ICMS Highlights

Edition 6
April 2016

Winter School on Complexity Science

INTERVIEW
/ Joanna Aizenberg

THE OLED OF THE FUTURE

INTERVIEW
/ George Whitesides

& more...

Institute for Complex Molecular Systems

TU/e Technische Universiteit Eindhoven University of Technology

Where innovation starts

ICMS Highlights

Dear reader,

In making this new ICMS Highlights, we look back on a vibrant Outreach Symposium 2016. It represents many of the ICMS values and we are very happy with the large number of participants. During the symposium, ICMS researchers discussed their science with invited external speakers and members of our industrial consortium. The need to exchange ideas beyond traditional disciplines is growing rapidly and for the ICMS this represents one of the primary objectives. The ICMS has formalized the long-lasting collaboration with the UCSB Materials Research Laboratory, while we will extend our international network.

Over the last few months, ICMS members played an important role in the launch of the Netherlands Platform Complex Systems. The research is strengthened with promising new projects. The teams of Bert Meijer and Anja Palmans, of Albert Schenning, Cees Bastiaansen and Tom Engels and of Patricia Dankers have each received an NWO NEWPOL grant. Patricia Dankers was also successful in the CVON call. On the personal side we are very pleased and proud of the ERC Starting Grant of Tom de Greef, the ERC PoC of Regina Luttge and EU Marie Curie fellowships for Junhong Yan, Nathan van Zee, and Chidambar Kulkarni.

TU/e is the place to be where innovation starts and where people matter. ICMS is proud to be part of it and as the world around us is changing continuously, ICMS will adapt where needed.

We hope you enjoy reading,

Sagitta Peters
Managing director

Bert Meijer
Scientific director

Calendar

April 22, 2016
Science day TU/e
Location: TU/e

May 20, 2016, 15.00 hr
ICMS Discussion meeting
Dr. Erik Steur
Location: Ceres

June 17, 2016, 15.00 hr
ICMS Discussion meeting
Dr. Wim Noorduin
Location: Ceres

July 15, 2016, 15.00 hr
ICMS Discussion meeting
SensUs team
Location: Ceres

October 13, 2016, 16.30 hr
Nobel Prize evening
Location: Zwarte Doos

January 19-20, 2017
ICMS Outreach Symposium
Location: Zwarte Doos

The complete calendar can be found on our website.

Content

Edition 6
April 2016

/ Joanna Aizenberg

Dreams of a *dynamic* building

The lab of prof.dr. Joanna Aizenberg, a materials scientist at Harvard University, offers spectacular examples of biomimetic materials. Her research includes slippery surfaces, bio-inspired optics, nanostructured surfaces, controlled self-assembly, wettability and biomineralization. The inspiration for all these topics comes from biology. From sea urchins to pitcher plants and deep sea sponges to desert beetles - nature proves to be an endless source of ideas.

Why is nature such an important source of inspiration for your research? After all, design and synthesis of novel molecules with new functionalities is at the heart of chemistry.

"The main reason is that nature knows how to create many different functionalities from one material. Most materials we now use are very good at only one function. They are either very hard or very flexible. Water resistant or they can breathe. But these materials cannot change, they are passive. My interest is in dynamic materials that can adapt to changing circumstances, and those materials are found everywhere in nature. We look to nature's engineering solutions and use those as a starting point to create our synthetic solutions. For that we need chemistry, in particular supramolecular chemistry. The work here at the ICMS is very inspirational for what we are doing. I am not a synthetic organic chemist, so in my classes on chemistry for applied physics, I always show the work of Bert Meijer's group to illustrate what you can create with non-covalent interactions in terms of strength and versatility."

In what kind of applications do you see a benefit of using dynamic materials?

"My dream is to create a whole building with a skin of dynamic materials. Just think about what we could do. Thermoreflective windows that respond to the amount of sunlight and can thus control the temperature inside. Windows that can create a liquid layer to prevent freezing. Walls that shed water when it rains, but can breathe when needed. This will help reduce structural damage to the construction due to water that remains in porous materials and crevices. It can also act as an anti-fouling agent because it prevents the growth of molds and fungi. All this will help to make the heating and cooling system as well as overall maintenance of such a building much more efficient and much more 'green'. Thinking even more wildly, what about walls that can very quickly respond to impact? For example from a bullet or a crashing car. There is an endless range of possibilities."

How do you ensure that such a dynamic skin keeps working? With all those different stimuli and the wide range of potential responses, where is the benefit for the system to keep performing as planned?

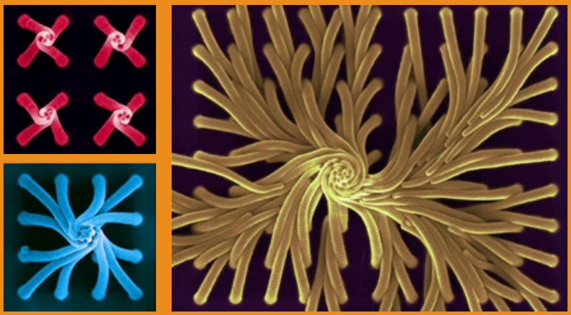
"You program the desired responses into the material itself. The information is in the building blocks of the material. There is no choice, it does either this or that. The challenge is that most functions are orthogonal: ensuring that a material is watertight does not easily combine with the need to breathe. One way is to create feedback loops in the material so that the response to one stimulus induces the necessary reaction to get the system back to its starting point."

The conventional way to solve a complex puzzle is to take it step by step and gradually introduce complexity. That seems to contradict the need to balance all those different functions.

"True, that approach will get you nowhere. You have to start with the complexity built in. Don't concentrate on finding the perfect conditions for one particular function, but work towards an optimal solution for all the required functions taking into account all the boundary conditions. That will not deliver the perfect solution for each separate function, but that is irrelevant because you the need the solution that fits this particular combination of functions."

In your lecture during the ICMS Outreach Symposium, you showed many fascinating examples of controlled self-assembly and patterned actuation. Hairy surfaces that can move tiny spheres around, for example. But all this is still on the nano and mesoscale. Is it feasible that we can scale these systems up to the level of a real-life building?

"The key is to know what is critical and what is not, and then focus on controlling the critical issues. I am convinced that it is easier to move to larger scales than it is to figure out how we can predict the behavior of materials on the nanoscale. To me, that is the real challenge here."



Winter School on Complexity Science

In December 2015, the Institute of Complex Molecular Systems (ICMS) opened its doors to 45 PhD students and postdoctoral researchers from all over Europe on the occasion of the Winter School on Complexity Science. Organized by ICMS, TU/e, and the Over Grenzen program of the Royal Dutch Academy of Science and Arts (KNAW), the winter school hosted world renowned experts in the fields of engineering, mathematics, physics, chemistry, and computer science. The program comprised of five days of tutorial and topical invited lectures, embracing the “inexhaustible baroque-like diversity of evolution scenarios, that are principal fingerprints of complex systems”, as phrased by Prof. G. Nicolis, the first speaker at the school. Co-sponsoring organizations were the Eindhoven Multiscale Institute (EMI) and the Dutch Institute of Systems and Control (DISC).

From the Newtonian paradigm to the complexity paradigm

Grégoire Nicolis: “Traditionally, the objective set by Science is to predict the future state of natural objects on the basis of their present state. More than three centuries ago Isaac Newton showed how with few theoretical concepts, like the law of universal gravitation, one can interpret the essence of planetary motions or predict accurately an eclipse of the sun thousands of years in advance. Following this historical achievement and some further major developments, the world was viewed as fundamentally simple, reducible to a collection of few fundamental elements animated by regular and predictable motions. This constitutes the essence of the so-called Newtonian paradigm. However, our everyday experience shows that there exist phenomena that are, manifestly, much less regular and predictable. For example we cannot accurately predict the weather more than a few days in advance, or the state of the planet earth 50 years from now, although they obey to the same laws of nature as the motion of celestial bodies. This realization opened the way to a first, rough idea of complexity, which perhaps still survives as such in our ordinary vocabulary, namely, that complexity is related to the complications arising when one deals with systems involving a multitude of variables and parameters blurring some underlying regularities. But over the years, following the discovery of unexpected behaviours in ordinary systems as well, obeying to laws known to their least detail and operating in the laboratory under strictly controlled conditions, the perception of complexity dramatically changed. From a mere metaphor to characterize intricate systems, it was recognized as a fascinating phenomenon deeply rooted into the laws of nature.”

