule ‘fragments’ of up to 300 dalton. The idea is to identify fragments that are capable of binding to a protein of the ‘14-3-3 protein family’. These then provide the leads for the development of drug molecules that can act as molecular glues. “We subsequently perform biophysical and structural analysis, and aim for compounds which we can test in cell culture to explore their potential as drugs.”

PARADIGM SHIFT

Sijbesma and Wolter are convinced that the future will learn this is a viable new approach for early-stage discovery of drugs that are more selective, more effective and less disturbing. Sijbesma: “In my view, the stabilization of PPIs has the potential to lead to a paradigm shift in our thinking about druggability. Our research provides the basis for this, in that we show that indeed molecules can be found that can act as stabilizers.” Although she predicts a huge expansion of targetable proteins in the coming years, she expects that establishing clinical relevance will require long-term efforts. Wolter: “The real challenge will be to convince pharmaceutical companies to adopt this approach. It can be hard to persuade them to change the way they have been thinking for the last 50 years.”



MATERIALS FOR REGENERATIVE MEDICINE

Probing cellular sensitivity

In 2018, ICMS and the department of Biomedical Engineering welcomed two new members, full professor Jan de Boer (The Netherlands) and assistant professor Vito Conte (Italy). De Boer leads the research group BioInterface Science (BiS). Conte performs research within the Soft Tissue Engineering and Mechanobiology group (STEM) led by Carlijn Bouten. Conte and De Boer have recently started collaborating on a project which, in their words, is nothing more than the scientific remake of the 'Princess and the Pea' story.

When answering questions about his new life at TU/e, Vito Conte cannot help but mention his new beard. "Do you like it? It's curly, with a salt and pepper touch". Yet, more has changed as a result of Conte's relocation to The Netherlands. Theoretical physicist by education, and with a PhD in biomechanical engineering, Conte started his academic career at King's College London. He then moved to the Institute for Bioengineering of Catalonia (IBEC), where he focused on the mechanics of epithelial morphogenesis during development and disease. He currently is junior group leader of the Mechanics of Development and Disease group at this institute.

Recently, Conte redirected his scientific interests towards synthetic morphogenesis (Latin for 'beginning of the shape'). This is also the main reason behind his new appointment at TU/e, he explains. Within the STEM group, Conte investigates how to exploit cell and tissue mechanics to control the in vitro morphing of tissues for regenerative and clinical purposes. And he keeps looking further, at new collaborations and potential new research directions.

COLLABORATIONS START WITH OPEN DOORS

"I have an open door policy", says De Boer, "and Vito stops by my office almost on a daily basis, always with a new idea in mind." And considered from the complementarity of their expertise, Conte's strive for collaboration is more than justified. "Our group", explains De Boer, "is devoted to understanding and applying basic cell biological principles at biointerfaces, with a particular interest for regenerative medicine". The BiS group does so by embracing a 'holistic approach' to both discovery and application, which combines high throughput technologies, computational modeling, and experimental cell biology. "Our goal", says De Boer, "is to streamline the wealth of biological knowledge to real clinical applications". A mission that goes hand in hand with establishing the Center for Therapeutic Biomaterials, a joint effort which bears the signature of various researchers from different fields within ICMS.

Jan de Boer (left) and Vito Conte

"THE COLLABORATIVE PROJECT OF DE BOER AND CONTE REPRESENTS A NICE EXAMPLE OF HOW TO UNCOUPLE CHEMISTRY FROM MECHANOBIOLOGY."

THE PRINCESS AND THE PEA

De Boer and Conte have recently started a collaborative project on the effect of topography and stiffness on cellular behaviour. De Boer: "We both supervise a master's student, Marc Mazur. We like to define this project as our 'Princess and the Pea' story'. Marc is using our topographies to cast hydrogels on top." The result is a structure of several adjacent topographies superposed with hydrogel layers of different thickness. As for the protagonist of the 'Princess and the Pea' story, kept awake in a stormy night by a pea hidden under layers and layers of thick mattresses, human cells are deposited on top of the hydrogels and tested for their sensitivity to the underlying topographic cues.

UNCOUPLING OF MATERIAL PROPERTIES

In materials science, the uncoupling of material properties remains a challenge. Nowadays, researchers often vary material stiffness by playing with chemistry. "For example", says De Boer, "softer and stiffer hydrogels can be created by varying the rate of crosslinking. Yet, when doing so, protein bindings will also change, and as a result affect cellular response." In this respect, the collaborative project of De Boer and Conte represents a nice example of how to uncouple chemistry from mechanobiology, by studying cellular behavior in response to stiffness, while keeping the material properties of the hydrogels the same.

News, awards & grants

Chemist Jan van Hest

CHOSEN AS A MEMBER OF ROYAL DUTCH ACADEMY OF SCIENCES

Jan van Hest, professor of bio-organic chemistry at the TU/e, joins the Royal Dutch Academy of Sciences (KNAW).

"In all his work, Van Hest combines innovative synthetic strategies with a clear vision of possible biomedical applications," the KNAW said.
Jan van Hest, professor of bio-organic chemistry at the TU/e, joins the Royal Dutch Academy of Sciences (KNAW). The KNAW is the most important Dutch society for top scientists. Van Hest, who has been working at TU/e since 2017 and is head of the Institute for Complex Molecular Systems in Eindhoven, is involved in the development of artificial cells and nanomedicines.

ERC Consolidator Grant to professor Willem Mulder

FOR HIS RESEARCH ON CANCER IMMUNOTHERAPY

Professor Willem Mulder was awarded a Consolidator Grant of €2.75 million by the European Research Council (ERC) for his research on cancer immunotherapy, an innovative cancer treatment based on empowering the human body's natural defenses. The awarded proposal focuses on the application of nanotechnology to current immunotherapy treatments, which show limited therapeutic power and serious adverse effects. Mulder will use the funds to solidify his recently established Precision Medicine group, at the TU/e Biomedical Engineering Department.

The European Research Council (ERC) announced the recipients of the Consolidator Grant Call of 2018 in November 2018. This year, 19 of the 291 awarded grants went to Dutch (12) and international (7) researchers working in the Netherlands. Professor Mulder: "I feel honored and very happy. This grant will be used to establish a research group at TU/e that focuses on the use of nanotechnology to visualize and regulate the immune system."

ICMS Fellowship

FOR NICHOLAS TITO

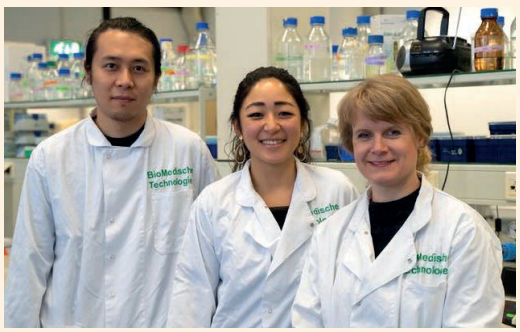
It is with great pleasure that we announce the appointment of dr. Nicholas Tito as an ICMS Fellow. Nick is inspired by entropy, and how life has evolved to exploit entropy for robustness in biological materials. He takes an active part in bringing both early-stage and experienced scientists together at conferences. In 2019, he will co-chair two Gordon Research Seminars, one in "Complex Active & Adaptive Material Systems", and another in "Liquid Crystals". Scientific outreach is also a part of Nick's career. He creates interactive and visual computer software that allows scientists and non-scientists alike to explore modelling at the microscale. His recent "Stochasm" app (https://stochasm-app.com) allows the user to interactively simulate complex emergent phenomena from simple (or complex) local interaction rules, acting as a platform for creating digital art from science in the process. Together with ICMS Fellows Danqing Liu and Ghislaine Vantomme, Nick will contribute to a dynamic and creative multidisciplinary atmosphere in the field of Complex Molecular Sciences.

