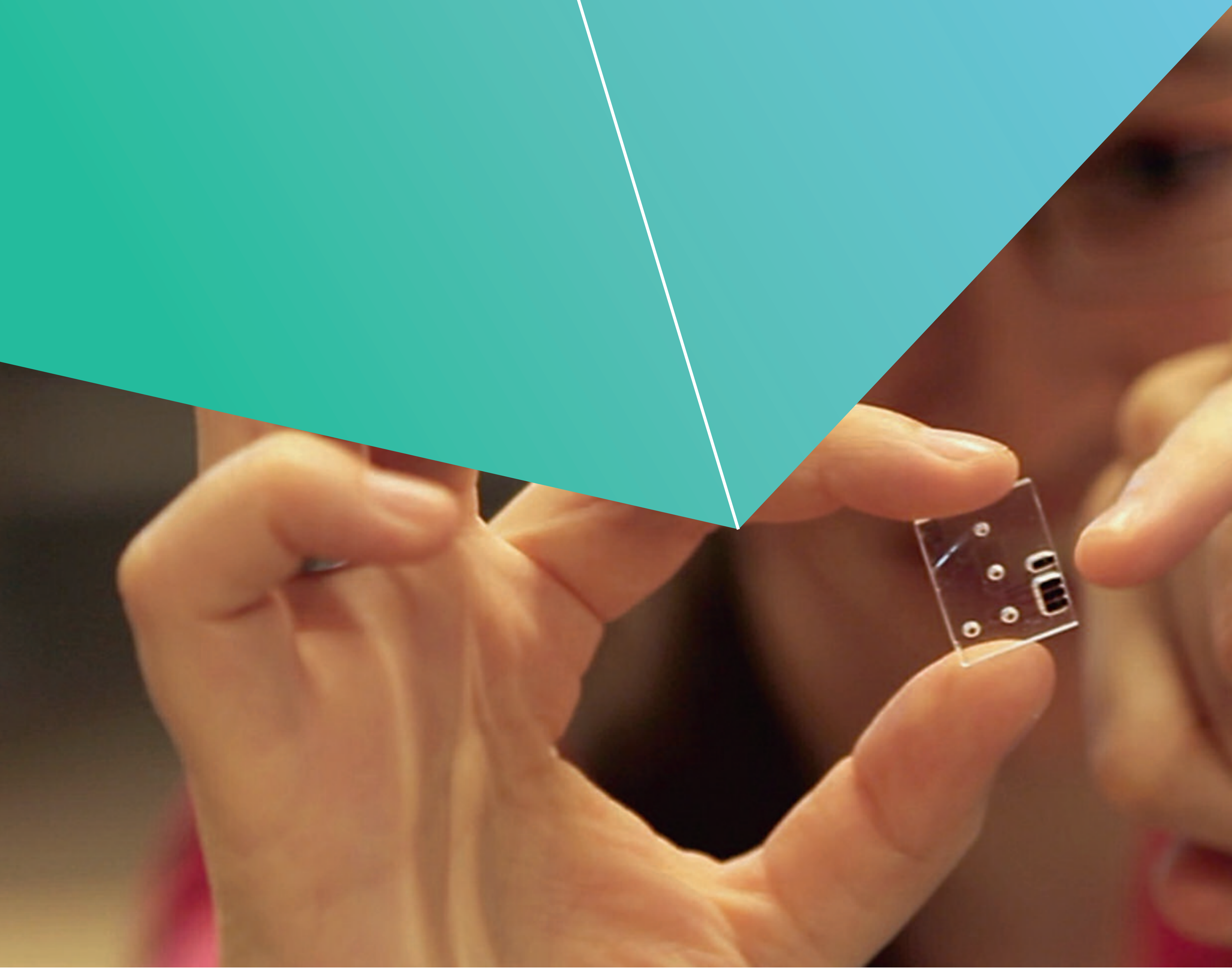
Where different worlds meet

MCEC OVERVIEW 2014 - 2015



MCEC

Netherlands Center for
Multiscale Catalytic Energy Conversion

Where different worlds meet

MCEC OVERVIEW 2014 - 2015

MCEC
Netherlands Center for
Multiscale Catalytic Energy Conversion

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"MCEC brings together a diverse range of scientists around one of the grand societal challenges: energy conversion."

By working on a multiscale science approach in the field of catalysis, chemists, physicists and engineers can bridge ten order of magnitude in length scales when connecting reactors with the intricate details taking place at the level of single atoms and molecules in individual catalyst particles.

We proudly present in this first MCEC report an overview of the various activities that we have developed during the first two years of our new research program. At the same time the report gives an idea about how we intend to move forward in building this research community.

This collaborative approach also explains why we invested a great part of the first years to build a solid basis for this curiosity-driven research program. We focused on setting up the content of the program in terms of specific research projects and project clusters, and fostering relationships among the MCEC members. This approach not just helped at the start of the projects, but also initiated a lot of scientific discussions.

After two years we now see that knowledge exchange among our members and students becomes more intensive and that new scientific collaborations have started. We believe that these scientific interactions will become even stronger in the years to come.

On behalf of the MCEC Management Team,

Prof. Bert Weckhuysen
Scientific Director

About MCEC

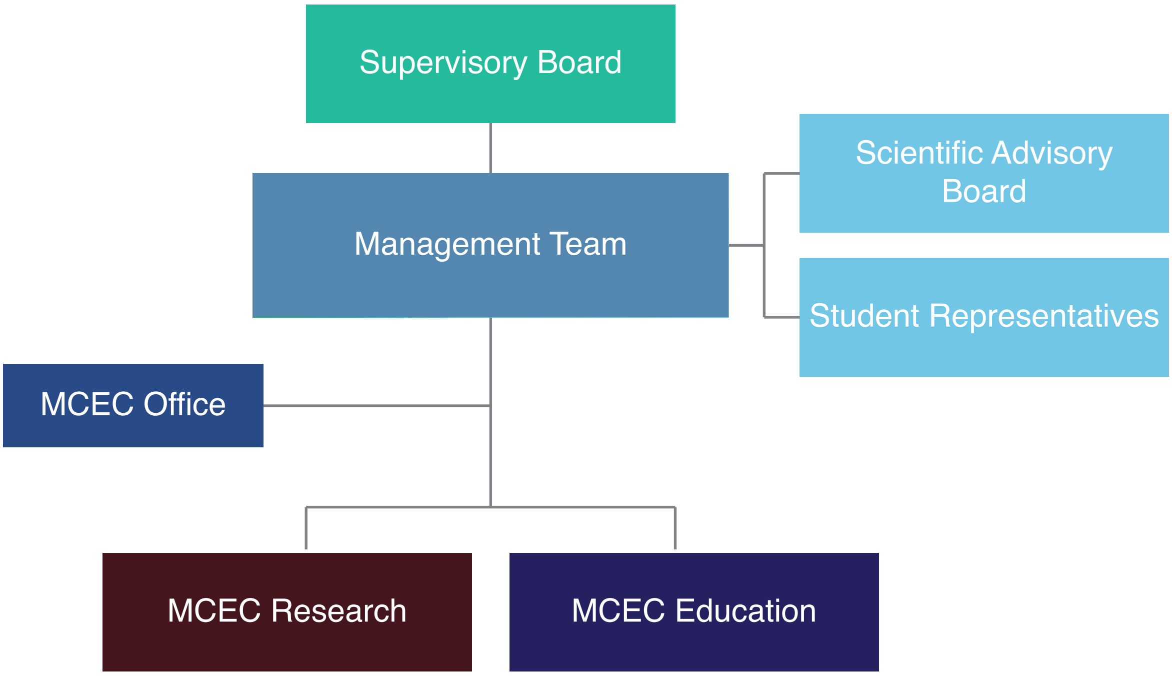
"Catalysis is an interdisciplinary science. Bringing scientists with different backgrounds together, provides ample opportunities to make new scientific breakthroughs."