Complexity: the whole matters more than the parts

Grégoire Nicolis: “The most fascinating aspect of complexity is its unifying power. The science of complexity lies at the crossroads of physics, mathematics, engineering, environmental life and human sciences. It embraces many disciplines and yet it constitutes a field of science in its own right with its specific laws and methodologies. And this is exactly where the challenge starts. Complexity requires the cross-fertilization of ideas and techniques from nonlinear science, statistical mechanics and thermodynamics, probability and numerical simulations. The marked added value resulting from this cross-fertilization confers to Complexity science its characteristic uniqueness and originality”.

Complexity in meteorology: the collaboration with Catherine Nicolis

As was the case in the past, for the excellent collaboration of Professor Nicolis with his wife Catherine Nicolis, leader in non-linear processes as applied in geoscience. Grégoire Nicolis: “In the monograph Foundations of complex systems we addressed, among others, the behaviour and the application of stochastic and deterministic non-linear systems in meteorology and climate dynamics. Working with Catherine was very instrumental in shaping my way of thinking, raising new intriguing questions particularly on the issue of prediction, and, most importantly, bridging the gap between fundamental science and applications to real-world problems of concern.”

Learning from the best: the Nobel laureate Ilya Prigogine

Grégoire Nicolis: “Being supervised by Ilya Prigogine during my PhD project and collaborating with him over a long time later was a real honour and a rare privilege. Besides his acknowledged outstanding scientific qualities, Ilya Prigogine had a superb intuition and an astounding humanistic culture. His personality was radiating a natural sense of leadership based on his brilliance, never on hierarchies of any kind.” The long lasting collaboration between Nicolis and Prigogine resulted in

Grégoire Nicolis

Grégoire Nicolis (1939) is Professor Emeritus in the physics and chemistry departments at the University of Brussels. After studying engineering at the National Technical University of Athens, he completed his PhD in Physics at the University of Brussels in 1965 under the guidance of the Nobel laureate Ilya Prigogine, noted for his pioneering theories on self-organizing systems and irreversibility. Following post-doctoral studies at the University of Chicago (1966-1967), Nicolis was appointed professor at the University of Brussels. His research interests include nonlinear dynamics, stochastic processes, non-equilibrium statistical mechanics, irreversible thermodynamics, self-organization, and the physical foundations of complexity.

several articles in internationally renowned journals and the monograph Exploring complexity (1987), which is nowadays still considered as the birth certificate of the complexity's vocabulary.

The ICMS experience

Grégoire Nicolis: "Over the last decades, complexity became a major scientific field in its own right, modifying considerably the scientific landscape through the creation of specialized journals, learned societies and institutes like the Interdisciplinary Center for Nonlinear Phenomena and Complex Systems in Brussels and the ICMS, here in Eindhoven. Workshops, seminars and winter schools like this are unique occasions for advanced training of a new generation of scientists. Complexity attracts audiences of an unprecedented diversity comprising mathematicians, biologists, chemists and physicists. Hopefully, this will stimulate active cooperation between scientists of the various groups and promote interdisciplinary learning."

"The most *fascinating* aspect of Complexity is its **UNIFYING POWER.**"


Alessandro Sorrenti


Pranav Madhikar


Upanshu Sharma


Jens Wehner


Valerie Voorsluijs

Alessandro Sorrenti
Institut de Science et d'Ingenierie Supramoleculaires, France: "My interests mainly concern the investigation of dissipative self-assembly mediated by enzyme switching. During this Winter School, I strengthened my knowledge on self-assembling from equilibrium conditions to far from equilibrium systems, by following the lectures and exchanging knowledge with young researchers from different fields. As emphasized by many of the lecturers, expanding supramolecular chemistry towards non-equilibrium thermodynamic is the new trend, which perfectly links to my current research approach."

Pranav Madhikar
TU/e, Eindhoven: "I enjoyed the introductory lecture of Prof. Nicolis because he explained some of the distinctive features of Complexity starting from a fundamental level. Sometimes, during the PhD, students tend to be too much result oriented, and to forget about the entertainment of the learning process. In this respect, this school was an interesting change of pace."

Upanshu Sharma
TU/e, Eindhoven: "I like to look at problems from the application point of view and, for this reason, the lecture of Prof. Maes about statistical mechanical treatment of response theory around non-equilibrium regimes was particularly inspiring for me. Also, this Winter School is the umpteenth demonstration of the interdisciplinary character of ICMS, a dynamic network of scientists promoting knowledge sharing with good initiatives."

"I mostly *enjoyed* all the networking and the BRAIN STORMING."

Jens Wehner
Max Planck Institute, Germany:
"I joined the Winter School because of my interest in complexity, and the lecture of Nicolis was the perfect introduction for the new-to-the-field like me. Also, it was a good occasion to meet new people and get some new inputs. Overall, as a visiting researcher at ICMS, I can say that this institute is one of the most stimulating places I have worked so far. I am a material scientist, and my research focuses on the transport and the thermodynamic properties of highly polar organic dyes via computational simulations. At ICMS my numerical knowledge improved even more, thanks to the daily support I receive from the highly qualified mathematicians I work with."

Valerie Voorsluijs
Université libre de Brussels, Belgium:
"During this Winter School I met many other PhD students and world renowned scientists. I mostly enjoyed all the networking and the brain storming, which I personally find more effective than studying individually from books. Also, having read many of the articles of Prof. Nicolis, attending one of his lectures in such a privileged audience was a real honour for me, a pure pedagogical experience."

ICMS TOP PUBLICATIONS

October 2015 – March 2016

1. *J.J. van Franeker, G.H.L. Heintges, C. Schaefer, G. Portale, W.W. Li, M.M. Wienk, P. van der Schoot, R.A.J. Janssen*
   Polymer solar cells: solubility controls fiber network formation
   J. Am. Chem. Soc. 137, 11783–11794 (2015)

2. *L.M. Pitet, E. Alexander-Moonen, E. Peeters, T.S. Druzhinina, S.F. Wuister, N.A. Lynd, E.W. Meijer*
   Probing the effect of molecular nonuniformity in directed self-assembly of diblock copolymers in nanoconfined space
   ACS Nano 9, 9594-9602 (2015)

3. *D. van der Zwaag, P.A. Pieters, P.A. Korevaar, A.J. Markvoort, A.J.H. Spiering, T.F.A. de Greef, E.W. Meijer*
   Kinetic analysis as a tool to distinguish pathway complexity in molecular assembly: an unexpected outcome of structures in competition
   J. Am. Chem. Soc. 137, 12677-12688 (2015)

4. *Y.L. Liu, T. Pauloehrl, S.I. Presolski, L. Albertazzi, A.R.A. Palmans, E.W. Meijer*
   Modular synthetic platform for the construction of functional single-chain polymeric nanoparticles: from aqueous catalysis to photosensitization
   J. Am. Chem. Soc. 137, 13096-13105 (2015)

5. *T.J. White, D.J. Broer*
   Programmable and adaptive mechanics with liquid crystal polymer networks and elastomers
   Nature Mater. 14, 1087-1098 (2015)

6. *C.P. Plaisance, R.A. van Santen*
   Structure sensitivity of the oxygen evolution reaction catalyzed by cobalt(II, III) oxide
   J. Am. Chem. Soc. 137, 14660-14672 (2015)

7\. *M. Scheepstra, S. Leysen, G.C. van Almen, J.R. Miller, J. Piesvaux, V. Kutilek, H. van Eenennaam, H.J. Zhang, K. Barr, S. Nagpal, S.M. Soisson, M. Kornienko, K. Wiley, N. Elsen, S. Sharma, C.C. Correll, B.W. Trotter, M. van der Stelt, A. Oubrie, C. Ottmann, G. Parthasarathy, L. Brunsveld*
Identification of an allosteric binding site for RORγt inhibition
Nature Commun. 6, 8833 (2015)

8\. *L.G. Milroy, M. Bartel, M.A. Henen, S. Leysen, J.M.C. Adriaans, L. Brunsveld, I. Landrieu, C. Ottmann*
Stabilizer-guided inhibition of protein-protein interactions
Angew. Chem. Int. Ed. 54, 15720-15724 (2015)