Eindhoven's own 'Semi-human Vase'

CONNECTS ART AND SCIENCE

The researchers made three different shapes of the vase. A special collaboration between designer Hongjie Yang and scientists Patricia Dankers and Dan Jing Wu from Eindhoven University of Technology has led to a series of unique, imaginative objet d'art: the 'semi-human vase'; a 3D-printed mold in the shape of three different vases cultured with patches of human cells stained in blue. This project was exhibited from 20th February till 15th April 2019 in the world-famous museum Centre Georges Pompidou in Paris. The project provoked the notion among visitors that the border between human and object is fading.


Half-menselijke vaasjes



(from left to right) Hongjie Yang, Dan Jing Wu and Patricia Dankers

COVER OF NATURE REVIEWS CHEMISTRY FOR

Albertazzi and the ICMS Animation Studio

Lorenzo Albertazzi, Associate Professor in the Molecular Biosensing for Medical Diagnostics group and member of the ICMS, has just published a review in the prestigious Nature Reviews Chemistry. The review entitled 'Super resolution microscopy as a powerful tool to study complex synthetic materials' includes an illustration from the ICMS Animation Studio, which was selected to be on the cover of the February Issue of the Journal.

Next-generation materials face diverging drivers

CONNECTING STRUCTURE WITH PROPERTIES REMAINS THE KEY CHALLENGE IN MATERIALS SCIENCE

The 2019 ICMS Outreach Symposium focused in part on 'Next-Generation Materials'. We talked about the future of the materials sciences field with keynote speakers Elisabeth Engel, George Malliaras and Paul Blom, and ICMS director Jan van Hest. What are the needs that drive the field, what are the envisioned applications of those next-generation materials, and how does that translate to research we need to do today?

(from left to right)
George Malliaras, Jan van Hest, Paul Blom, Elisabeth Engel and Esther Thole

"TO MOVE TOWARDS MULTIFUNCTIONALITY, WE NEED TO TACKLE THE LACK OF DYNAMIC BEHAVIOR."

Talking about the promise of next-generation materials implies that the current materials are not delivering what we hope, need or expect. What is the major problem of the current materials and how are the next-generation materials going to offer solutions? First topic on the list: biomedical materials. Elisabeth Engel, group leader at the Institute for Bioengineering of Catalonia (IBEC) kicks off. "Let me first stress that there is still a lot we don't understand about the current materials, in particular how they interact with the cells in our body. But we do know that our current materials are limited. Take for example load bearing materials. We now use titanium which is very strong but offers no additional effect. We need something that not only matches the mechanical properties of bone but is also bioactive, biofriendly, and able to stimulate the growth of new tissue."

According to Engel, the main limitation of the current materials is that they only offer one specific property or function. "We have strong materials that adequately perform that one function, but they cannot do anything else. They are not multifunctional." To move towards multifunctionality, we need to tackle the lack of dynamic behavior, says Jan van Hest, scientific director of ICMS and professor of Bio-organic Chemistry at Eindhoven University of Technology. "The current materials are static, their properties remain unchanged. However, for tissue engineering and tissue remodeling, you would like the properties to change over time and adapt to the new requirements. Not only the mechanical properties but also the functionalities of the signaling elements that are connected to the regenerating tissue. Such materials could be considered next-generation, but I agree with Elisabeth that in order to take that step we need to better understand why our current materials are not as ideal as they should be."

EXPLORE NEW ROADS

All these drawbacks raise the question if we should stay focused on the materials that we have and try to improve them. Is that worthwhile or do we need a different conceptual approach to get to genuinely new, innovative materials? Engel feels that this is too much of a generalization. "Some materials we now have work fine for the current applications", she says. But new needs and requirements are just around the corner. Engel: "There is, for example, the increasing problem of antibiotic resistance, which drives the need for new antimicrobial materials." And there are new roads in regenerative medicine that we want to explore, says Van Hest. "When you think about organ regeneration material development becomes a lot more complex. Different cell types need to come together, the matrix material will need an intricate design, so what the best type of material will be really is an open question. Maybe there is not one material that offers the solution; we might need a combination of materials and perhaps a combination of approaches. >>

For some applications, we may even need to look beyond just the materials and incorporate multiple functionalities in a device. I think the difference between material and device is becoming less distinct."

The latter notion is particularly relevant to the work of George Malliaras, Prince Philip Professor of Technology at the University of Cambridge. His research focuses on bioelectronics; materials that can interface with neurons. The need for new materials in this field is very clear, he says. "The current technologies rely on inorganic materials such as metals and silicon, which are mechanically hard and unable to conduct ions. This means that we are dealing with a mismatch in both mechanical and electrical properties. Addressing this mismatch requires materials that are soft, deformable and stretchable, and can make contact with the body without creating a mechanical load. At the same time, these materials should be able to conduct the signals that are used by biology, meaning small metal ions and more complex biomolecules." When asked what the major obstacles are that he encounters, Malliaras' answer is - surprisingly - not about technical intricacies. "The key issue in the field is that there have to be compelling advantages to move to in vivo studies and get a new material into the clinic", he says. "But once that step is taken, you have to stick to that particular material. There is no room for adaptations." This is difficult for scientists as they prefer to work on multiple materials, tune their properties and study the results. Malliaras: "When you embark on the journey toward clinical translation, you have to stay focused on that one material you started with, which is probably not the best and certainly will not be the best by the time you reach the end of the track. You know that new, better, more promising materials will have been developed by then, but you cannot change along the way. As a result, many materials that offer a much better performance will never make it to the clinic."

LOWER THE BARRIER

This sounds incredibly frustrating, but Malliaras is very down-to-earth about it because there is a logical explanation. "You have to pool resources to bring a material to maturity, it is simply not feasible to do that for every material. The research will continue and you will find better materials, but at a certain point you have to choose one that you stick with." The fact that it may not be the best is acceptable as long as it turns out to be good enough. That will pave the way for other materials, as Malliaras explains. "If one organic bioelectronics material makes it to the clinic, it will lower the barrier for others. You need a successful application to keep a field afloat. It goes the other way around as well because it would be a disaster for the field if we don't manage to deliver commercial organic bioelectronics applications." He compares this to the impact of OLEDs on the overall field of organic electronics. "The commercial success of OLEDs has carried the whole field and allowed it to be what it is today. Without those applications, the field would be much smaller."

Paul Blom, professor of Molecular Electronics and director of the Max Planck Institute for Polymer Research (MPIP), recognizes the diverging drivers sketched by Malliaras. "We scientists like to come up with something completely new, something that was not there before and that can do new things", Blom says. "On the other hand, new materials can emerge because they offer an immediate advantage to existing ones, such as lower costs or easier production. You don't necessarily need a completely new material to offer a solution. For example, if your material allows for much cheaper production of solar cells, it will be very attractive for industry even when the material does not offer a better or even a similar performance. The key driver is not always the need for a truly innovative material. Costs and ease of production are very important for industry."

But when practical needs and requirements are in the lead, doesn't that pose a risk to research? Don't we need fundamental breakthroughs anymore? Blom: "Well, you cannot plan a fundamental breakthrough, it often happens by coincidence. And the more people work on something, the higher the chances that a breakthrough is found. That requires funding and to ensure that you need objectives that industry and funding agencies are willing to pay for. If people work for ten years on a topic, and nothing remotely useful comes up, then investments will dry up. Industry will lose interest and it will become difficult to get proposals granted and so forth. The field will die, and all the attention will shift to the next hype."