The wish for a sustainable world has become indispensable in our society. Within MCEC, chemists, physicists and engineers join forces to tackle one of this century's most challenging questions: How can we make our energy carriers and materials in a more sustainable manner?

Catalysis is an essential part of that answer. Our research program on Multiscale Catalytic Energy Conversion, named MCEC, aims to develop novel as well as more efficient catalytic processes to produce the fuels and materials of the future. The research takes place at all relevant scales, from atoms to reactors, and intends to provide the scientific basis for redesigning the traditional chemical processes.

MCEC not only combines three scientific disciplines of chemistry, physics and engineering, but the program also interconnects around fifty talented researchers, internationally renowned seniors and up-and-coming juniors, of the three universities involved: Utrecht University (UU), Eindhoven University of Technology (TU/e) and University of Twente (UT). The program has the added advantage of being at the center of their long-term research strategies: Sustainability (UU), Energy (TU/e) and Nanotechnology (UT).

Key to the success of MCEC, we believe, lies in scientific collaboration beyond the existing boundaries of disciplines and institutions. That's why we stress the importance of multidisciplinary research and education. We find it important to equip our researchers with a broad set of skills, knowledge and experience. And as a long-term goal, we want to contribute to the training of a new generation scientists and engineers, who will proceed their careers in academia or in the industry, thus contributing to a more sustainable society.



In short, MCEC aims to:

- provide a world-class research environment with expert guidance;
- facilitate effective interaction and free exchange of knowledge and information within the center; and
- attract, educate and inspire the most talented researchers.

In doing so, MCEC aims to be more than a research center: it is a platform where promising ideas can be initiated and shaped, and where collaborations come into being.

The developed experimental and theoretical methods, and related base knowledge, will not be limited to catalytic energy conversion routes. They're also highly relevant and equally applicable to other research fields, such as that for fuel cells, batteries, diagnostic devices, photonic and plasmonic devices, nanoscale electronics, drug delivery systems and energy conversion and storage materials. Therefore, we expect that the scientific breakthroughs within our program will lead to knowledge utilization in other fields of science as well.

MCEC is a so-called Gravitation Program: a ten-year research program, directly funded by the Dutch Ministry of Education, Culture and Science (OCW). A Gravitation Program brings the best researchers in the Netherlands together in consortia; renowned scientists who have carried out innovative and influential research in their field. In the case of MCEC, it provides the partners of UU, TU/e and UT with a unique opportunity to do fundamental research related to catalysis - thus establishing a long-term and strategic collaboration in the field of chemical conversion processes, to be able to produce the fuels, chemicals and materials of the future.

MCEC is led by the Management Team (MT) that is chaired by Scientific Director Prof. Bert Weckhuysen (UU) and supported by Managing Director Emke Molnar (UU) and MCEC office. The MT meets five times a year and is responsible for the overall management of the MCEC program, while the Supervisory Board (SB) - consisting of the representatives of the three participating universities – monitors the progress of the program.

In the fall of 2014, MCEC established a Scientific Advisory Board (SAB), which provides advice and recommendations to the Management Team regarding the short and long-term plans and activities of the program. The seven SAB members cover the different disciplines in the program, and are experienced in setting up and/or leading multidisciplinary consortia.

Management Team

Prof. Bert Weckhuysen (Utrecht University)
Scientific Director

Prof. Alfons van Blaaderen (Utrecht University)

Prof. Rutger van Santen (Eindhoven University of Technology)

Prof. Hans Kuipers (Eindhoven University of Technology)

Prof. Detlef Lohse (University of Twente)

Prof. Albert van den Berg (University of Twente)

Supervisory Board

Prof. Gerrit van Meer (Utrecht University)
Dean Faculty of Science

Prof. Frank Baaijens (Eindhoven University of Technology)
Rector Magnificus

Prof. Dave Blank (University of Twente)
Chief Scientific Ambassador

Scientific Advisory Board

Prof. Gert-Jan van Heijst (Eindhoven University of Technology)
Chairman

Prof. Klavs Jensen (Massachusetts Institute of Technology)
Vice-chairman

Prof. Daan Frenkel (University of Cambridge)

Prof. Lynn Gladden (University of Cambridge)

Prof. Jacques Magnaudet (Institut de Mécanique des Fluides de Toulouse)

Prof. Jens Nørskov (Stanford University)

Prof. Robert Schlögl (Fritz Haber Institute of the Max Planck Society)

2016 →→ Prof. Emiel Hensen (Eindhoven University of Technology) will join the Management Team.
2016 →→ Prof. Unni Olsbye (University of Oslo) will join the Scientific Advisory Board.

Yearly meetings

Board meetings

Both the Scientific Advisory Board and the Supervisory Board are scheduled to meet once a year. The first SAB meeting was in November 2015. The first SB meeting is planned for 2016.

Strategic meeting

Our MCEC members are the principal scientists who supervise PhD and/or PD projects. Once a year, the MCEC MT and members meet to discuss their view on our program. The main goal of these Strategic Meetings is to update all parties involved about important scientific and/or organizational subjects, and to share ideas about possible activities and future developments. The Strategic Meeting is always combined with one of the three other yearly meetings:

MCEC Annual Meeting

Around April, during a two-day retreat, our PhD's and PD's present their research and future goals with an individual pitch and poster.

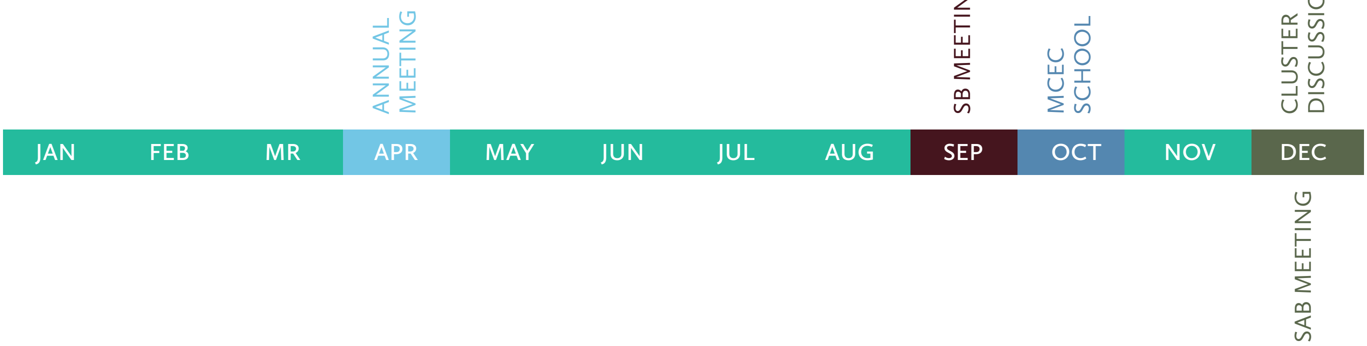
MCEC Cluster Discussions

The PhD's and PD's discuss their work and scientific collaborations along the framework of the MCEC project clusters (see page 21). This two-day event usually takes place in December.