9\. *M.J. Webber, E.A. Appel, E.W. Meijer, R. Langer*
Supramolecular biomaterials
Nature Mater. 15, 13-26 (2016)

10\. *D.E.P. Muylaert, G.C. van Almen, H. Talacua, J.O. Fledderus, J. Kluin, S.I.S. Hendrikse, J.L.J. van Dongen, E. Sijbesma, A.W. Bosman, T. Mes, S.H. Thakkar, A.I.P.M. Smits, C.V.C. Bouten, P.Y.W. Dankers, M.C. Verhaar*
Early in-situ cellularization of a supramolecular vascular graft is modified by synthetic stromal cell-derived factor-1α derived peptides
Biomaterials 76, 187-195 (2016)

11\. *T.N. Do, W.Y. Choy, M. Karttunen*
Binding of disordered peptides to kelch: insights from enhanced sampling simulations
J. Chem. Theory Comput. 12, 395-404 (2016)

12\. *J.M. Clough, A. Balan, T.J. van Daal, R.P. Sijbesma*
Probing force with mechanobase-induced chemiluminescence
Angew. Chem. Int. Ed. 55, 1445-1449 (2016)

13\. *N.K. Gupta, A. Pashigreva, E.A. Pidko, E.J.M. Hensen, L. Mleczko, S. Roggan, E.E. Ember, J.A. Lercher*
Bent carbon surface moieties as active sites on carbon catalysis for phosgene synthesis
Angew. Chem. Int. Ed. 55, 1728-1732 (2016)

14\. *L.L.C. Olijve, K. Meister, A.L. DeVries, J.G. Duman, S. Guo, H.J. Bakker, I.K. Voets*
Blocking rapid ice crystal growth through nonbasal plane adsorption of antifreeze proteins
Proc. Nat. Ac. Sci. U.S.A. published online (2016)

15\. *M.M.K. Hansen, L.H.H. Meijer, E. Spruijt, R.J.M. Maas, M.V. Rosquelles, J. Groen, H.A. Heus, W.T.S. Huck*
Macromolecular crowding creates heterogeneous environments of gene expression in picolitre droplets
Nature Nanotechnol. 11, 191-197 (2016)

16\. *L.M. Stevers, C.V. Lam, S.F.R. Leysen, F.A. Meijer, D.S. van Scheppingen, R.M.J.M. de Vries, G.W. Carlile, L.G. Milroy, D.Y. Thomas, L. Brunsveld, C. Ottmann*
Characterization and small-molecule stabilization of the multisite tandem-binding between 14-3-3 and the R-domain of CFTR
Proc. Nat. Ac. Sci. U.S.A. published online (2016)

17\. *E.W.A. Visser, L.J. van Ijzendoorn, M.W.J. Prins*
Particle motion analysis reveals nanoscale bond characteristics and enhances dynamic range for biosensing
ACS Nano published online (2016)

18\. *P.J.M. Stals, C.-Y. Cheng, L. van Beek. A.C. Wauters, A.R.A. Palmans, S. Han, E.W. Meijer*
Surface water retardation around single-chain polymeric nanoparticles: critical for catalytic function?
Chem. Sci. 7, 2011-2015 (2016)

19\. *M.H. Bakker, C. Lee, E.W. Meijer, P.Y.W. Dankers, L. Albertazzi*
Multicomponent supramolecular polymers as a modular platform for intracellular delivery
ACS Nano 10, 1845-1852 (2016)

20\. *M. Moraingthem, R. Arts, M. Merkx, A.P.H.J. Schenning*
An optical sensor based on a photonic polymer film to detect calcium in serum
Adv. Funct. Mater. 26, 1154-1160 (2016)

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

NEWS, AWARDS & GRANTS

REGINA LUTTGE

receives ERC PoC Grant

Dr. Regina Luttge, associate professor in the research group Microsystems, has received a € 150,000 Proof-of-Concept Grant from the European Research Council (ERC) to develop a micro-bioreactor for brain cells.

The Proof-of-Concept Grants are awarded to researchers who have previously received another ERC grant for their research. With the newly awarded grant they can further develop, patent or investigate whether there is a market for any discoveries arising from that research.

DPD-2016 AWARDS

for ICMS members

During the Dutch Polymer Days 2016, Bas van Genabeek won the Plenary Lecture Award for his lecture entitled “Synthesis and self-assembly of discrete dimethylsiloxane-lactic acid diblock co-oligomer; New materials for nanolithography”. Koen Nickmans won the Poster Presentation Award in the category Technology. The Workshop Lecture Award in the category Biomedical went to Sabrina Zaccaria. The Dutch Polymer Days (DPD) were held March 7th-8th 2016 in Lunteren.

COLLABORATION MRL AND ICMS FORMALIZED

The Materials Research Laboratory (MRL) of the University of California, Santa Barbara and the Institute for Complex Molecular Systems (ICMS) have been collaborating for many years. Recently this partnership has been formalized via a Memorandum of Understanding.

In the coming years MRL and ICMS will further strengthen their collaboration in research and education in the area of functional supramolecular systems and high-tech materials. This might include sharing of research facilities, exchange of bachelor, master and PhD students and staff members, in addition to starting joint research projects.

NWO NEWPOL

projects for ICMS members

NWO Chemical Sciences has granted funding for six projects in the field of new polymers, of which three are associated with ICMS members. These grants are part of the public-private collaboration program NEWPOL and worth about € 140,000 each. The research projects will be executed in collaboration with the Dutch Polymer Institute (DPI) with the principal aim of developing new polymer materials that can help in fulfilling the societal and industrial needs of sustainability and multi-functionality.

The projects are:

- Polymers becoming smart - prof.dr. Albert Schenning, prof.dr.ing. Cees Bastiaansen and dr.ir. Tom Engels
- Supramolecular biomaterials for stem cell expansion - prof.dr. Bert Meijer and dr.ir. Anja Palmans
- Super active anti-microbial material for tissue repair - dr.dr. Patricia Dankers and dr. Bas Zaat (AMC, Amsterdam)

SENSUS

student competition update

SensUs is a new international student competition being organized by students at TU/e. Every year SensUs defines a specific goal for the teams; this year's challenge is to develop a compact system that detects creatinine in blood plasma. Creatinine is an important biomarker for kidney function. At five universities in Europe, multidisciplinary student teams are developing molecular biosensing systems.

All teams are now up and running, working hard to make an innovative sensing system. On September 9^{th}-10^{th} 2016 all teams will convene in Eindhoven to demonstrate their prototypes during a public event. After the pilot year 2016, more universities will be invited to join. The SensUs competition provides a platform that encourages corporation between universities, companies and healthcare partners.

For more information: **www.sensus.org**

MINISTER BLOK

visited Ceres and Eindhoven architecture

Minister Stef Blok of Housing and Civil Service visited Eindhoven on February 1^{st} 2016 at the invitation of the BNA (Royal Institute of Dutch Architects). The added value of architects at rezoning and transformation was the central theme of the day.

As part of the program, Minister Blok visited among others Strijp-S and Science Park TU/e, including the building Ceres, which was awarded the Building of the Year Award by BNA in 2013.

Three ICMS researchers acquire

MARIE CURIE GRANTS

Three ICMS researchers have each acquired a personal grant from the Marie Skłodowska Curie Actions (MSCA) of the European Horizon 2020 subsidy program. These Individual Fellowships range from € 166,000 to € 178,000 for two years.

Corona around nanoparticles – Dr. Junhong Yan
Increasingly GPs and hospitals are using small devices to do tests on patients. In many new test approaches nanoparticles are used, which are particles much smaller than a micrometer. However, one problem is that nanoparticles in biological fluids such as blood attract proteins, which tend to create a shell (or 'corona') around the nanoparticles and thereby hinder their action. In this project, Yan will investigate how exactly this happens by labeling proteins with DNA and monitoring their interactions.

Fighting tumors on the spot – Dr. Nathan van Zee
A highly promising new therapy to tackle tumors is to administer a drug in an inactive form and then activate it through a chemical reaction at exactly the location of the tumor, for instance by using a synthetic enzyme. In this project, Van Zee aims to enhance the properties of potential candidates for this function, single chain polymer nanoparticles.

Organic spintronics – Dr. Chidambar Kulkarni
In spintronics the magnetic properties of electrons (the 'spin') are used to store data in a computer memory rather than by electrical charge as in electronics. While most research tends to focus on inorganic materials as active components, Kulkarni will be investigating 'organic' variants in the form of supramolecular assemblies.