"YOU CANNOT PLAN A FUNDAMENTAL BREAKTHROUGH, IT OFTEN HAPPENS BY COINCIDENCE."

"THE UNDERLYING QUESTION OF MATERIAL SCIENCES IS HOW TO DERIVE PROPERTIES FROM STRUCTURE."

Van Hest emphasizes that developing new materials is not the only road toward innovation. "I think there is still a lot to gain by integrating and combining existing materials and concepts. That way you can create materials with completely new properties that offer new possibilities for applications. This is something we stimulate within ICMS. Some researchers have questions or ideas but don't know what materials are available, whereas other researchers have materials but don't know where they could be useful for." The surging interest in biohybrid materials is a case in point, says Blom. "There is a lot of activity in combining synthetic and biological materials to make functional devices, and I believe in it. There are so many concepts that chemists and physicists know about but don't know how to use it in biology, and there are many biologists who have ideas but don't know what physics and chemistry can offer. We can go a long way by bringing those views together. You need someone who can make something, someone who understands it, and someone who knows where and how to use it. You really need all three- if one is missing, you will not get there."

COMPLEX MODELS

It is now time to also include researchers from mathematics and informatics to the endeavor, says Engel. "ICMS is doing that already and it allows building much more complex models to study phenomena on the interface between cells and materials. Instead of trying to understand the effect of one single stimulus at a time, we can now simultaneously explore several stimuli in various target cells without the time consuming culturing of all these cells. Modelling will save a lot of time and money and helps you to better target the interface you're interested in." She feels that it will take some time for these new fields to get embedded in the material sciences. "Chemists and biologists have been talking to each other for quite some time already. Now that mathematicians are entering, we need time to get to know one another and understand each other's language. Then we can together find a way to target a common objective. It takes time to get from multidisciplinary research to truly interdisciplinary research."

Such a new approach is also needed in view of the overall change in the position of material sciences in relation to pressing societal and economic issues. Materials have become a focal point from many different perspectives, such as circularity and sustainability. "It requires a new way of thinking", says Van Hest. "There are new users, new applications, new functionalities, and sustainability is a key driver." A clear example is the focus on degradation, according to Blom. "Now you see many groups studying degradation products and processes, but in the past that was considered a problem for industry. Academics were not supposed to work on that type of problems. However, industrial labs have disappeared, so when academics don't step in, new materials will never reach an application. We now need to deliver materials and technologies that are much more mature than what was sufficient in the past."

HOW TO DERIVE PROPERTIES FROM STRUCTURE

Does all this imply that we need a revolution in material sciences? And if so, what are then the most pressing questions we need to address? Such questions are too broad for Malliaras. "This can only be answered in the context of specific applications. You need a well-defined problem first, and then that will allow you to translate requirements into material parameters that can guide optimization. Only when you decide on the application can you extract the properties you need." But can we still talk about materials sciences as a field, or is it becoming so application-driven that there are no common denominators anymore? Are there no generic problems that material scientists face, regardless of the specific topic they work on? Malliaras: "Material sciences is an extremely broad field. Materials that are applied in a gas turbine are completely different from those that will be used in the body. Yet, the underlying question of material sciences is how to derive properties from structure, and that applies to both these applications." Connecting structure with properties is the basic denominator, says Van Hest. "We now need to study that relationship in increasingly complex environments, which means that we need to understand more parameters and understand which parameters we need to measure. But in the end it still boils down to the structure-properties connection. We need to understand how to move forward, both conceptually and empirically, towards better materials."

GRIP ON COMPLEXITY

Decoding social contagion with the help of network data science

Huijuan Wang wants to discover the mechanisms behind the spread of user activities on interdependent social networks. At the ICMS Outreach Symposium on Monday March 11, she presented her ambition to model this ‘social contagion’ and provided a foundational understanding of its emergent effects.

Huijuan Wang was born in Harbin, China. She obtained both her MSc and her PhD on the robustness of networks in Electrical Engineering from Delft University of Technology, both with the distinction cum laude. She is now a tenured assistant professor with the Multimedia Computing Group at the same university, focusing on network data science. Together with Linda Douw of Amsterdam UMC she recently initiated the Dutch chapter of the Network Science Society (www.netsci.nl), which kicked off with a national symposium on May 7, 2019.

UNDERSTANDING THE SPREAD OF MISINFORMATION

The concept of social contagion refers to the explosion of online social networks, each of which supports the spread of information, opinion and behaviour. This can be accompanied by the spread of misinformation and even social riots. "If society wants to control such emergence of collective behaviour, or even just explain the phenomena", Huijuan says, "it's crucial to develop an understanding of the interacting patterns between networks."

'Decoding' the process of social contagion is quite a challenge. Huijuan wants to develop a methodology starting from models that have already been studied in dynamic networked systems such as the outbreak of epidemics or neural processing. Crucial to her approach is the use of online available open source data combined with machine learning and time series analysis in a stochastic data modelling approach. "There are all kinds of network metrics that describe diverse features in the data. We have to ask how they relate to each other and which ones can evaluate our social contagion model best. That is an integral part of my research, to establish metric correlation patterns. As it turns out, these often are network or data dependent."

For Huijuan the combination of network science with data science creates the new field of 'network data science'. It will push the boundary of network science by addressing the interaction between spreading processes that explains not only the average but also the diversity of user activities and thus the emergence of active users or networks. "The acquired knowledge will enable us to develop strategies to minimize unwanted effects or even develop technology to battle issues such as social segregation."

Theses

OCTOBER 2018 - APRIL 2019

Folding polymer chains: an interplay of supramolecular interactions
GIJS TER HUURNE
October 1, 2018
PhD advisors:
prof.dr. E.W. Meijer,
dr.ir. A.R.A. Palmans,
prof.dr.ir. I. K. Voets

Functional supramolecular polymers in water
SJORS WIJNANDS
October 8, 2018
PhD advisors:
prof.dr. E.W. Meijer,
prof.dr. M. Merkx,
dr.ir. A.R.A. Palmans

Propagating fractures in swelling ionized hydrogels: XFEM analysis
JINGQIAN DING
October 9, 2018
PhD advisors:
prof.dr.ir. D.M.J. Smeulders,
prof.dr.ir. J.M.R.J. Huyghe,
dr.ir. J.J.C. Remmers

Structure-property relationships in bimodal UHMW PE
SARAH LAFLEUR
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PhD advisors:
prof.dr. A.P.H.J. Schenning,
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dr. J.R. Severn

Mechanics of growth and remodeling in native and engineered cardiovascular tissues
PIM OOMEN
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Ultrafast electron microscopy and spectroscopy using microwave cavities
WOUTER VERHOEVEN
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dr.ir. P.H.A. Mutsaers

Nucleation and growth of magnetite in bioinspired environments
GIULIA MIRABELLO
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Light-induced oscillating topographies in liquid crystal coatings
MATTHEW HENDRIKX
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The journey of supramolecular polymers to biomaterials: from fundamental studies to applications
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Processing organic photovoltaic layers from and on water
FALLON COLBERTS
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Towards understanding of cartilage damage development around focal defects and implants
ASHLEY HEUIJERJANS
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ROLAND VAN VLIEMBERGEN
October 31, 2018
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Self-assembly modulation of π-conjugated architectures in water
JURGEN SCHILL
November 12, 2018
PhD advisors:
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prof.dr. A.P.H.J. Schenning