MCEC School

MCEC School is an integrated, five-day program with 6 ECTS (2 ECTS each yearly, with a certificate of attendance). The first MCEC School was held in October 2015 and will be followed by a second and third MCEC School in respectively 2016 and 2017 (read more on page 38).

Yearly meetings



MCEC community

MCEC is a consortium of both young and more established researchers with various scientific backgrounds, working together in our interuniversity research center to conduct excellent research. That requires a strong network and the organization of a wide range of communal activities.

It is therefore important that such activities are initiated, organized and facilitated by the MCEC Office, with the direct involvement of MCEC members. Since collaboration is key, we've launched lab tours as an integrated part of our program. Community members visit each other in their work environment to gain more insight in their respective expertise and also to get acquainted with the facilities and instrumentation available in Eindhoven, Enschede and Utrecht. Scientific lectures are part of the lab tour as well.

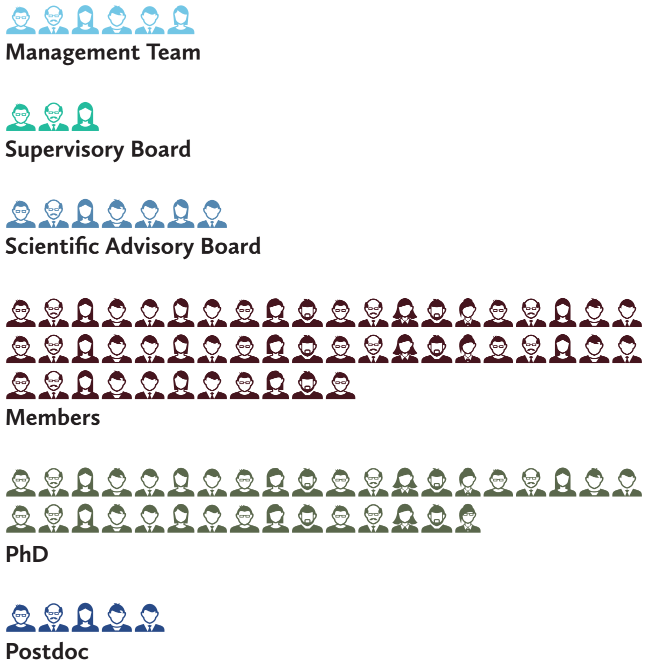
These kind of activities enable members to form (and feel part of) a community. Regularly, there are also local meetings at the three MCEC locations. These small gatherings mostly focus on a certain research topic, theme or discussion. During the lab tours and other meetings, our community members get the chance to come to know one another better, to exchange knowledge, to develop new ideas – and of course to see the possibilities that collaboration can offer.

Our community stays informed via 'MCEC Matters', our internal digital newsletter, and 'MCEC Management Matters', a short summary of the topics discussed during the MT meetings. By doing so, we aim to create an open as well as transparent research consortium.

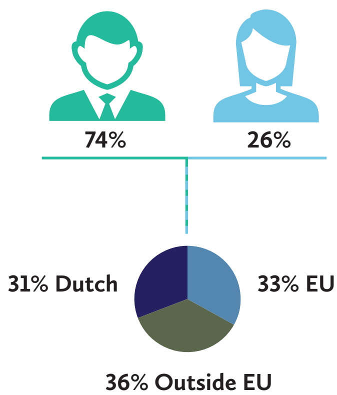
Diversity

We do believe that we should stay aware of both cultural and gender diversity within our program; whether it be on a representational and organizational level, or in recruitment and selection. We hope for example that visible female role models make for a higher number of female PhD candidates. Therefore, we invite and encourage female MCEC members as well as members with different cultural backgrounds to take place in our teams, so they become more visible in the community and get responsibility on specific subjects of advice to the MT.

MCEC community



PhD's and Postdocs

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MCEC teams

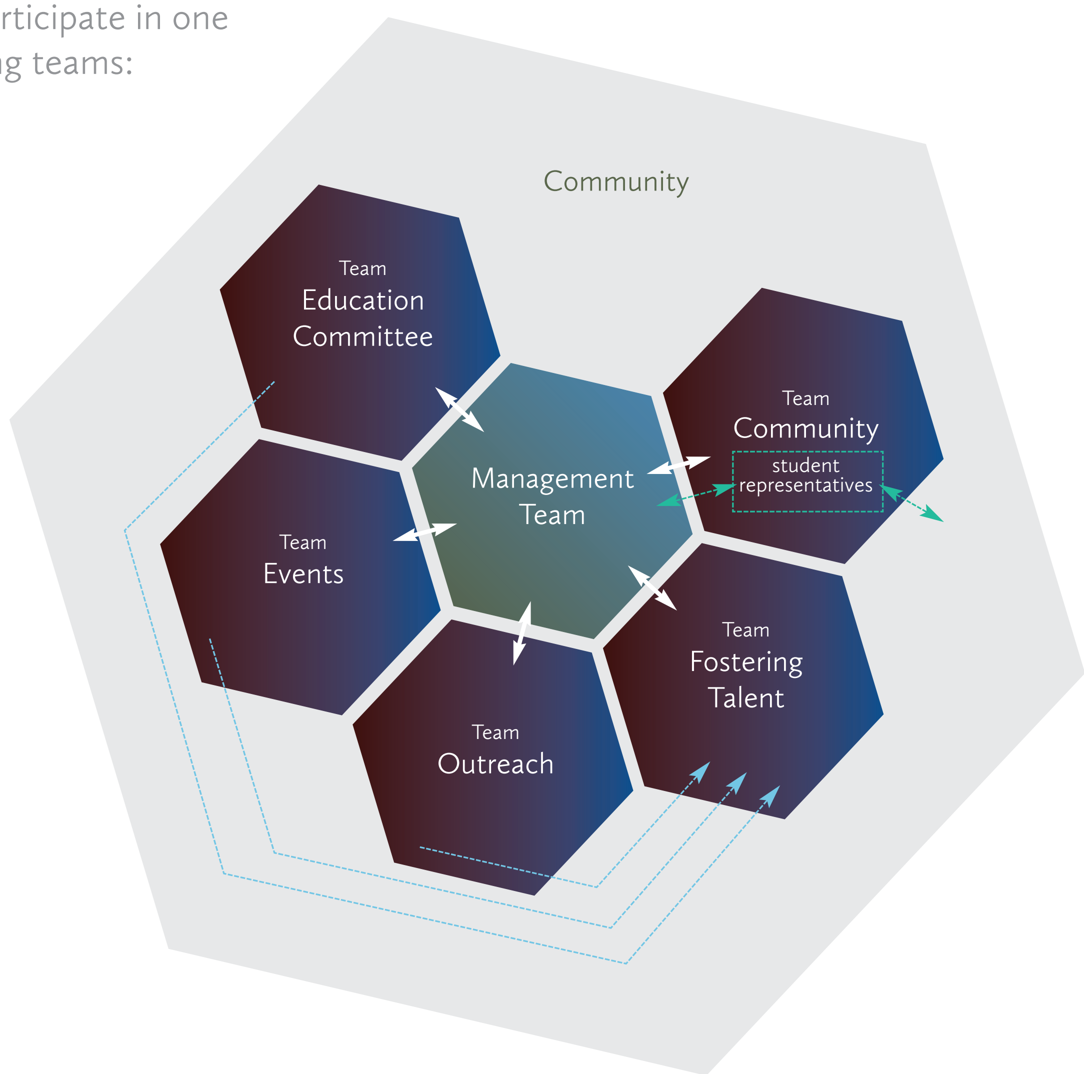
Meaningful collaborations don't arise out of nowhere. To get a grasp of the possibilities and to be inspired, getting to know one another personally and professionally is one criterium, being aware of the available knowledge and facilities is another. We can make sure the conditions to do so are there. But in the end, the creative thinking required for the challenging scientific research MCEC takes on, cannot be enforced top-down.