Launch of

NETHERLANDS PLATFORM COMPLEX SYSTEMS (NPCS)

The formal launch of the Netherlands Platform Complex Systems (NPCS) by the founding partners, Utrecht University (UU), the Netherlands Organisation of Scientific research (NWO), and the Netherlands Organisation for Applied Scientific Research (TNO) took place on November 27th 2015. The purpose of the NPCS is to bring together all stakeholders from academia, industry and policy makers within the complex systems research, thereby generating national and international impact.

NPCS aims to organize, structure and facilitate researchers in complex systems, and to promote educational, societal and industrial use of complex systems knowledge. Rutger van Santen and Henk Nijmeijer are members of the board of Netherlands Platform Complex Systems (NPCS) and have also been strongly involved in the start of this new platform.

Outreach Symposium 2016

The fifth annual ICMS Outreach Symposium was held on January 21 and 22, 2016. With this symposium, ICMS presents to its members and the outside world an overview of the ongoing research within the institute's themes, with lectures from TU/e and invited speakers.

This year the symposium was visited by more than two hundred and eighty scientists from the ICMS, Dutch academia, and European industry. This clearly indicates the impact of the various fields in fundamental research as well as its societal and economic value.

Bio-inspired engineering was the theme of the first day. Marileen Dogterom (Delft University), Karen Christman (University of California San Diego), Tonny Bosman (SupraPolix), Mikko Karttunen, and Kees Storm, amongst others, gave lectures to highlight the different research interests of the ICMS.

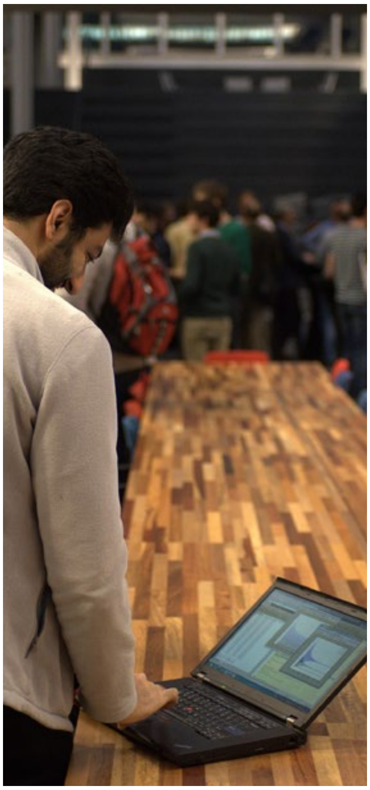
The second day was organized together with the Dutch Gravitation Program "Functional Molecular Systems". Here an expert view on future developments was presented by world-leaders in the field including Joanna Aizenberg (Harvard University), Chris Hunter (Cambridge University), and George Whitesides (Harvard University). Theme leaders from the Gravitation Program illustrated the progress made within the consortium.

The combination of lectures, poster sessions, and several moments for informal discussion enabled the exchange of knowledge and ideas. The next Outreach Symposium will be held on January 19 and 20, 2017. We are looking forward to your attendance.

Visited by more than

280

scientists from ICMS, Dutch academia and European industry



NEXT OUTREACH SYMPOSIUM

JANUARY 19 & 20 2017

CLARIANT DSM BRIGHT SCIENCE. BRIGHTER LIVING. سابك sabic SupraPolix SyMO-Chem

Industrial consortium

With the industrial consortium ICMS reaches out. Mutual benefits are being sought by combining industrial research and development with more fundamental sciences. While the industrial members stay up to date with the most recent developments, ICMS scientists get inspiration for their research. As part of the membership company coworkers can visit lectures and workshops, use the Advanced Study Center, participate in courses, and access the state of the art infrastructure at ICMS. To further promote knowledge exchange, ICMS organizes a yearly Outreach Symposium.

Interested to learn more about the consortium? Please contact us.

> THERE IS A LOT OF 'ME TOO' SCIENCE GOING ON

/ George Whitesides

Time to tackle the complex problems

Chemists need to explore new horizons and embrace new topics according to prof.dr. George Whitesides of Harvard University. Throughout his research career, he has made it a point to enter new areas again and again. "It is intellectually very stimulating to be posed with a problem that you don't have a clue about."

In your 2015 essay 'Reinventing chemistry' in Angewandte Chemie, you state that the chemistry field has become complacent and needs to reinvent itself in order to stay relevant. What happened?

"For decades, there was more than sufficient funding for chemistry research, both in academia and in industry. Those were relatively easy times for scientists, you hardly needed to justify your research plans. But those days are long gone, while many academics today still behave as if they are simply entitled to funding. There is a lot of 'me too' science going on. In the US, I often experience that truly novel ideas are not embraced by the scientific establishment, but are seen as a threat. Let me immediately state that here at the ICMS and also within the Functional Molecular Systems program, things are really different. These scientists have the guts to take on new challenges and they are tackling good problems."

What makes a problem a 'good' problem?

"A good problem is not simple. For a long time, chemistry has focused on 'simple' problems. Studying one molecule, highly purified, in a well-defined environment will surely teach you a lot, but it is not real. Nothing in real life is simple. The most urgent, and most interesting, problems are never simple. But chemistry was always happy to leave the complex problems to other fields, like physics and informatics. We should get out of our comfort zone and develop a new view on what the interesting problems for chemistry are."

In your essay, you mention a whole list of topics that chemistry should focus on. From dissipative systems to clean water, from origins of life to megacities. What can chemistry contribute to these problems?

"What chemistry can do really well is dealing with complexity and detail at the same time and we should exploit that in tackling a whole range of problems that are generally not associated with chemistry. Take megacities. Chemists are used to working with large numbers and with flows and fluxes. The transport problems on a molecular level share many similarities with the transport problems in megacities. Another example, the living cell. That is a huge collection of molecules that are in itself not alive. Yet, together, they create a living system. How? That is an intriguing problem for chemistry. In my view, it is intellectually very stimulating to be posed with a problem that you don't have a clue about."

How can we initiate such a change in the current line of thinking?

A smile appears: "Well, it is a waste of time trying to change the middle-aged men that are now in charge. Focus on young people. They are eager, full of energy and do not yet carry a history of achievements and failures. Allow young researchers the freedom to pursue their ideas and offer them the support and confidence to take risks. Failing is allowed. What we all should realize is that a research group is not only a collection of individuals with ideas, it is also a social organization. Complex problems require the input of many different people. You need an open setting where everybody is bringing something to the table and each contribution should be equally appreciated and valued. The conventional hierarchy in which students learn to reproduce what the 'master' has done is not the right approach. Today's students will be working on problems that we cannot even imagine right now, we need to prepare them for that, not for doing what we have done."

THE TRANSPORT PROBLEMS ON A MOLECULAR LEVEL SHARE MANY SIMILARITIES WITH THE TRANSPORT PROBLEMS IN MEGACITIES.

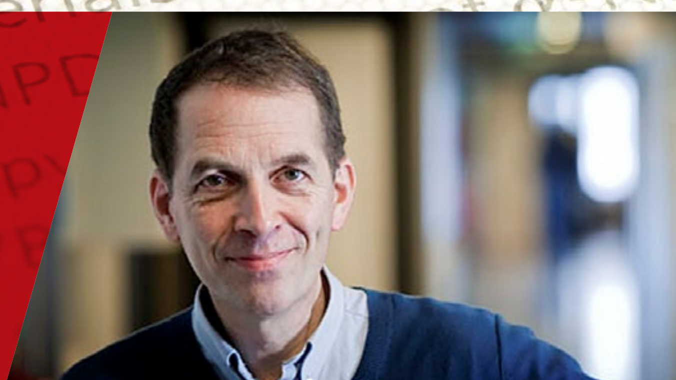
The kind of real life problems you propose are frowned upon by many academics.