Supramolecular control over recognition of proteins and cells
SAM VAN DUN
November 19, 2018
PhD advisors:
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dr.rer.nat. C. Ottmann

Enabling motions with impacts in robotic and mechatronic systems
MARK RIJNEN
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ANTONETTA (GITTA) BUSKERMOLEN
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DARIO DI CARLO RASI
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HAO SU
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SERGIO SPAANS
March 13, 2019
PhD advisors:
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JOHANNA MELKE
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High performance scalable data center and computer network architectures based on distributed fast optical switches
FULONG YAN
April 11, 2019
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April 24, 2019
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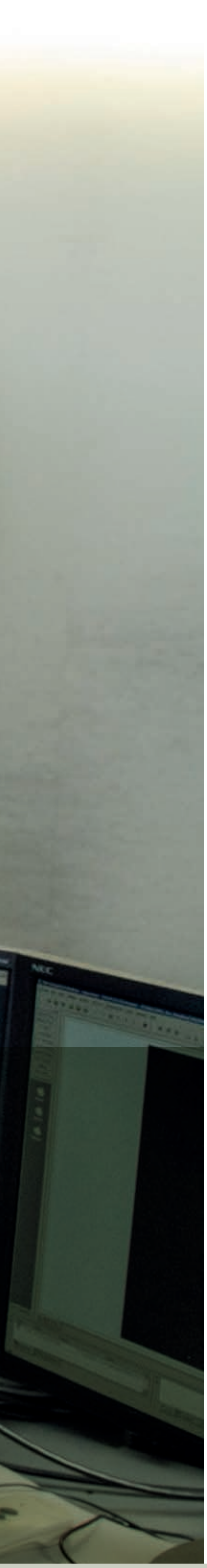
ADVANCED ANALYSIS
OF COMPLEX
MOLECULAR SYSTEMS

A new pathway to vesicle formation

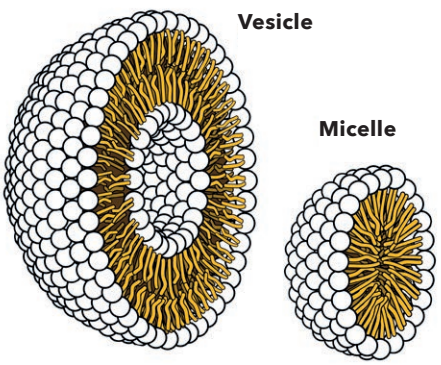
LIQUID-PHASE NANO-DROPLETS ARE AT THE ONSET OF SUPRAMOLECULAR ASSEMBLY



Alessandro Ianiro (left) and Hanglong Wu

In a recent paper in Nature Chemistry, Alessandro Ianiro and Hanglong Wu provide new fundamental insight in the self-assembly process of vesicles. Research of the two ICMS PhD students shows that nano-droplets, consisting of the molecular vesicle-building blocks in the liquid phase, are crucial to vesicle formation. Their remarkable finding results from a fruitful combination of advanced theoretical computation with real-time monitoring using liquid- phase transmission electron microscopy.

Over the years, vesicle formation from amphiphilic building blocks has been studied quite extensively by many researchers worldwide. Being able to control vesicle size and shape is of importance for a variety of applications, for instance in cosmetics and medicine. However, although a certain consensus exists regarding the mechanisms of vesicle formation, in many cases the results turn out to be irreproducible and inexplicable.



In short, two main pathways have been proposed that both start with the supramolecular assembly of small initial micelles. In one pathway these merge together to form flat disk-like structures, which in turn bend into vesicles. In the other pathway, the initial micelles attract further building blocks from solution. While growing, they rearrange into vesicles that gradually incorporate solvent in their core. The first pathway predominantly occurs at high copolymer concentrations, the second at low concentrations.

ELABORATE SIMULATION

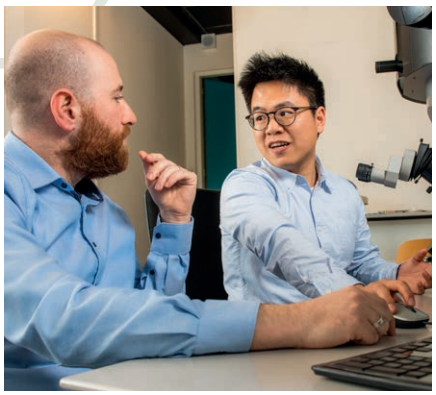
When performing a comprehensive analysis of the literature concerning vesicle formation, Alessandro Ianiro was surprised but also challenged by the lack of consistency. "I find it becomes really interesting if there is any irreproducibility. However, many researchers do not really ask themselves why their results are different from others even if they are using the same experimental set-up." The pathway now presented by Ianiro and Wu provides a sounder base for understanding experimental results. It does not merely replace the previously proposed pathways, but in fact unifies these in a new, richer frame. It started with Ianiro setting out to simulate vesicle formation based on a theoretical analysis that postulated the occurrence of liquid-liquid phase separation. He thus identified a crucial initial phase of nano-droplets consisting of the amphiphilic building blocks in the liquid phase. Further elaborating his model, he was able to incorporate both pathways already presented in literature. In fact, the new model perfectly predicts whether vesicle formation proceeds according to the one or the other pathway. >>

"WHEN WE PRESENT OUR IMAGES OF VESICLE FORMATION AT CONFERENCES, THE FIRST REACTION GENERALLY IS ONE OF DISBELIEF."

EXPERIMENTAL OBSERVATION

The question, of course, was whether Ianiro's theoretical model could be supported by experimental observation. This is where Hanglong Wu comes in, and his expertise in liquid-phase transmission electron microscopy (LP-TEM). By applying a dedicated 'imaging cell' he was able to confirm the occurrence of the nano-droplets and substantiate the mechanism of subsequent vesicle formation. "In many cases, the very first phase where the liquid phase droplets are formed occurs very fast and only for a short period of time", Wu says. "So it is not surprising that many researchers have missed its importance."

What's more, in a common Cryogenic Transmission Electron Microscopy (Cryo-TEM) experiment it usually takes a few minutes to fast freeze the sample before the first images can be obtained. By using the liquid phase cell in LP-TEM, which allows for

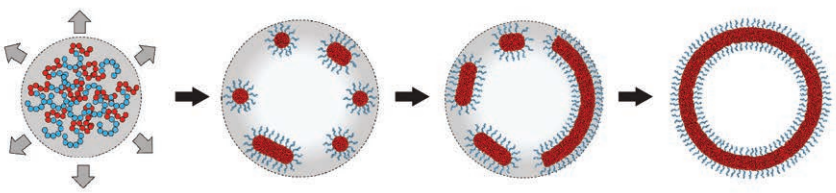


ultimate control over solvent mixing, 'live' imaging of vesicle formation can start at the first nanosecond. Even so, it took dozens of trials to yield a handful of meaningful experiments. "Often papers are written based on just one successful experiment", Wu says. "Since we were able to observe multiple vesicle-forming events and were able to relate these to a series of carefully designed control experiments, we are confident that we are looking at the truth and not at an artefact."