That's why we find it important that our community is involved in the organization of the MCEC program. We want them to learn different aspects of working in and running a multidisciplinary program like MCEC, and feel a sense of responsibility for the program's success. We ask them to think about (and share) new ideas that are not solely concerning their own scientific research. Whether it be organizing a lab tour, finding ways to encourage and reward

"The challenge of our team is to achieve a true community feeling, that should lead to a level of multidisciplinary collaboration within the larger frame of MCEC. We organize monthly informal Friday afternoon drinks, teambuilding exercises during the MCEC School, and excursions to interesting and for our research relevant companies. The power of Team Community is that it has a real bottom-up approach, as it is organized for and by PhD students. Our vision is that by creating a true MCEC team-spirit we will contribute to this program in a way that will lead to more than the sum of the individual PhD and PD projects."

MATHIEU ODIJK, CHAIR OF THE TEAM COMMUNITY

Members of the MCEC community participate in one of the following teams:



talent, communicating with the general public or enthusing young pupils for the field of science – it all belongs to being part of MCEC.

Teams were formed with balance in mind: in every team, members of the different disciplines and research groups are represented.

Team Community

Team Community has seven PhD members and is led by Mathieu Odijk (UT). Being one of MCEC's Assistant Professors on a tenure track position, Odijk plays an important role in our program. Team Community is responsible for organizing social activities, especially for the PhD's and PD's (which are supported by the MT with an allocated budget). They contribute to our internal newsletter 'MCEC Matters' with interviews and a current selection of interesting research papers. Two members of this team function as student representatives as well (see the facing page).

2016 →→ A special forum for scientific (but also non-scientific) discussions is in the making: an online application to support the discussions and knowledge exchange within the PhD community, as a means to enhance communication.

Team Education Committee

The Education Committee is chaired by Hans Kuipers (TU/e). This team of scientists was responsible for setting up and monitoring the first MCEC School (2015) and guided PhD students during their work on the case studies as tutor. Additionally, the team advises the MT on other education-related topics, such as how to foster multidisciplinary discussion among students and which (online) tools or work forms should be used for educational purposes.

2016 →→ The Education Committee will organize the following MCEC Schools in 2016 and 2017.

Team Events

The starting points of Team Events were: a) to facilitate interaction between different disciplines, groups and projects, b) to strengthen collaboration and stimulate new ones, c) to link PhD and PD projects to existing collaborations where needed, and d) to make suggestions about how to work towards joint projects and publications as tangible results. Team Events developed the concept, and helped to set up the program for the different science-related meetings; most importantly the yearly Annual Meeting, Cluster Discussion and Strategic Meeting. The team works closely together with the Managing Director on the program of these events as well as on the planning of the first open symposium.

2016 →→ In order to gain more focus and deepen the knowledge on a specific research topic, we will organize open symposia. The focus in these symposia lies on a multiscale and multidisciplinary approach, regardless of the scientific topic.

Team Fostering Talent

2016 →→ The activities of Team Fostering Talent will be developed and specified during 2016. This team is about initiating and working out ideas on how to attract and inspire talent and reward meaningful collaborations. MT member Albert van den Berg will lead this team.

Team Outreach

2016 →→ The first activities for Team Outreach, that will be led by Ivo Filot (TU/e) as one of MCEC's Assistant Professors, are planned for the end of 2016. This team will work out a plan for external communication and appearance and, even more important, for the involvement of our PhD students in outreach activities with focus on secondary school students. We believe that this specific target group is important to educate and stimulate to get inspired for (choosing) science. It also gives us the opportunity to train our PhD students in explaining complex research content to a general public, which is increasingly important in the career of a scientist.

Student representatives

Anne-Eva Nieuwelink (UU) and Aditya Sengar (TU/e) are MCEC's student representatives. They provide feedback to the MT about existing and planned activities, and thus effectively act as a sounding board for the MT. Their feedback and critical, but constructive approach are always very much appreciated because we fully believe our program benefits greatly from them.

Aditya Sengar (TU/e)

"MCEC needs proper communication channels among all of its members; between all disciplines, and at all levels. The PhD students are clearly at the heart of these scientific communication channels. They are the people that are growing their scientific knowledge and thus want to learn about the progresses in various research fields. With MCEC being a diverse community, I'm motivated to make sure that people from different aspects of science learn about other fields.

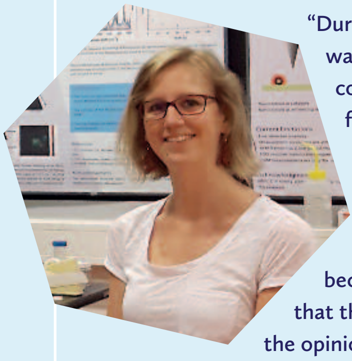
As student representatives, we've been asked to review the 2016 MCEC School, and to give suggestions on the layout of the plan and what type of lectures should be incorporated in the School. Also, the involvement in the outreach and fostering talent activities is something I'm really looking forward to. Spreading a message to our society, apart from the MCEC scientific community, and being able to communicate with them, is certainly a very important part in the development of all of us.

We aim at reaching a point where students working in one part of the country can efficiently communicate with the ones in the other part of the country without having to call upon their guides for this linkage. This requires relations to be built carefully by setting up meetings among student bodies with both a scientific perspective and a social event in mind.

At the moment, we're working on an internal forum to increase the interactions among all MCEC members. More importantly, it is necessary to make people aware of each other's work and how they can contribute, help or collaborate. Knowledge exchange should be the primary goal of our community here.

Sharing knowledge, materials and ideas has helped humans to deal with all kinds of social challenges and has enabled them to develop. Science is pretty similar to that. We need support from different fields to grow as a person both socially and professionally. Otherwise, the scientific knowledge gathered will always remain unidirectional."

Anne-Eva Nieuwelink (UU)



"During the first MCEC School there was a brainstorm about communication. I really liked the fact that communication between PhD students within the MCEC consortium is a key to its success. I volunteered to be a student representative because I believe it is very valuable that the MCEC staff members ask for the opinion of their PhD students. Since all the matters that we get to evaluate are there to improve our own skills, knowledge or research, I am convinced of the benefits of constructive feedback.

Aditya and I are asked to share our thoughts on, for example, potential activities of the new teams Outreach and Fostering Talent, and the program of the MCEC School. Instead of solely via email, the contact with the organization and scientific staff is personal. After last year's MCEC School, there were some points of improvement suggested by the PhD students. As student representatives we were glad to notice that the Education Committee implemented a lot of the community's suggestions when making their plans for the 2016 MCEC School.

Furthermore, I've been active as student representative without the MCEC staff specifically asking me for feedback. For example, I like to ask around how others are holding up with several issues. When I come across something of which I think the MT should know about, I report it.

For me, the most important part of being a student representative is to carefully think through what my own ideas are and, in addition, collect opinions from other PhD students. I hope to share the general opinion instead of bluntly giving my own. People often use the opportunity of feedback to push their own opinion through. However, that's not the idea of being a student representative. I would be very happy if the other PhD students know that I'm their student representative and come to me with their concerns, questions or suggestions."