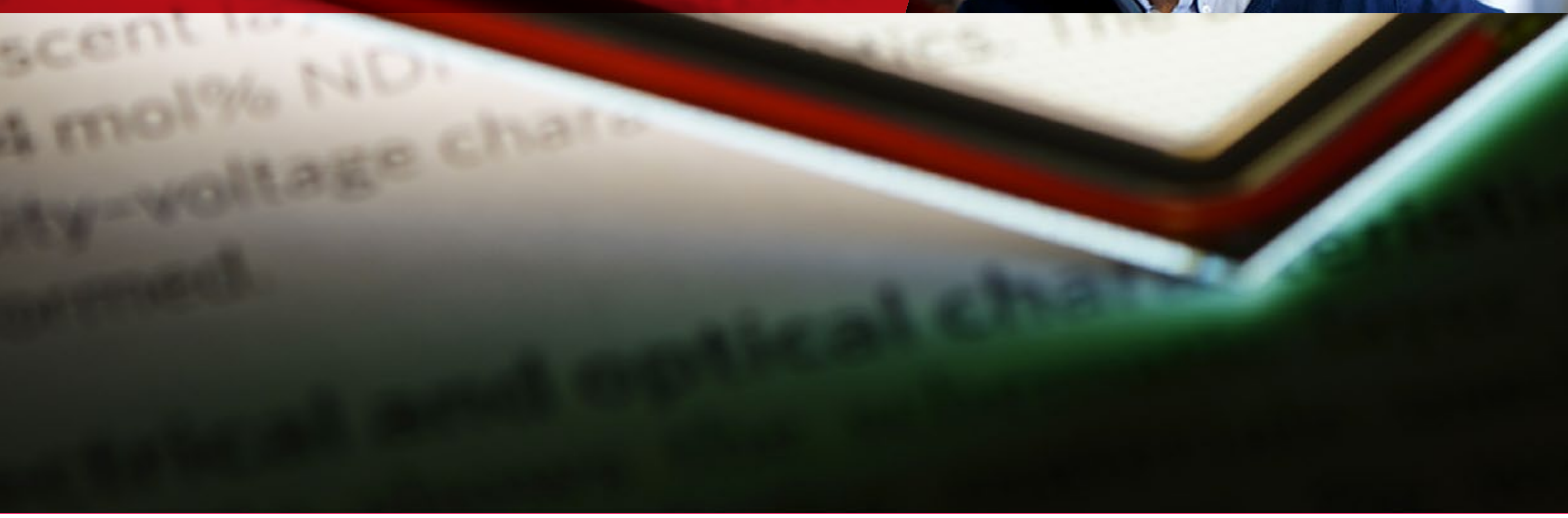
"I find the discussion on fundamental versus applied research completely uninteresting and irrelevant. When you have no answer to the question 'Who cares?' about your research, you are in the danger zone. You should ask yourself whether you are really that much smarter than everyone else."

/ Reinder Coehoorn

The OLED of the *future*

Physicist Reinder Coehoorn and his colleagues are trying to figure out the science behind an organic thin film that emits light. As it turns out, there is a lot more to it than just understanding the emission process.





Coehoorn: “Often, people think that organic materials such as plastics do not have electrical conductivity, since plastics are normally used as insulators. To them, it seems magical that a current can be passed through specific types of organic materials, which can then emit light. But to scientists, the detailed mechanism of the light emission is also still a bit of a mystery. We are working to understand all the subprocesses of the OLED and how these subprocesses interact with each other.”

Virtual OLED

Coehoorn and his colleagues have developed a model and a simulation tool that work exactly like the OLEDs. “In combination with physical experiments, this virtual OLED makes it possible to investigate whether our assumptions about how certain aspects work are true or not. It suggests new strategies for improving OLEDs.”

The virtual OLED is a result of a four-year European collaboration project and of a subsequent Dutch project within the NanoNextNL program. “To our pleasant surprise, the first time we combined everything we knew in the virtual OLED, the result of the computer simulation matched the result of a real-life experiment really well,” Coehoorn tells enthusiastically.

Balancing properties

“There are different subprocesses of an OLED that need improvement,” starts Coehoorn. “For example, the high efficiency OLEDs we make these days have insufficient lifespan. We can also make OLEDs that have a long lifespan, but they have a low efficiency.”

“In our research, we are trying to find out what limits the efficiency, and ultimately also the lifespan,” explains Coehoorn. “We hope to be able to use our OLED simulation tool to better analyze our experimental results and to develop models that predict the performance of OLEDs. These models can then be used to develop OLEDs with both long lifespan and high efficiency. It will also give more fundamental physical information about how OLEDs work at the molecular scale. This is of great value for science and industry at the same time.”

When improving OLEDs, there are a lot of aspects that need to be taken into account. Coehoorn: “You have the physics of the processes occurring in OLEDs, but you cannot forget about the science of the materials, for example. That is why we’re doing this research in ICMS, as there are colleagues who know exactly how the materials behave.”

The bigger picture

Coehoorn: “Of course, as a scientist, I’m curious about how nature works. That question is too broad for one person to answer, but you can work on a little part of it. But I think it is also very important to keep the bigger picture in mind. Why are you looking into this one aspect? Is this really the most important thing to do? And what will be the longer-term impact of our research program?”

In keeping his eye on the bigger picture, Coehoorn noted that their work on OLEDs can have applications in other fields as well. “If we figure out a combined experimental and computer simulation approach to understanding OLEDs in all their complexities, we might use that approach to understand other complex organic systems as well,” states Coehoorn. “Which elements interact and how? That is what we want to know.”

Outside the TU/e

Reinder Coehoorns work is broader than the university in Eindhoven. He is a Distinguished Professor at the Electronic Paper Display Institute in Guangzhou, China, where he will be starting a group to work on the development of flexible OLEDs. Closer to home, Coehoorn is very active on the board of NanoNextNL. He is engaged with the development of a long-term Dutch program for nanotechnology, which has some distinct focus areas. “For example: nanotechnology for nanofabrication, clean energy, reduced energy consumption, medical systems, and food. We need to keep our knowledge infrastructure up-to-date in order to maintain our leading position.”

More about this research

P. Bobbert, R. Coehoorn, Europhysics News 44 21-25 (2013)

M. Mesta, M. Carvelli, R.J. de Vries, H. van Eersel, J.J. van der Holst, M. Schober, R. Coehoorn e.a. Nature Materials, 12, 652-658 (2013)

FACTS

The light-emitting layer in an OLED can be as thin as

100 nanometers

Organic transistors and

organic solar panels

are under development

/ Remco van der Hofstad

Dealing with variability and modeling complex networks

The group of probabilist Remco van der Hofstad works on two related subjects: first they are investigating various problems in which variability is central, and second they study complex networks. Probability is the common aspect of these two subjects.

FACT

The brain can be seen as a complex network because it contains some

100 billion neurons

that are connected to one another

"For a mathematician, the spreading of a ***rumor***, a viral marketing campaign and the **SPREADING OF A DISEASE** basically look the same."

Complex networks can describe a variety of systems such as the Internet or the brain. Research in complex systems focuses on how the network structure influences behavior in such networks: how fast will something – such as a rumor or a disease – spread in a network and how does this depend on network characteristics? Or, how can the human brain learn how to speak again after someone has had a stroke? Even though the networks are quite different, questions such as these can be solved in the same way at a mathematical level. Van der Hofstad and his colleagues investigate these systems to see how network properties might influence the bigger picture.

Variability issues

Researchers working with Van der Hofstad do more than just study complex networks, however. Their work can be of benefit to electrical engineers and physicists, for example, in solving probability problems. Reality is not always the same as theory. Experiments always contain variability, and these natural fluctuations in a system have to be taken into account appropriately. For example, Van der Hofstad's group collaborates with chemists at ICMS working on molecular chemistry. In their experiments, the chemists expected to observe a certain molecular exchange in a 2D supramolecular fiber. Instead, they found something much more random. Thus, they wanted to know the origin of this random behavior, and as a result turned to Van der Hofstad and one of his former-PhD students Robert Fitzner for help.

Helping to find the answer

Van der Hofstad, with his intuition for probability, notices that the behavior was indeed random, but crucially not independent. This is highly confusing for non-mathematicians, but in effect it means that the process had more inherent structure than expected. Fitzner extracted key characteristics from the system and used them in the design of a computer simulation. This allowed him to test the influence of certain exchange patterns within the system on the random behavior. By comparing the simulation results (if the process works this way, the result should look like that) to the results of the laboratory experiments (it looks like this), the chemists could rule out some of the predicted molecular exchange patterns along the fiber as the origin of the random response in the system. In fact, the simulations did not match the chemist's expectations which were based on existing experimental literature. This finding eliminated proposed causes while helping the researchers to focus on the exact causes of this unexpected behavior.