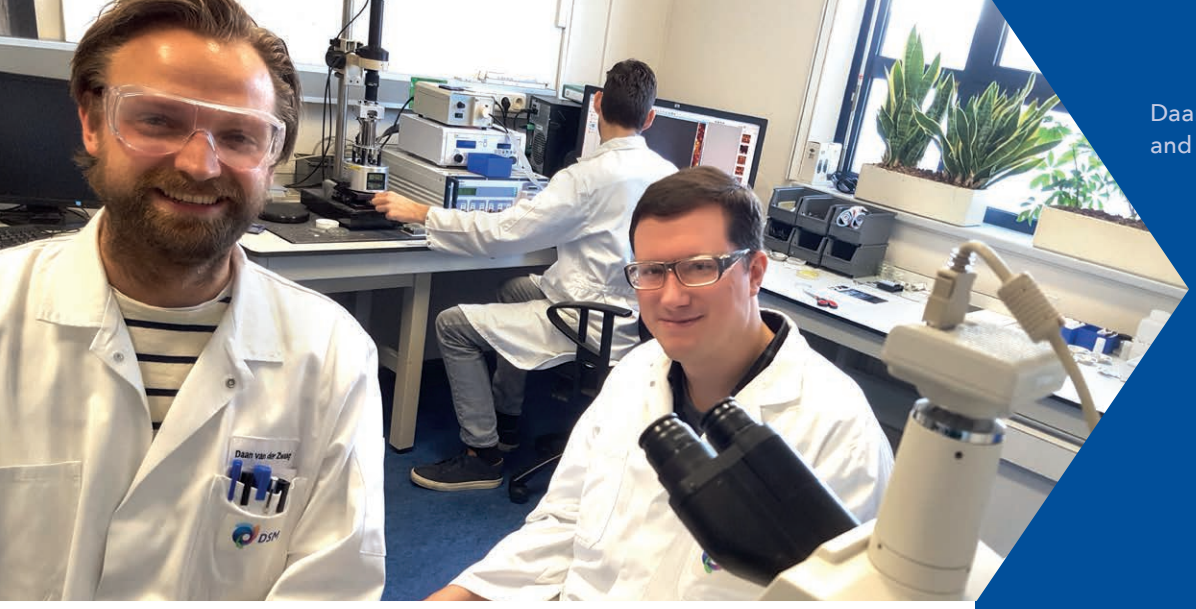
DISBELIEF AND AWE

The development of the LP-TEM for observation of soft matter has really pushed the boundaries of materials research, Wu argues. "When we present our images of vesicle formation at conferences, the first reaction generally is one of disbelief. People are in awe because of the high contrast and the degree of detail that we can observe." Of course, he adds, the theoretical computations performed by Ianiro were just as crucial. In fact, is the interplay between the two that really brought the breakthrough forward. "It is the fruitful feedback loop between theory and experiment that advances the science", says Ianiro. "Just developing theory shows nothing, so you need experiments. On the other hand, without an explanatory theory, performing experiments does not provide you with any insight."

The new model predicts crucial parameters of vesicle formation, such as the distribution of building blocks and membrane thickness, and provides an understanding of what controls the particle diameter. This in itself is crucial to the development of applications such as embedding drugs in vesicles for controlled drug delivery. Adding to this, the discovery of the precursor nano-droplets provides new opportunities for controlling the sizes, shapes, morphologies and internal structures of self-assembled aggregates. This will open new perspectives for the design of vesicular nanocontainers in technological applications.



Schematic of the self-assembly from nano-droplets (left), intermediated by micelles and cylinders and plates (middle), into a liposome (right). *Image: Alessandro Ianiro | Nature Chemistry.*



Daan van der Zwaag (left) and Patrick Stals

DSM Coating Resins

INDUSTRIAL CONSORTIUM

Royal DSM is a global purpose-led, science-based company in Nutrition, Health, and Sustainable Living. DSM's purpose is to create brighter lives for all. With its products and solutions, DSM addresses some of the world's biggest challenges whilst simultaneously creating economic, environmental and societal value for all its stakeholders; customers, employees, shareholders, and society-at-large. DSM delivers innovative solutions for human nutrition, animal nutrition, personal care and aroma, medical devices, green products and applications, and new mobility and connectivity.

facts

DSM WAS FOUNDED IN
1902

WITH APPROXIMATELY
23,000
EMPLOYEES

TOGETHER WITH ITS ASSOCIATED COMPANIES DELIVERS ANNUAL NET SALES OF ABOUT
€10 BILLION

ICMS collaborates closely with the DSM Business Group Resins & Functional Materials (DRF), which supplies innovative resins solutions for paints and coatings, fiber optic materials, and 3D printing. DRF is a global leader in the development and production of sustainable coating technologies by offering waterborne, UV, powder and plant-based coating resins with clear sustainability and performance advantages over solvent-borne coatings. In this way our company is addressing global macrotrends, for example in Nutrition & Health – by offering innovative coatings for food-packaging; in Climate & Energy – by offering coatings with low carbon footprint and volatile organic content; and in Resources & Circularity – by offering recycling solutions for multicomponent products (Niaga®) and plant-based resins (Decovery®).

For DSM, the collaboration with ICMS offers the opportunity to study the complex interactions that multi-component systems such as waterborne resins display. Having been trained at ICMS ourselves, this platform also enables us scientists to stay in touch with the latest techniques and developments in complexity science, and apply these to promote sustainable industrial innovation. Finally, we hope to contribute to guiding the excellent science performed at ICMS towards maximum societal impact.

Three fellows, three continents, three disciplines

(from left to right) Danqing Liu, Nick Tito and Ghislaine Vantomme

ICMS Highlights spoke to three ICMS fellows from three continents working in three disciplines (material science, chemistry, and physical/theoretical modelling). Together, they testify to the multidisciplinarity of ICMS and the multicultural environment of the institute. Meet Danqing Liu, Ghislaine Vantomme and Nicholas (Nick) Tito, and read more about their thoughts, their motivations and their dreams.

WHAT IS GOING ON IN YOUR RESEARCH TODAY?

Nick: My inspiration is entropy, and how life has evolved to exploit entropy for robustness in biological systems and materials. I love thinking about how to design new soft materials and nanostructures that capitalize on entropy, rather than oppose it, for achieving exciting functionality. For instance, natural structures like viruses, cells, or large proteins interact and chemically communicate with each other by means of many independent binding units, often called 'ligands' and 'receptors'. I'm interested in how such multivalent structures compete for binding onto the same target. Ultimately, we try to harness these principles via clever chemical design for our own goals, e.g. more selective drugs, biological sensors, or microscopic probes.

"MEMBERS OF THE ICMS ARE OPEN, CREATIVE, AND INSPIRED."

Danqing: With my broad background in various disciplines (electrical, mechanical and chemical engineering), I see myself as a materials scientist. In my work, I attempt to fill the field between molecular sciences, such as synthetic organic chemistry, and more macroscopic materials dimensions including morphology and shape control. I seek to transfer or even amplify the responsive effects of a single molecule to the macroscopic level of a device. This is realized by incorporating the functional molecules into suitable and cooperative host materials, such as liquid crystals.

Ghislaine: Self-assembly needs to be controlled in the laboratory to obtain >>

the functional structures needed to realize a precise function. Therefore, as an organic chemist, my aim is to understand, control and manipulate molecules into complex hierarchical architectures, so that we can offer strategies to build complexity into materials. This is, of course, a huge challenge, full of unknowns. My seatbelt is fastened and I am ready for an exciting journey!

TO WHAT EXTENT DOES YOUR FELLOWSHIP WITH THE ICMS HELP?

Nick: Members of the ICMS are open, creative, and inspired. It's the perfect place for theorist like myself to have a direct and vibrant connection with talented people that can make "invisible paper dreams" a reality. The Institute is really a "one-stop shop" for expertise in chemical synthesis, analytical measurement, imaging/characterization, biological study, and even animation.