Freddy Rabouw

Utrecht University
MCEC tenure track
Assistant Professor Multiscale Science on Heterogeneous Catalysis

“Starting January 2017, I will be working with both physicists and chemists. My background has been a combination of these two fields: I have worked with fast and intense lasers to study the properties of materials (physics), but also on developing new methods for nanoparticles synthesis (chemistry). This has taught me to ‘speak both scientific languages’. Within the MCEC program I will act as a bridge between chemists and physicists. I hope to learn more from both sides, about heterogeneous catalysis as well as studying chemical reactions from chemists, and about material self-assembly and fluid dynamics from physicists.

As a first research project, I will develop spectroscopic techniques to study catalyst materials and chemical reactions on a wide range of time- and length scales, by combining pulsed lasers with microscopy. This will teach us how, when and where a solid catalyst does its job most efficiently, and thus how a solid catalyst should be designed ideally. I will start by immersing myself in the groups of Soft Condensed Matter and Inorganic Chemistry and Catalysis at Utrecht University, and also visit the MCEC research groups of the University of Twente and Eindhoven University of Technology. In this way, I will learn more about the possibilities and challenges within the MCEC program, and come up with concrete ideas for scientific collaborations.”

Read Freddy Rabouw’s entire contribution on his scientific research on page 42.

Overview 2014-2015

December, 2013
Funding decision
MCEC is officially announced as one of the Gravitation Programs. During the ceremony, Minister Jet Bussemaker (Education, Culture and Science) awards the main applicants of the MCEC program, who are the current members of the MT, with the Gravitation Grant.

March, 2014
Shaping the program
The most promising research topics to include in the program are discussed among the MT, MCEC members and other involved scientists of the participating universities. Specific attention is given to the multidisciplinary nature of the program, which is not only reflected in the scope of the research, but also in the way of guidance and supervision. By September 2014, 40 projects (35 PhD and 5 PD positions), categorized under 6 project clusters, are allocated.

August, 2014
Establishment of the Scientific Advisory Board
The SAB will provide advice and recommendations to the MT regarding the progress, and the short and long-term plans and activities of the program.

September 1, 2014
Official start of the MCEC program

November 5-6, 2014
MCEC kick-off
The opening symposium of MCEC is held at the 'Winkel van Sinkel' in Utrecht. More than a hundred guests are present. The launch is a two-day event, the second day for MCEC members only. During the Strategic Meeting they discuss their contribution to the program, the setup of the yearly succession of MCEC Schools, and the possibilities to strengthen existing and establish new scientific collaborations.

March-April, 2015
Community get-together at TU/e, UT and UU
In order to involve both MCEC members and students in our organization, Hans Kuipers (MT member and chairman of the Education Committee) presents the plans for the first MCEC School, and Emke Molnar (Managing Director) discusses the setup of the MCEC teams.

April, 2015
Mathieu Odijk appointed on MCEC position
Mathieu Odijk (UT) is appointed as Assistant Professor on Micro- and Nanodevices for Chemical Analysis, on an MCEC tenure track position.

June 10, 2015
First MCEC lab tour at UU
PhD's, PD's and MCEC members attend this one-day event, organized to bring the community together, to learn more about the different research topics and disciplines involved in the MCEC program, as well as to visit the facilities and research setups at each location.

June, 2015
Start-up of three MCEC teams
Of the five MCEC teams, the teams Education Committee, Community and Events are the first to start.

August 20, 2015
Second MCEC lab tour at UT

August 31, 2015
Visit of Minister Bussemaker

Minister Jet Bussemaker comes to Utrecht for a visit to the four NWO Gravitation programs coordinated by UU: MCEC, the Netherlands Earth System Science Centre (NESSC), Cancer Genomics Centre Netherlands (CGC) and the Consortium on Individual Development (CID). MCEC is the main organizer of this event.

October 12-16, 2015
MCEC School

The first MCEC School is held in Driebergen. This five-day program consists of several lectures of different disciplines, provided by MCEC members and invited guest lecturers from the Netherlands and abroad. Discussion sessions, case studies, teambuilding workshops and social activities are also part of the program.

November 30-December 2, 2015
MCEC at CHAINS

MCEC presents itself at CHAINS 2015 together with the other Dutch Gravitation Programs in the field of chemical sciences: the Research Center for Functional Molecular Systems (FMS) and the Institute for Chemical Immunology (ICI). Six MCEC members contribute to this event as keynote speaker, chair or regular speaker at several sessions, and six PhD students present their poster.

November 30, 2015
SAB and Strategic Meeting

SAB and MT come together and discuss the scientific themes, goals and program organization. This is followed by the second Strategic Meeting, in which the MT and members of the MCEC community discuss their view on the progress and development of the program.

December 7, 2015
Kick-off ARC CBBC

The Advanced Research Center Chemical Building Blocks Consortium (ARC CBBC) is officially announced by Minister Henk Kamp (Economic Affairs). The two Gravitation Programs MCEC and FMS form the scientific base of this new public-private partnership. Bert Weckhuysen and Ben Feringa (FMS) are the main initiators of this national research center. MCEC will follow up on the developments and strengthen the collaboration with ARC CBBC in order to facilitate knowledge transfer for its students and members.

December, 2015
Ivo Filot and Freddy Rabouw appointed on MCEC positions

2X

Ivo Filot (TU/e) is appointed on a tenure track position as Assistant Professor on Computational Catalysis. Freddy Rabouw (UU) is appointed on a tenure track position as Assistant Professor on Multiscale Science on Heterogeneous Catalysis (starting 2017).

January 15, 2016
Third MCEC lab tour at TU/e

Scientific staff positions

Our program has three tenure track Assistant Professor positions, which we consider as key positions. The aim is to embed the candidates in the universities for a longer term than the initial length of the MCEC program itself. Candidates are selected based on their scientific quality as well as on their ambition and ability to bridge disciplines and build new collaborations between the research groups in our program. The selected candidates will also be involved in the organizational aspects of the program. They have a key role in the community and the opportunity to develop their leadership skills in the challenging consortium that MCEC is. Learn more about our Assistant Professors Freddy Rabouw (UU) on page 12, Mathieu Odijk (UT) on page 18 and Ivo Filot (TU/e) on page 34.

Furthermore, at the end of 2014 the University of Twente appointed two part-time professors on an MCEC position:

- Prof. Xuehua Zhang (affiliated at RMIT University, Melbourne, Australia)
  Title of the position: Surface and Colloidal Science and Engineering
- Prof. Roberto Verzicco (affiliated at Tor Vergata, University of Roma, Italy)
  Title of the position: Simulation of Turbulence

Future plans

2016

Inventory of the research setups and instruments

MCEC technician Relinde Moes (UU) is going to conduct an inventory of the research setups and instruments which are used on the different MCEC locations and are therefore available for our members and students. This inventory contributes to our efforts to encourage further collaboration.

2016

Fourth tenure track Assistant Professor position

The Management Team aims to announce a fourth tenure track Assistant Professor position at the University of Twente.

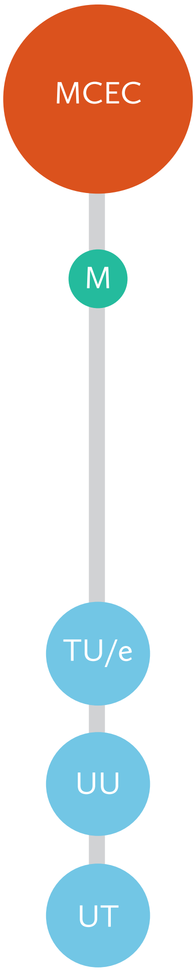
2016

MCEC Annual Meeting

All PhD's and PD's will present their individual project progress at the first MCEC Annual Meeting in April 2016. We will also present the first MCEC Poster Prize winner.