Model versus reality

The model built by Van der Hofstad and Fitzner is simpler than reality, but that is the very definition of a model. It is often irrelevant that a model is not precisely correct – what is more important is that the model is useful. Sometimes, a model can provide you with insight that a real experiment cannot. This is why Van der Hofstad and his colleagues encourage researchers to knock on their doors if they have questions about complex networks or variability.

More about this research

L. Albertazzi, D. van der Zwaag, C.M.A. Leenders, R. Fitzner, R.W. van der Hofstad, E.W. Meijer, Science 344, 491-495 (2014)

R.W. van der Hofstad, Random Graphs and Complex Networks Vol. I. Book, will be published summer 2016

EPL Update

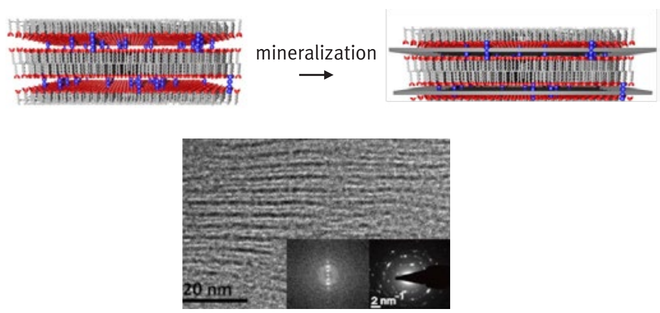
Multi materials and additive manufacturing programs kicked off

The board of the Eindhoven University of Technology recognizes the significant industrial bilateral contracts in the field of polymer science and technology and has awarded the Eindhoven Polymer Laboratories (EPL) with € 1,8 million Impuls funding to support interdisciplinary and interdepartmental research in two programs, “Multi Materials” and “Additive Manufacturing.”

Multi materials

In the program “Multi Materials,” EPL has defined five challenging projects that connect different methodologies and expertises. Two projects are led by research groups in Chemical Engineering and Chemistry. In the first project the researchers propose to use synthetic organic matrices to generate hybrid ultrathin, quasi-2D crystals of zinc oxide within a responsive hierarchically-organized organic matrix to study and exploit their piezo-electric and optoelectronic properties. This approach will provide a generic route with tunable dimensions regardless of the specific chemistry and conventional crystal habits of the material. The second project aims at developing theory for multi-component supramolecular systems where one of the components is capable of forming one-dimensional supramolecular polymers that can selectively bind each other. Applications will involve mixing these structures with other structures such as polymers and nanoparticles. Are mixtures of supramolecular systems with other components stable? The groups will hence work on theory for predicting the phase stability.

The physics department will focus on research on vitrimers, which are an exciting new class of polymer networks in which the crosslinks are dynamic by means of a connectivity-preserving exchange mechanism. While different exchange materials may provide higher-



Ultrathin quasi-2D Bottom: TEM image showing ultrathin $CaCO_3$-infiltrated smectic layers. Inset left: FFT revealing a layer spacing of ~6.4 nm and a crystal thickness of ~2 nm; Inset right: electron diffraction pattern showing crystallization of the initially amorphous film (Sommerdijk / Schenning groups, rsc advances 2016) performance alternatives to many current polymer materials, their combination of (re)formability and toughness renders them particularly interesting as base materials for additive manufacturing. This links directly to the EPL's research efforts in additive manufacturing. Biomedical researchers will apply layer-based material processing to create biodegradable, self-expandable stents. Again, supramolecular technology provides the toolbox to embed functionalized building blocks into the materials. In this way, tissue regeneration can be controlled by which specific cell types can be captured from the blood to steer healthy vascular regeneration. However, the effects of these layer-based methods on the mechanical integrity of the resulting stents need to be further studied.

Researchers in mechanical engineering will focus efforts on producing polymeric systems for effective and efficient EMI shielding by using functionalized two-component multi-layer systems in which both components consist of a similar PMMA matrix, but one is enriched with conductive fillers such as carbon nanotubes or graphene sheets. A key question in this project is whether EMI shielding efficiency remains present while the material is strained. This aspect will be investigated by in-situ conductivity and EMI shielding characterizations during material extension.

Additive manufacturing

Additive manufacturing techniques are revolutionizing the way that 3D polymeric objects with complex shapes are being produced. The eight PhD students in this program, working in EPL groups in the Mechanical Engineering (W) and Chemical Technology departments (ST) are developing basic academic knowledge that will improve 3D printing processes and help bring applications to market. Projects range from investigating fundamental material and rheological properties, material characterization, and development of novel printing materials.

Two of the students, Eveline Maassen (ST) and Rosaria Anastasio (W), work closely together with a team at TNO to improve materials and processes for stereolithography. As a resin is cured layer by layer in this photopolymerization technique, the material is prone to building up stresses during the polymerization. Eveline will focus on the elimination or at least mitigation of this stress, while Rosaria will focus on the careful analysis of the intrinsic mechanical properties of single and multiple layers of the printed materials.

Other projects concentrate on the experimental characterization and computational modeling of the sintering process in selective laser sintering (SLS). Although this technique is widely used, the fundamentals of the sintering process are still poorly understood. Two PhD projects (W), one with an experimental focus and the other with a modeling focus, aim at a fundamental understanding of the particle fusion process, which could ultimately lead to improvements in the process and resulting products. In order to better understand the material behavior before and after sintering, a parallel project (W) has started on the investigation of the intrinsic mechanical properties and possible morphologies of melt-processed and sintered nylon-12, one of the most widely used polymers in SLS.

All in all, both programs have a coherent package of research topics from which we expect to see exciting new science and technology.

Eveline Maassen and Rosaria Anastasio analyze photopolymerization products at the Multi-Scale lab of Mechanics of Materials

NEWS, AWARDS & GRANTS

ERC Starting Grant for

TOM DE GREEF

Tom de Greef has been awarded a Starting Grant of some € 1.8 million by the European Research Council (ERC). De Greef's work concentrates on synthetic biology, a field in which he is working on a method for the quicker reprogramming of cells.

Tom de Greef will be working on a method to significantly accelerate research in the field of synthetic biology. Synthetic biology concerns reprogramming cells so that they can exercise other functions, for example for medical purposes. Currently, researchers constantly make minor adjustments to the biochemical networks of the cell and then examine the effects. This time-consuming procedure in general takes several weeks.

De Greef wants to take some of this research outside of the cell itself, bringing the biochemical networks outside the cell in order to subsequently optimize the molecular interactions so that they are much faster by using the very latest microfluidic methods. Then by placing the biochemical networks back into the cell, he can see whether they behave similarly there. He hopes that the reprogramming of cells for therapeutic applications can be accelerated in this way. It is also an approach that provides more insight into the molecular processes and the information-processing behavior of biochemical networks in the cell.

BERT MEIJER

elected as AAAS Fellow

The American Association for the Advancement of Science (AAAS) Council elected 347 Fellows during 2015, in recognition of their contributions to innovation, education, and scientific leadership. Bert Meijer has been acknowledged for his contribution to advancing science in chemistry and has therefore been elected as an AAAS Fellow.

The AAAS is an international non-profit organization dedicated to advancing science for the benefit of everyone.

500TH ICMS

affiliated paper published

Since its start, ICMS keeps a list with publications which are published with ICMS as (co-)affiliation. October last year we reached the 400th ICMS publication and now we can announce that the 500th ICMS publication has recently been published in PNAS magazine. Congratulations to Ilja Voets and co-authors!

L.L.C. Olijve, K. Meister, A.L. DeVries, J.G. Duman, S. Guo, H.J. Bakker, I.K. Voets, Blocking rapid ice crystal growth through nonbasal plane adsorption of antifreeze proteins, Proc. Nat. Ac. Sci. U.S.A. published online (2016).