Ghislaine: I see every day new examples that chemistry is not just a matter of molecules but also of people. That's exactly what I find in the ICMS: a friendly environment to exchange and to learn. At the beginning of my postdoc here, I worked with Danqing on liquid crystals networks. With her, I learned a lot on how to make devices and why it is so important to control the molecular organization of materials to reach new properties.

Danqing: I've started my collaboration with Ghislaine in 2016 with the aim to come to new functions in soft materials such as complex but pre-set triggered deformation relevant for soft robotics. Together with Nick, I gained more insight into the mechanism of our actuation processes by his molecular dynamic models. And recently I started a collaboration with researchers from the departments of Mechanical Engineering and Biomedical Technology, to expand further on the soft robotics focus area.

WHAT WILL YOUR FUTURE LOOK LIKE?

Nick: I really believe that the most exciting and important advances happen when scientists join forces, rather than work in isolation. I hope to one day have a university research group here in the Netherlands that reflects this outlook. I would love to foster early-stage researchers from all walks of life to pursue their scientific ambitions, and I'd like to make sure they have loads of opportunities to be scientifically mobile and social both within and beyond the Netherlands."

Danqing: I envisage to make materials that can feel, sense, behave and act as human skins, but with enhanced sensitivity and accuracy. And ultimately, the materials will have the capability to communicate with each other by exchanging mechanical and/or chemical information without human intervention.

Ghislaine: I hope we will continue doing what we enjoy the most: to learn from each other's, to explore new ideas and to guide students. We are very lucky to work in an institute where the first concern is to do great science.

"I REALLY BELIEVE THAT THE MOST EXCITING AND IMPORTANT ADVANCES HAPPEN WHEN SCIENTISTS JOIN FORCES."

Danqing Liu, ICMS fellow since 2015, was recently appointed assistant professor in the Stimuli-responsive Functional Materials & Devices group in the Department of Chemical Engineering and Chemistry.

Nicholas (Nick) Tito became an ICMS fellow in 2019. He is affiliated with the Theory of Polymers and Soft Matter Group in the Department of Applied Physics.

Ghislaine Vantomme, ICMS fellow since 2018, was recently appointed assistant professor in the Macro-organic Chemistry group in the Department of Chemical Engineering and Chemistry.

Key publications

SEPTEMBER 2018 - MARCH 2019

01. A THERMODYNAMIC MODEL FOR MULTIVALENCY IN 14-3-3 PROTEIN-PROTEIN INTERACTIONS
L.M. Stevers, P.J. de Vink, C. Ottmann, J. Huskens, L. Brunsveld
J. Am. Chem. Soc. 140, 14498–14510 (2018)

02. BILAYER-TERNARY POLYMER SOLAR CELLS FABRICATED USING SPONTANEOUS SPREADING ON WATER
F.J.M. Colberts, M.M. Wienk, R. Heuvel, W. Li, V.M. Le Corre, L.J.A. Koster, R.A.J. Janssen
Adv. Energy Mater. 8, 1802197 (2018)

03. DNA-BASED NANODEVICES CONTROLLED BY PURELY ENTROPIC LINKER DOMAINS
D. Mariottini, A. Idili, M.A.D. Nijenhuis, T.F.A. de Greef, F. Ricci
J. Am. Chem. Soc. 140, 14725–14734 (2018)

04. EFFECT OF TRIPLET CONFINEMENT ON TRIPLET-TRIPLET ANNIHILATION IN ORGANIC PHOSPHORESCENT HOST-GUEST SYSTEMS
A. Ligthart, X. de Vries, L. Zhang, M.C.W.M. Pols, P.A. Bobbert, H. van Eersel, R. Coehoorn
Adv. Funct. Mater. 28, 1804618 (2018)

05. INTEGRATIVE EPIGENETIC TAXONOMY OF PRIMARY PROSTATE CANCER
S. Stelloo, E. Nevedomskaya, Y. Kim, K. Schuurman, E. Valle-Encinas, J. Lobo, O. Krijgsman, D.S. Peeper, S.L. Chang, F.Y. Feng, L.F.A. Wessels, R. Henrique, C. Jeronimo, A.M. Bergman, W. Zwart
Nat. Commun. 9, 4900 (2018)

06. MECHANICS OF ELASTOMERIC MOLECULAR COMPOSITES
P. Millereau, E. Ducrot, J.M. Clough, M.E. Wiseman, H.R. Brown, R.P. Sijbesma, C. Creton
Proc. Natl. Acad. Sci. U. S. A. 115, 9110–9115 (2018)

07. NEAR-INFRARED TANDEM ORGANIC PHOTODIODES FOR FUTURE APPLICATION IN ARTIFICIAL RETINAL IMPLANTS
G. Simone, D. Di Carlo Rasi, X. de Vries, G.H.L. Heintges, S.C.J. Meskers, R.A.J. Janssen, G.H. Gelinck
Adv. Mater. 30, 1804678 (2018)

08. PLASMON RULERS AS A PROBE FOR REAL-TIME MICROSECOND CONFORMATIONAL DYNAMICS OF SINGLE MOLECULES
E.W.A. Visser, M. Horacek, P. Zijlstra
Nano Lett. 18, 7927–7934 (2018)

09. POLYMORPHISM IN BENZENE-1,3,5-TRICARBOXAMIDE SUPRAMOLECULAR ASSEMBLIES IN WATER: A SUBTLE TRADE-OFF BETWEEN STRUCTURE AND DYNAMICS
N.M. Matsumoto, R.P.M. Lafleur, X. Lou, K.-C. Shih, S.P.W. Wijnands, C. Guibert, J.W.A.M. van Rosendaal, I.K. Voets, A.R.A. Palmans, Y. Lin, E.W. Meijer
J. Am. Chem. Soc. 140, 13308–13316 (2018)

10. QUADRUPLE JUNCTION POLYMER SOLAR CELLS WITH FOUR COMPLEMENTARY ABSORBER LAYERS
D. Di Carlo Rasi, K.H. Hendriks, M.M. Wienk, R.A.J. Janssen
Adv. Mater. 30, 1803836 (2018)

11. RATIONALLY DESIGNED SEMISYNTHETIC NATURAL PRODUCT ANALOGUES FOR STABILIZATION OF 14-3-3 PROTEIN-PROTEIN INTERACTIONS
S.A. Andrei, P.J. de Vink, E. Sijbesma, L. Han, L. Brunsveld, N. Kato, C. Ottmann, Y. Higuchi
Angew. Chem. Int. Ed. 57, 13470–13474 (2018)

12. STRAIN-STIFFENING IN DYNAMIC SUPRAMOLECULAR FIBER NETWORKS
M. Fernandez-Castano Romera, X. Lou, J. Schill, G. ter Huurne, P.-P.K.H. Fransen, I.K. Voets, C. Storm, R.P. Sijbesma
J. Am. Chem. Soc. 140, 17547–17555 (2018)

13. TRACKING LOCAL MECHANICAL IMPACT IN HETEROGENEOUS POLYMERS WITH DIRECT OPTICAL IMAGING
G.A. Filonenko, J.A.M. Lugger, C. Liu, E.P.A. van Heeswijk, M.M.R.M. Hendrix, M. Weber, C. Mueller, E.J.M. Hensen, R.P. Sijbesma, E.A. Pidko
Angew. Chem. Int. Ed. 57, 16385–16390 (2018)

14. A UNIFIED VIEW ON NANOSCALE PACKING, CONNECTIVITY, AND CONDUCTIVITY OF CNT NETWORKS
K. Gnanasekaran, C. Grimaldi, G. de With, H. Friedrich
Adv. Funct. Mater. 29, 1807901 (2019)