Finances

The funding for the MCEC program was awarded in the letter of the Dutch Ministry of Education, Culture and Science (OCW), dated December 13, 2013. The financial plan that the Netherlands Organisation for Scientific Research (NWO) - as the intermediate between the Ministry of OCW and the MCEC program - agreed on, contains the following budget:



Total € 31.967.200.000,-

Management and general activities

These costs consist of (e.g.):

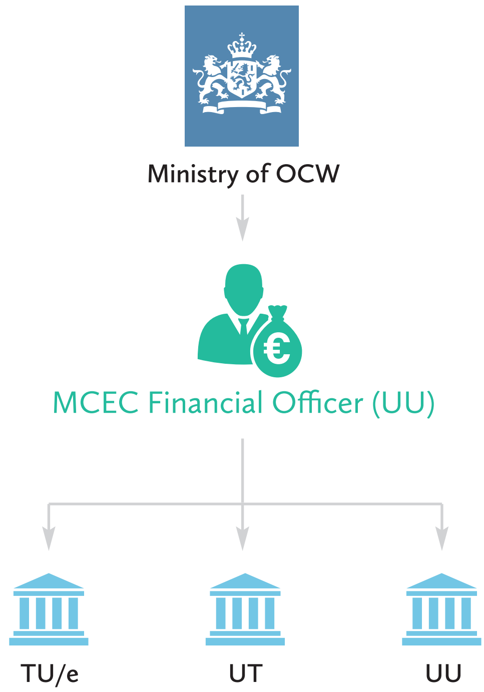
→ running the MCEC support office;
→ setting up the fostering talent program;
→ organizing meetings, workshops and Schools for the MCEC community;
→ investing in knowledge utilization and outreach activities.

Research and education

This amount is meant for:

→ appointing PhD's and PD's, including material budget and personnel education budget for each appointed person;
→ investments in new research setups and equipment;
→ the appointment of tenure track Assistant Professors including a start-up fund of € 100.000,- each.

The MCEC Financial Officer coordinates the budget payment between:



Mathieu Odijk

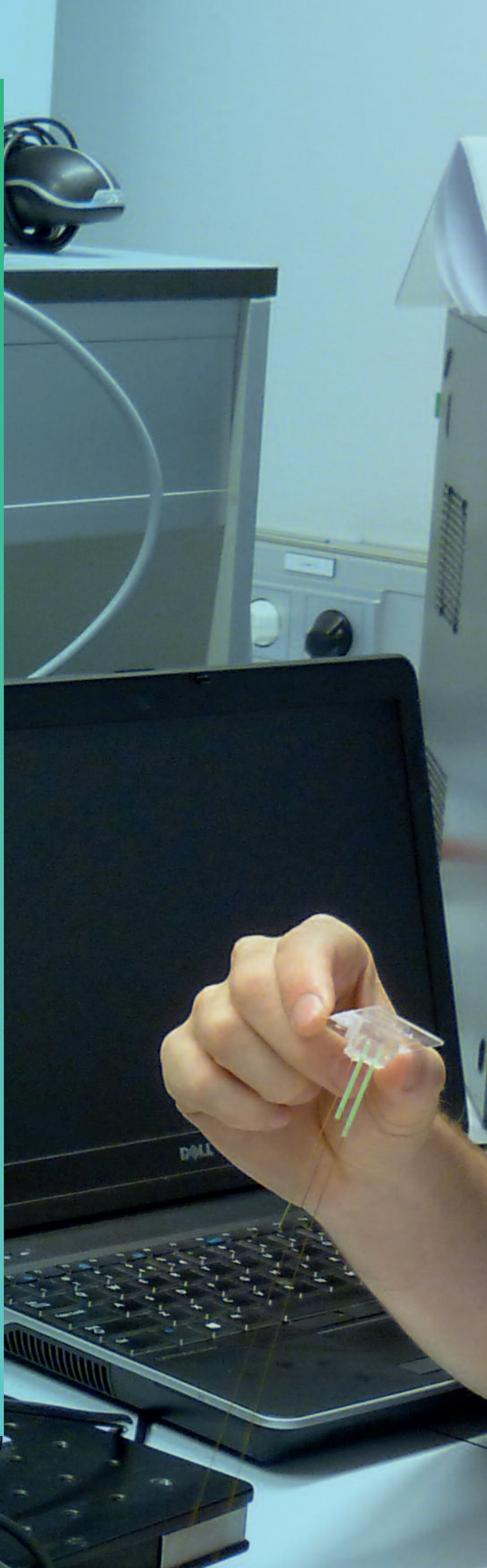
University of Twente
MCEC tenure track
Assistant Professor Micro- and Nanodevices for Chemical Analysis

"When the barriers of scientific disciplines come down, that's when science becomes promising. In my tenure track at MCEC, I focus on microreactor design and microfluidics, and how they can be used for catalysis. Microreactors are extremely small reaction vessels of a few micrometer or even less. They are made in the Nanolab cleanroom at the University of Twente, with high-tech fabrication techniques for micro- and nanotechnology.

The downscaling of a reactor to these tiny proportions gives us an enormous advantage in our research, because it allows us to have better control of chemical reactions in the unique conditions we create at the lab. By using my expertise in microreactor design, microfabrication, microfluidics and chemical analysis, and putting it to use in heterogeneous catalysis, I hope to push out scientific frontiers.

In the future I would like to apply spectroscopic techniques to study electrochemical reactions on microfluidic chips and/or electrodes. Within MCEC, I'm already working on a self-initiated project where SERS and SEIRAS, two forms of spectroscopy, are combined to study reactions in biomass conversions. But the devices we need to develop for this project might also be of use for the study of solar fuels in the future."

Read Mathieu Odijk's entire contribution on his scientific research on page 43.



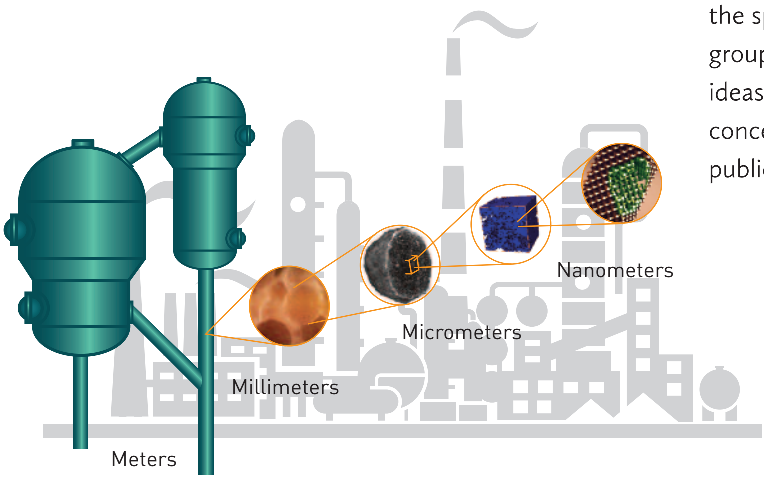

HP Impedance/Gain-Phase analyser
For general use
BIOS48

Research

Within our MCEC program, scientists are working on long-term research to come up with innovative solutions for energy conversion. The ultimate goal for us is to create a more sustainable world. The current use of non-renewable resources, such as natural gas and crude oil, as well as the gradual shift to new, more sustainable resources, such as biomass, call for a redesign of our traditional chemical conversion processes.