THESES ICMS

November 2015 – March 2016

1

Mechanochemical scission of transition metal-ligand bonds in coordination polymers

Abidin Balan

November 11, 2015
PhD advisors:
prof.dr. R.P. Sijbesma
& prof.dr. E.W. Meijer

2

Device physics of organic light-emitting diodes: interplay between charges and excitons

Harm van Eersel

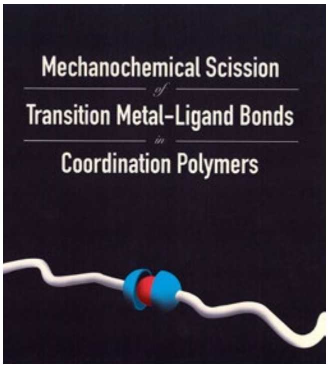
November 16, 2015
PhD advisors:
prof.dr. R. Coehoorn
& prof.dr.ir. R.A.J. Janssen

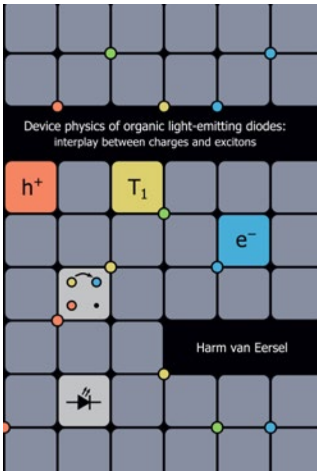
3

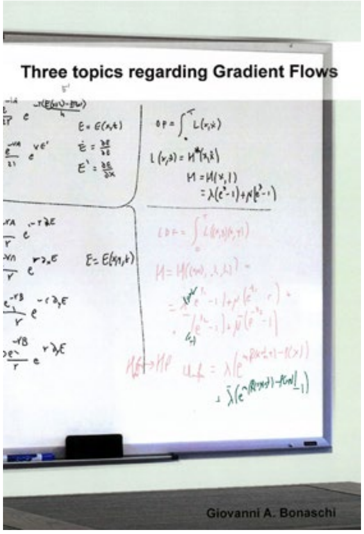
Three topics regarding Gradient Flows

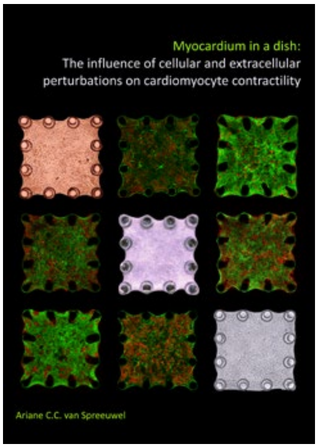
Giovanni Bonaschi

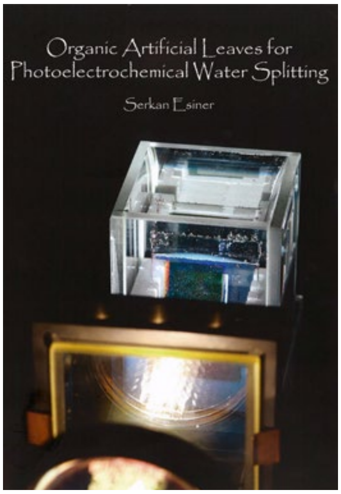
November 23, 2015
PhD advisors:
prof.dr. M.A. Peletier
& prof.dr. G. Savaré

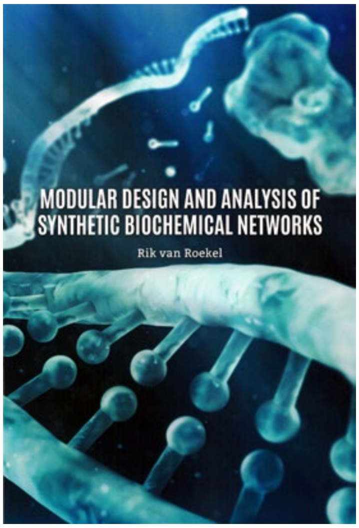












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Myocardium in a dish: The influence of cellular and extracellular perturbations on cardiomyocyte contractility

Ariane van Spreeuwel

November 24, 2015
PhD advisors:
prof.dr. C.V.C. Bouten
& dr. N.A.M. Bax

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Organic artificial leaves for photoelectrochemical water splitting

Serkan Esiner

December 9, 2015
PhD advisors:
prof.dr.ir. R.A.J. Janssen
& dr.ir. M.M. Wienk

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Modular design and analysis of synthetic biochemical networks

Rik van Roekel

December 10, 2015
PhD advisors:
prof.dr. P.A.J. Hilbers
& dr.ir. T.F.A. de Greef

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Towards a tissue engineered heart valve for life

ir. Bart Sanders

January 14, 2016
PhD advisors:
prof.dr.ir. F.P.T. Baaijens
& prof.dr.dr. S.P. Hoerstrup

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Microfluidics for cell analysis applied to study cell mechanics and high throughput screening

Guansheng Du

January 12, 2016
PhD advisors:
prof.dr.ir. J.M.J. den Toonder
& prof.dr. Q. Fang

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Out-of-cleanroom magnetic artificial cilia

Ye Wang

January 14, 2016
PhD advisors:
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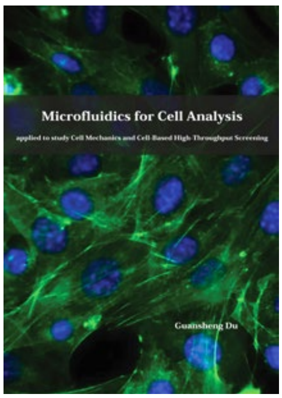
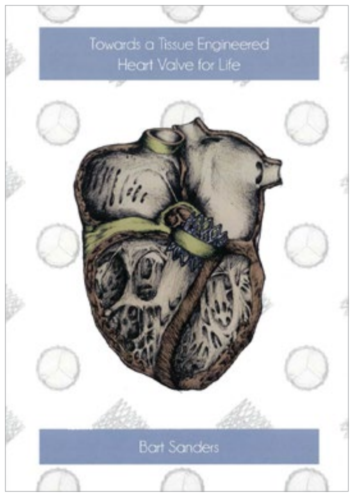
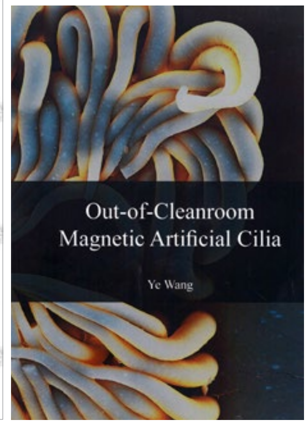
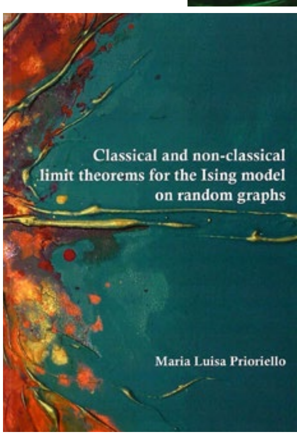
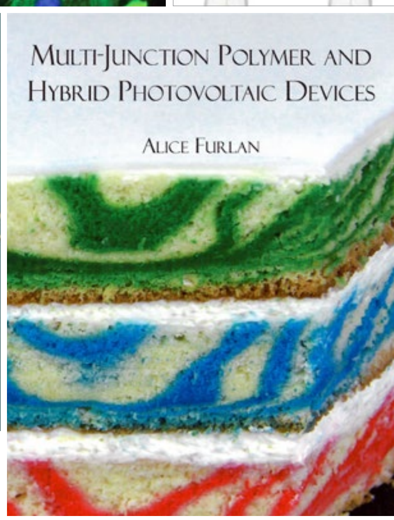
& prof.dr.ir. P.D. Anderson

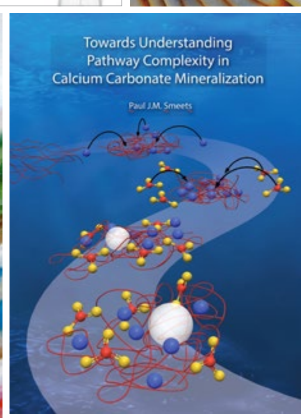












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Classical and non-classical limit theorems for the Ising model on random graphs

Maria Luisa Prioriello

January 27, 2016
PhD advisors:
prof.dr. R.W. van der Hofstad
& prof.dr. C. Giardina

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Multi-junction polymer and hybrid photovoltaic devices

Alice Furlan

February 25, 2016
PhD advisors:
prof.dr.ir. R.A.J. Janssen
& dr.ir. M.M. Wienk

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Towards understanding pathway complexity in calcium carbonate mineralization