15. EVOLUTIONARY APPROACHO CONSTRUCTING A DEEP FEEDFORWARD NEURAL NETWORK FOR PREDICTION OF ELECTRONIC COUPLING ELEMENTS IN MOLECULAR MATERIALS
O. Caylak, A. Yaman, B. Baumeier
J. Chem. Theory Comput. 15, 1777–1784 (2019)

16. MIMICKING ACTIVE BIOPOLYMER NETWORKS WITH A SYNTHETIC HYDROGEL
M. Fernandez-Castano Romera, R. Gosatl, H. Shaikh, G. ter Huurne, J. Schill, I.K. Voets, C. Storm, R.P. Sijbesma
J. Am. Chem. Soc. 141, 1989–1997 (2019)

17. NANOIMMUNOTHERAPY TO TREAT ISCHAEMIC HEART DISEASE
R. Duivenvoorden, M.L. Senders, M.M.T. van Leent, C. Perez-Medina, M. Nahrendorf, Z.A. Fayad, W.J.M. Mulder
Nat. Rev. Cardiol. 16, 21–32 (2019)

18. REDEFINING NEAR-UNITY LUMINESCENCE IN QUANTUM DOTS WITH PHOTOTHERMAL THRESHOLD QUANTUM YIELD
D.A. Hanifi, N.D. Bronstein, B.A. Koscher, Z. Nett, J.K. Swabeck, K. Takano, A.M. Schwartzberg, L. Maserati, K. Vandewal, Y. van de Burgt, A. Salleo, A.P. Alivisatos
Science 363, 1199–1202 (2019)

19. RELATING FRONTIER ORBITAL ENERGIES FROM VOLTAMMETRY AND PHOTOELECTRON SPECTROSCOPY TO THE OPEN-CIRCUIT VOLTAGE OF ORGANIC SOLAR CELLS
R.E.M. Willems, C.H.L. Weijtens, X. de Vries, R. Coehoorn, R.A.J. Janssen
Adv. Energy Mater. 9, 1803677 (2019)

20. REMOVAL OF MICROPARTICLES BY CILIATED SURFACES-AN EXPERIMENTAL STUDY
S. Zhang, Y. Wang, P.R. Onck, J.M.J. den Toonder
Adv. Funct. Mater. 29, 1806434 (2019)

21. THE CONSTRUCTION OF SUPRAMOLECULAR SYSTEMS
G. Vantomme, E.W. Meijer
Science 363, 1396–1397 (2019)

News, awards & grants

Max Planck Institute

FOR POLYMER RESEARCH AND ICMS JOIN FORCES

The Max Planck Institute for Polymer Research (MPIP) and the Institute for Complex Molecular Systems (ICMS) recently organized a joint one-day workshop on State-of-the-art Characterization tools. By joining forces in this area, we aim at going beyond current characterization capabilities. As our molecules, materials and systems continuously increase in complexity and dynamics, creative combinations of characterization tools are essential for a deeper understanding of structure-property relationships. This could for example be enabled via correlative analysis with high-end techniques. Experts from both organizations had lively in-depth discussions on which opportunities the following state of the art characterization techniques had to offer: solid state NMR, scanning probe techniques, electron and super-resolution microscopy and X-ray techniques. It became clear that applying these advanced characterization tools is of particular interest to both MPIP and ICMS in the areas of molecular devices and bio-inspired materials engineering. Industry also participated in the workshop to get acquainted with and inspired by our current and future capabilities. The success of this workshop has made both organizations committed to jointly further explore and advance the design, synthesis, characterization, and application of complex molecular systems.

Bert Meijer

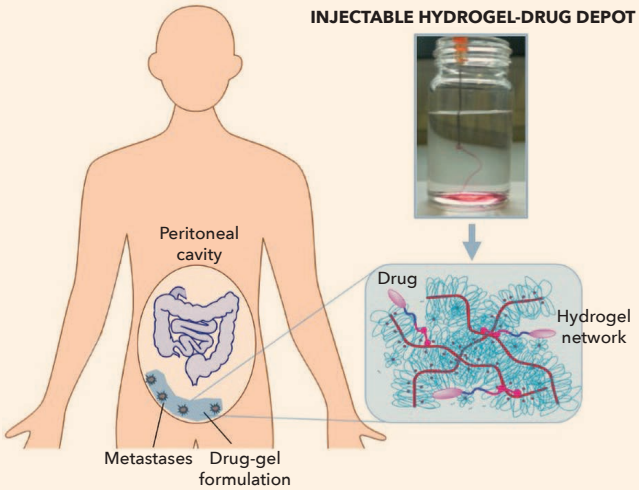
ENTERS THE AMERICAN ACADEMY OF ARTS AND SCIENCES

Bert Meijer amongst the new members of the Academy, which honors exceptionally accomplished individuals across disciplines and professions.

Bert Meijer, professor of Organic Chemistry at TU/e, has been elected as a member of the American Academy of Arts and Sciences, an honorary society that recognizes and celebrates excellence across disciplines and professions. Meijer will be inducted at a ceremony in October 2019 in Cambridge, Massachusetts.

KWF RESEARCH GRANT FOR

TU/e, Maastricht UMC and Catharina Cancer Institute



Maastricht UMC, Catharina Cancer Institute and TU/e receive funding from KWF to start preclinical validation of an innovative supramolecular hydrogel that enables local continuous intraperitoneal chemotherapy in peritoneal cancer. A KWF research grant was awarded to a consortium of Maastricht UMC, Catharina Cancer Institute, and TU/e for the development of a new strategy to improve intraperitoneal chemotherapy for patients with peritoneal cancer. Within this consortium professor Nicole Bouvy (Maastricht UMC), professor Ignace de Hingh (Catharina Cancer Institute) and professor Patricia Dankers (TU/e) join forces to start preclinical validation of an innovative supramolecular hydrogel that enables continuous local intraperitoneal chemotherapy. The material underlying this new therapy for peritoneal cancer is developed at the TU/e by researchers in the group of Patricia Dankers.

Molecular casings makes DNA-computing in blood viable

BY PROTECTING IT FROM ENZYME ATTACK

DNA molecules can potentially be reprogrammed to help do useful things, like detecting diseases and releasing drugs. But until now this so-called DNA computing was impossible in blood, as human enzymes degrade the molecules almost instantly. Biomedical Engineer Tom de Greef from Eindhoven University of Technology together with researchers from Radboud University, University of Bristol and Microsoft Research have solved this issue by creating a protective molecular casings, in which they created functioning DNA-based computational circuits. This compartmentalization approach has a nice bonus: it also increases the computing speed. The results are published in Nature Nanotechnology.

MOLECULAR DEVICES

Responsive soft materials for microfluidics, and more

Albert Schenning (left) and Jaap den Toonder

Jaap den Toonder and Albert Schenning cooperate on the next generation of microfluidic systems that contain active components but do not require bulky auxiliary arrangements. Key to these systems are light responsive polymers developed by Schenning. The cooperation between Den Toonder, engineer, and Schenning, polymer chemist, is one of synergy and inspiration.

In the research portfolio of Den Toonder's Microsystems group, an important focus is on manipulating fluids in microfluidic systems. Such systems are of relevance to lab-on-a-chip devices, for instance for bedside medical diagnostic application. They consist of intelligently designed geometries of branching and interconnecting flow channels with strategically microstructured surfaces. Although this enables all kinds of mixing and separation processes, such systems basically operate in a passive manner. Den Toonder wants to be able to devise the next generation of microfluidic systems containing active components such as valves and mixing chambers. "The challenge here is to integrate those components in the microfluidic system without compromising it's practical use", Den Toonder explains. And until now that has seldom been the case. The use of piezoelectric components, for instance, requires an electric auxiliary unit for power supply and electronic control. The same holds for micropneumatic systems.