The wish for a more efficient and sustainable production of transportation fuels, chemicals and materials, requires the development of smart catalysts and related catalytic processes. These processes have to perform with optimal transport of heat and mass at every possible scale: from the atomic level of the catalyst material to that of the actual reactor. The ultimate program aim? Developing radically improved catalytic energy conversion processes, which are capable of efficiently converting the feedstocks of today and tomorrow.

Multiscale science approach to catalysis



MCEC has defined three scientific and three technological challenges. By crossing and interconnecting these challenges, MCEC fosters both disciplinary and multidisciplinary frontier research. Each challenge focuses on the fundamental questions of the nanoscopic, mesoscopic and macroscopic scales of the catalytic process.

Our program consists of forty PhD and Postdoc projects. Each project is led by one MCEC member and supervised by at least two other MCEC members, all with different backgrounds and from different disciplines. Each project is included in one of the six so-called project clusters:

- → Biomass Conversion
- → Syngas Conversion
- → Future Methodologies in Catalysis & Solar Fuels
- → Fluidic Systems
- → Nanoreactors
- → Nanobubbles

A project cluster is always coordinated by two MCEC members. The subdivision in clusters makes sure that meetings, knowledge transfers and possible multidisciplinary collaborations can easily be organized.

Working along this organizational structure is definitely helping the collaboration to emerge, however this is not limited to a specific project cluster. In 2014 and 2015, the exchange between our students and supervisors grew due to the specifically organized visits of the different research groups to each other's locations. These meetings led to new ideas of shared experiments and agreements were made concerning joint activities and possible future joint publications.

Overall structure of the MCEC research program, including the three scientific and technological challenges:

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

The six distinct project clusters fitting in the initial structure of the MCEC research program:

Biomass Conversion

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Fluidic Systems

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Syngas Conversion

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Nanoreactors

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Future Methodologies in Catalysis & Solar Fuels

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Nanobubbles

Scientific Challenges \ Technological Challenges	Syngas & Methane Chemistry	Biomass Conversion	Solar Fuels
Mastering Catalytic Events			
Mastering Complex Multiscale Structures			
Mastering Mass & Heat Flows			

Biomass Conversion

8 PROJECTS

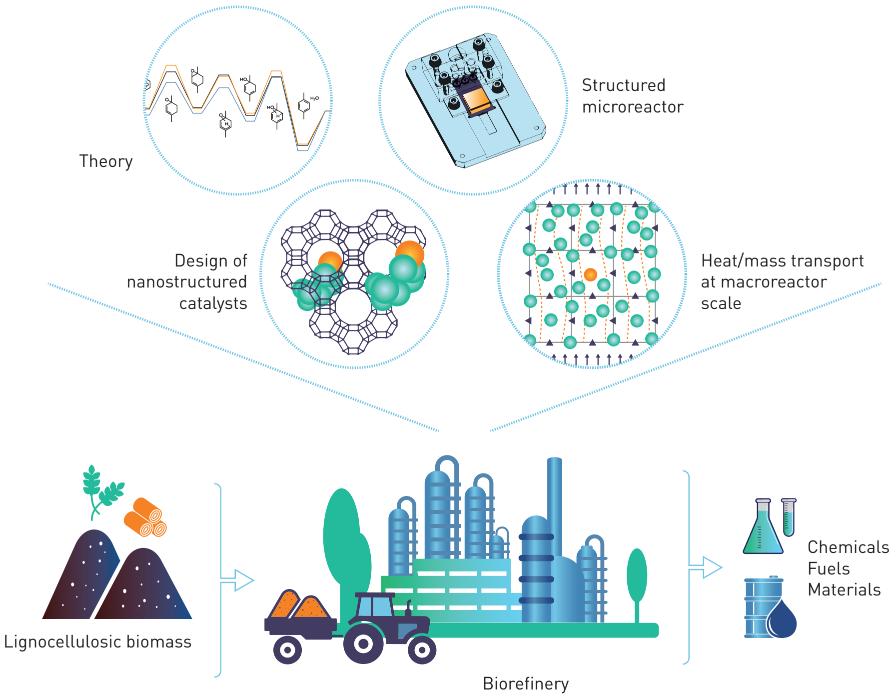
Coordinated by Pieter Bruijnincx & Niels Deen

Fostering the shift towards a bio-based economy is an important topic within the MCEC program. In this project cluster, a consortium of researchers investigates the conversion of the non-edible fraction of biomass into useful products, such as chemicals, materials and transportation fuels.

Catalyst design is aided by theoretical and multiscale modeling studies. By doing this, all relevant time- and length scales are considered. At the nanoscale an optimal design of the internal structure of the multifunctional catalyst is needed to achieve high product selectivity and to counteract catalyst deactivation, which takes place due to the presence of e.g. water and/or coking.

At the micro- and mesoscale one requires a proper understanding of the interplay between mass transfer and kinetics, which takes into account the external structure of the catalyst. Finally, at the reactor scale the interplay between flow phenomena, mass transfer and reaction is needed to make a priori predictions of the reactor performance.

The research carried out in this cluster will lead to new recipes for catalyst composition and structure formulations, a quantitative descriptive model for mass transfer and kinetics for specific catalyst structures, and first-principle tools for reactor performance prediction.



Integrated and structured Fluid Catalytic Cracking reactor

Lijing Mu (TU/e)

"We will develop a detailed reactor model that predicts the performance. The model can be used to test different process scenarios and provides insight into the heterogeneity of the reactor mixture."

Surface heterogeneity and interfacial transport

Aura Visan (UT)

"Understanding the influence of surface heterogeneity, both geometrical as well as chemical, on the fluid dynamics and mass transport near the catalytic surface for an optimum interface design."

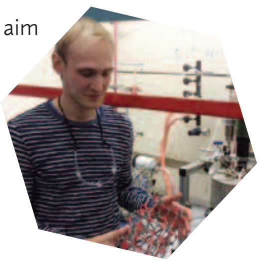
In-situ studies porous materials synthesis

Jan Wiesfeld (TU/e)

"Investigating formation mechanisms of porous inorganic materials in order to synthesize efficient and selective catalysts for biomass conversion in a controlled fashion."

Catalytic biomass conversion by porous oxides

Evgeny Uslamin (TU/e)



"In this project we aim to investigate reaction mechanisms and structure-activity relations underlying the biomass transformation processes on porous oxides. We develop theory of catalytic biomass conversion by studying well-defined systems."

Bio-oil to chemicals and fuels

Beatriz Luna Murillo (UU)

"Bio-oil from non-edible biomass can serve as feedstock for conventional fluid catalytic cracking process (FCC) for commodity chemicals production; however, co-feeding bio-oil results in catalyst deactivation. We will study this process in detail combining experimental and spectroscopic approaches."

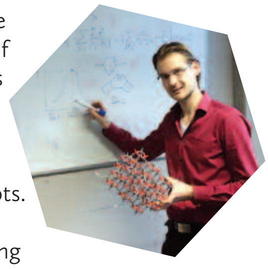
Acidic water in zeolite pores

Katarina Stanciakova (UU)

"In this project we will systematically address the problem of zeolite degradation upon water attack by means of molecular modeling. Our work should contribute to the development of a more stable and water resistant catalyst for biomass processing."

Theory of Lewis acid zeolite catalysis for biomass conversion

Roderigh Rohling (TU/e)



"In this project we develop theory of catalytic biomass conversion and focus on formulating new reactivity concepts. We study new enzyme-mimicking mechanisms beyond single-site models for zeolite-based chemocatalysts."