Paul Smeets

March 9, 2016
PhD advisors:
prof.dr. N.A.J.M. Sommerdijk
& dr. J.J. De Yoreo

Institute for Complex Molecular Systems

New technologies by mastering complexity

Mastering complexity requires a deep understanding on how matter – both natural and artificial – self-organizes into functional molecular systems. The Institute for Complex Molecular Systems, established in 2008, brings together mathematics, physics, biology, chemistry and engineering to stimulate education and research in this emerging field of science. Interdisciplinarity is the core of ICMS; with the input from leading specialists in different branches, new avenues are explored. Our mission is to be a leading institute for research and education in the engineering of complex molecular systems.
We do this via:

- Performing top research
- Training of talented young scientists
- Being the hotspot for interdisciplinary science activities of TU/e
- Foundation and housing of the Advanced Study Center

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2. Bio-inspired engineering (program leaders prof.dr.ir. Menno Prins and dr.dr. Patricia Dankers)
3. Complexity Hub (program leaders prof.dr. Rutger van Santen and prof.dr. Mark Peletier)

ICMS hosts the *Advanced Study Center*. This serves as an intellectual home to scientists from all over the world, hosting discussions on the theme of complexity. It is the home of *Eindhoven Multiscale Institute* (EMI) and *Eindhoven Polymer Laboratories* (EPL).

We aim at offering an ideal training environment for young students and scientists to prepare themselves for a career in science and engineering in a world of increased complexity. Therefore, master and PhD students can participate in *certificate programs*, in addition to their departmental programs. The relationship with industry is strengthened via the *Industrial Consortium* – where science meets innovation.

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.

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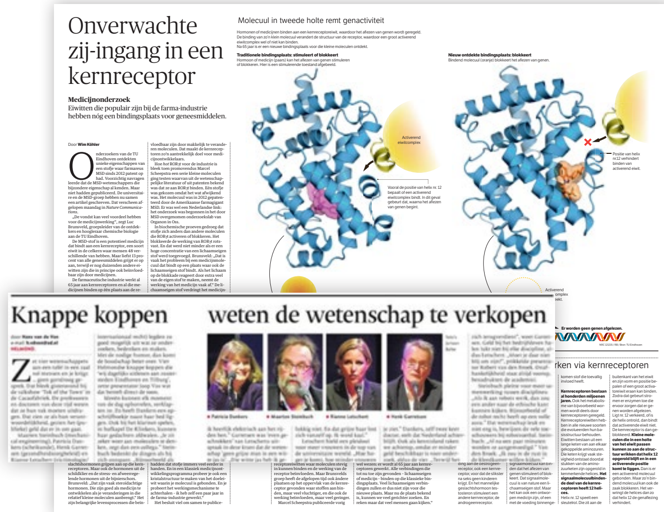
Onverwachte zij-ingang in een kernreceptor

Medicijnonderzoek
Eiwitten die populair zijn bij de farma-industrie hebben nóg een bindingsplaats voor geneesmiddelen.

Molecuul in tweede holte remt genactiviteit

Knappe koppen weten de wetenschap te verkopen

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

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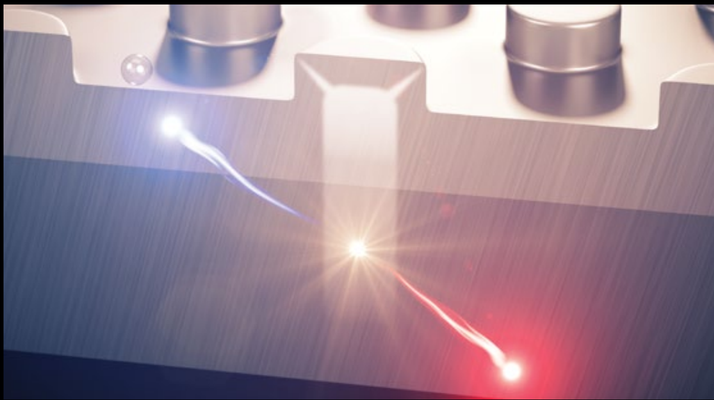
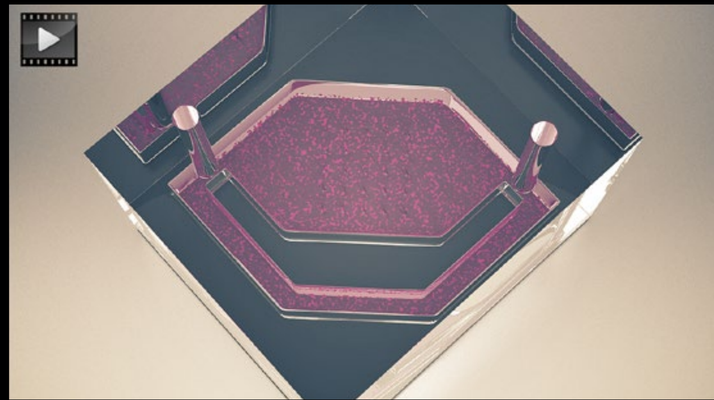
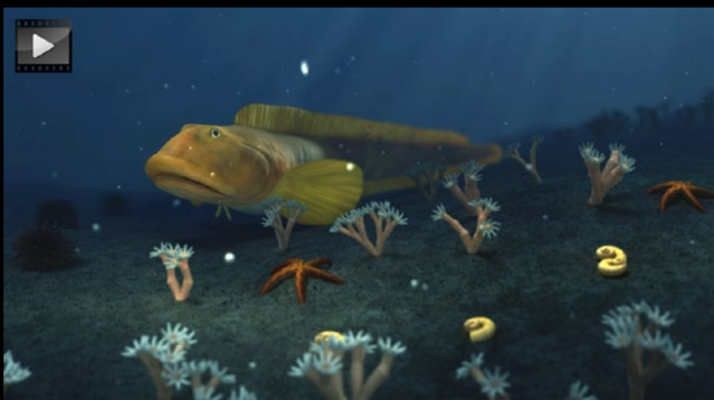

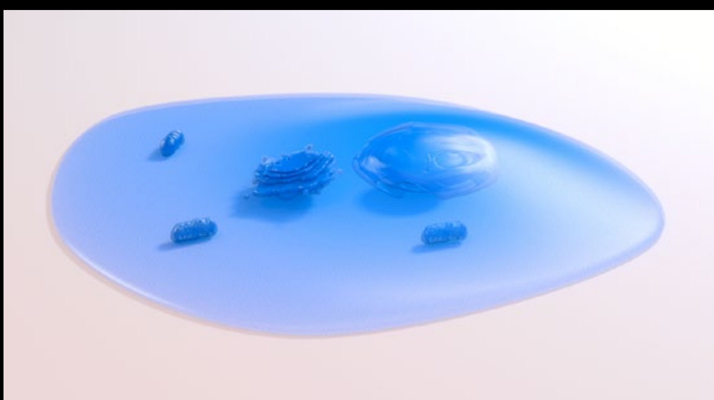

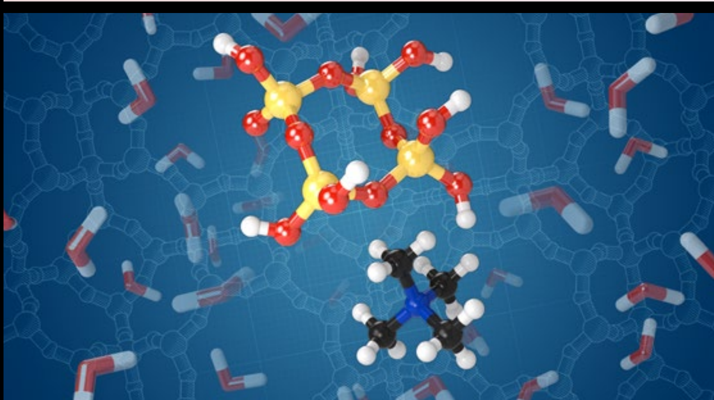
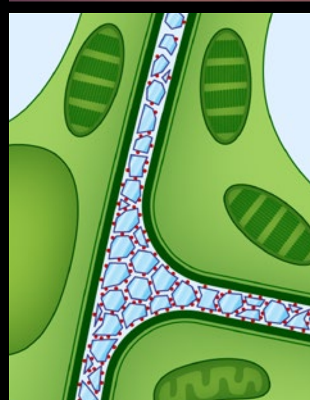

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