LIGHT RESPONSIVE MATERIALS

Fortunately, it takes just a three-minute walk across the TU/e campus to Albert Schenning's group for Stimuli Responsive Functional Materials and Devices. The group has extensive knowledge of light responsive polymer materials that offer the perspective of untethered active microfluidic components. "To ultimately bring microfluidic systems to market they have to be biocompatible, disposable and cheap", says Schenning. "Polymers then are the obvious materials. What's more, when we use the right molecular components we can make polymers responsive to light. This offers a great opportunity of creating active components that can control the flow, switch it on and off, and modulate its characteristics."
The Schenning group already designed a microvalve that opens when illuminated - using a simple microlaser as the only auxiliary system. Schenning: "Getting rid of expensive and bulky auxiliary systems in microfluidic systems indeed is an important driving force for the development of light responsive materials". He values the cooperation with Den Toonder: "In developing our materials we maintain a complete chain-of-knowledge approach spanning from synthesis to device fabrication. Jaap provides us with the engineering perspective that is crucial for materials development. He shows us what novel materials are needed and how these have to perform. It's up to us to translate that into a particular molecular design."
The inspiration is mutual, says Den Toonder: "When new materials with new functionalities are developed, we start thinking about the possibilities and opportunities for our devices."
Once in a while, the two of them get together for a brainstorm which almost always inspires them both to develop new ideas, new materials and new devices.

"WHEN NEW MATERIALS WITH NEW FUNCTIONALITIES ARE DEVELOPED, WE START THINKING ABOUT THE POSSIBILITIES AND OPPORTUNITIES FOR OUR DEVICES."

The cooperation goes way beyond microfluidics. Den Toonder for instance also researches microsystems in the biological domain, for culturing of cells or even micro-tissues - notably organoids, miniaturized and simplified version of organs with realistic and functional micro-anatomies. For this, Schenning sets out to develop new responsive materials. The hydrogel-based polymers he has until now been working on have the drawback of being sensitive to water and other fluids. This can, of course, be solved by adding fluid resistant coatings, but that complicates the design of both materials and device. He hopes to explore new horizons by using polymeric liquid crystal materials that offer both compatibility with fluids and superb responsiveness.

EYE FLUID DRAINAGE

Another challenging cooperation between the two is a recently initiated research project together with eye surgeons at Maastricht UMC. It concerns glaucoma, one of the main causes of blindness. The disease involves the increase of intraocular pressure caused by restricted eye fluid drainage. To a certain extent, the use of drugs can provide relief. However, at a more advanced stage of the disease, a surgical procedure is needed where a microscopic tubular drain is inserted in the eye. This, however, is a fixed solution where the required amount of drainage cannot be (fine)tuned. Den Toonder: "The idea is now to use a light-responsive material so the diameter of the drainage tube can be set using a laser, allowing control over the amount of drainage". To Schenning this poses quite a challenge: "The material will have to retain its conformation after illumination, whereas the materials that we now design return to their original state when the laser is switched off. And of course it has to be biocompatible and durable, able to withstand the scrutiny of clinical testing." In industry, he adds, there's a declining interest in researching such fundamentally novel materials. "This implies that really innovative solutions depend on the research that we perform here at the university."

Reflection on the ICMS Friday afternoon discussion session

BY JAIME GÓMEZ RIVAS

The investigation of complex systems requires, unavoidably, a multidisciplinary approach. Complex molecular systems need complex experimental techniques for their examination; complex theories can be tested with these experiments, and, eventually, complex phenomena or devices with improved functionalities can be realized. This working philosophy can be only realized in an organization that encourages scientific discussion and facilitates the interaction between scientists with different background but common interest. This is exactly what the ICMS Friday afternoon session enables.

In the discussion session that I chaired, I wanted to discuss the relevance of ultrafast optical techniques for the investigation of photo-excited molecular systems and devices. The background of my group is on nanophotonics and advanced spectroscopy, and our goal is to exploit strong interactions between light and matter to modify fundamental properties such as charge transport or energy transfer. For us it is important to know where the limits are for the performance of organic materials in optoelectronic devices, and what are the bottlenecks in this field. It is also interesting to share our expertise on ultrafast spectroscopy and near-field imaging,

Jaime Gómez Rivas

Around 20 ICMS members participated in the discussion session

and to discuss whether these techniques can also make an impact on the research of complex molecular systems.

Around 20 ICMS members participated in the discussion session, including permanent staff, PhD students and postdocs. Several conclusions were drawn from the discussion. For instance, the effect of grain size and interfaces in perovskite solar cells is not yet well understood. Ultrafast imaging of the charge transport in these devices can shed light onto the processes that limit the efficiency, but care needs to be taken when comparing devices operating at normal conditions with devices investigated under extreme conditions (e.g. 1 sun illumination vs. intense illumination with short pulses). The development of multi-scale imaging and spectroscopic techniques is also important for understanding the physical properties at a microscopic (single molecule) level and the impact that these properties have at a macroscopic (device) level. These techniques are not standard and need to be developed. Also, the determination of optical constants at intermediate frequencies (THz, far-IR) is interesting to test molecular models.

In summary, one hour of discussion gave us ideas for one full year!

"FOR US IT IS IMPORTANT TO KNOW WHERE THE LIMITS ARE FOR THE PERFORMANCE OF ORGANIC MATERIALS IN OPTOELECTRONIC DEVICES, AND WHAT ARE THE BOTTLENECKS IN THIS FIELD."

ICMS Industrial Challenge 2020

Next year will see a new edition of the ICMS Industrial Challenge that offers master's students the opportunity to be involved with industrially relevant research projects.

Set up on the initiative of Ilja Voets and Menno Prins, now being coordinated by Loai Abdelmohsen, the ICMS Industrial Challenge connects industry and academia and provides the industry with a 'thought force' generating impactful out-of-the-box creative solutions.

During the ICMS Outreach Symposium held March 11-12, five companies (DSM Coating Resins, Tianhe Resins Europe, Stahl, SABIC, and LifeTec Group) presented a total of eight challenges. To give an idea on the variety of subjects, the students were invited to work on: Developing a sustainable material for food preservation; Enhancing the recyclability of coatings; Finding a sustainable additive for the production of low-wear plastics; and Developing Cardiac Bio Simulators.

Currently, the recruitment of students is underway - they can register until August for their favourite challenge. September will see the formation of student teams taking up each challenge, and in January 2020 the best teams will be selected to compete at next year's ICMS Annual Symposium for the three ICMS Industrial Challenge Awards: the Science Award (scientific depth), the Innovation Award (industrial impact) and the Audience Award (the public's favourite).

"CURRENTLY, THE RECRUITMENT OF STUDENTS IS UNDERWAY - THEY CAN REGISTER UNTIL AUGUST FOR THEIR FAVOURITE CHALLENGE."

DSM
Jurgen Scheerder
Principal Scientist

LifeTec Group
Mattia D'Alessi
R&D engineer

Tianhe Resins Europe
Feng Li
Managing Director
Europe

Stahl
Frank Brouwer
Senior Green
Technology Chemist

LifeTec Group
Dave Wanders
R&D engineer

Institute for Complex Molecular Systems (ICMS)

CREATING FUTURE TECHNOLOGIES BY MASTERING COMPLEXITY

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

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

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

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

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

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

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

ICMS in PRESS

EDITORIAL
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