Polyalcohol reforming to synthesis gas as logistic fuel for mobile fuel cell applications

Vetrivel Shanmugam (TU/e)

"The aim of this project is to understand the coke formation mechanism at the surface of mesoporous silica supported metal nanoparticles under conditions of oxidative steam reforming of polyalcohols to synthesis gas as logistic fuel."

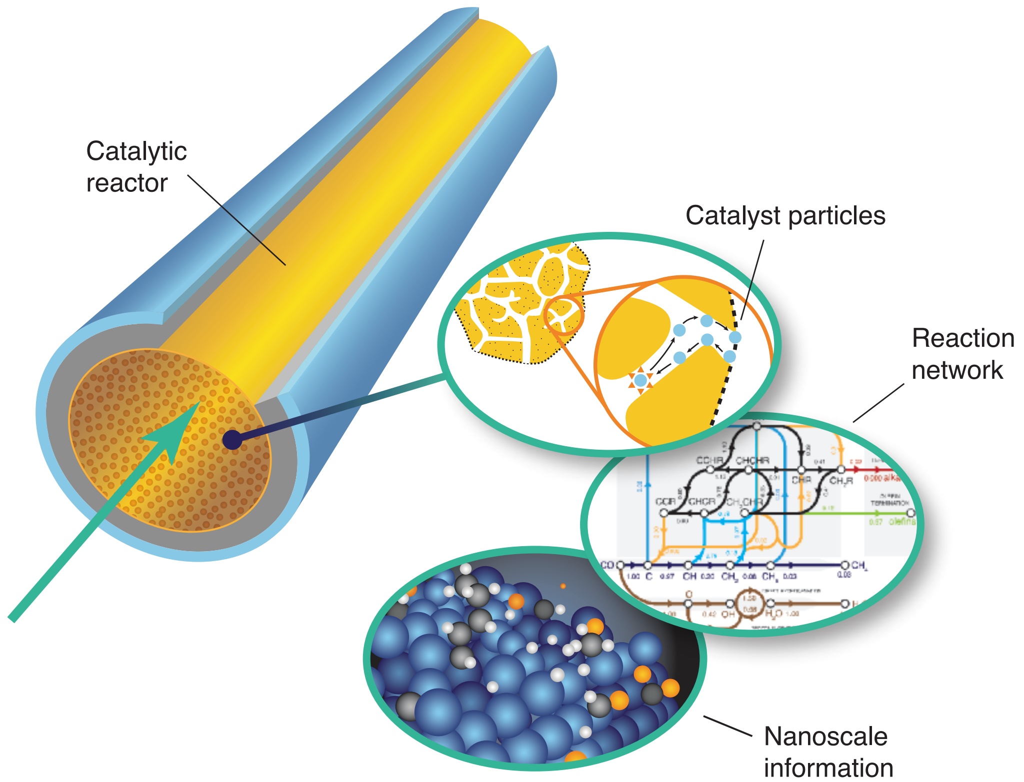
Syngas Conversion

6 PROJECTS

Coordinated by Hans Kuipers & Rutger van Santen

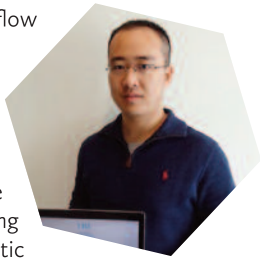
The process challenge in syngas conversion towards base chemicals, such as transportation fuels or aromatics, is to beat the selectivity problem of methane production. Recent studies have demonstrated that there are large heterogeneities in catalyst composition and physical properties. As a result, the concentration and flow profiles will be highly complex.

The catalytic engineering challenge is to model and control this multiphase process of gas, liquid and solids. Methods are needed for catalyst synthesis of the complex multicomponent materials that are accurate on the nanoscale as well as larger length scales. Multiscale modeling that integrates microkinetics with the response to reaction and flow medium as well as in-situ and ex-situ characterization techniques is a necessity, and adequate model approaches should be discussed and developed.



MC-DNS study of coupled heat and mass transfer with catalytic surface reaction

Jiangtao Lu (TU/e)



“Modeling of the flow of reactants and products around catalytic particles as well as intraparticle transport and the reactions occurring there. Real catalytic processes can be optimized based on the prediction of this computer simulation.”

Direct conversion of synthesis gas to aromatics

Lennart Weber (UU)

The synthesis of aromatic compounds from synthesis gas (a mixture of hydrogen and carbon monoxide, derivable from renewables) is accomplished by short olefins production via Fischer-Tropsch synthesis followed by aromatization in zeolite pores in a one-step catalytic process.“

Kinetics and mechanism of syngas chemistry

Robin Broos (TU/e)

“The aim of this project is to combine a nanoscale description of the individual reaction steps in the Fischer-Tropsch reaction obtained by quantum-chemical calculations with a reactor engineering model to predict the overall catalyst performance.”

Influence of wall corrugation on mass transfer in liquid catalytic reactors

Aditya Sengar (TU/e)

“In catalytic reactors, solid surfaces are usually corrugated on length scales of micrometers. A fundamental investigation of the coupled convection-diffusion-reaction mechanisms in the boundary layer near such corrugated walls is undertaken.”

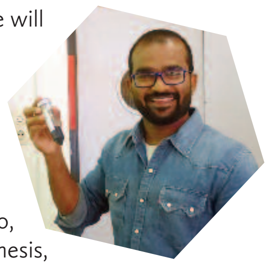
Liquid-phase TEM and cryo-TEM of fundamentals of catalyst assembly

Petra Keijzer (UU)

“In this project melt infiltration and deposition precipitation of metals or metal precursors will be investigated at the fundamental level for the assembly of solid catalysts for a wide range of conversions.”

Supraparticles for catalysis

Ramakrishna Kotni (UU)



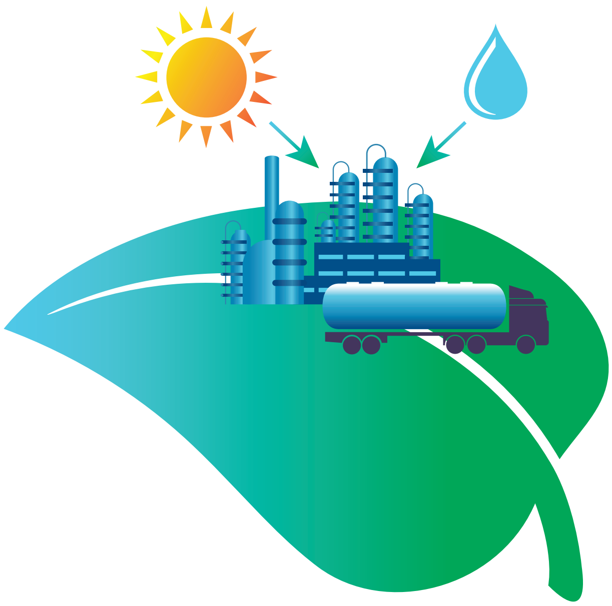
“In this project we will mainly focus on visco-elastic high shear processing to obtain relatively monodisperse droplets. To do so, first the NP synthesis, using existing procedures, will need to be optimized for FT catalysis (particles size, composition, stabilizer removal).”

Future Methodologies in Catalysis & Solar Fuels

6 PROJECTS

Coordinated by Alfons van Blaaderen & Emiel Hensen

Of the three technological challenges we take up in the MCEC program, catalytic processes aiming for solar fuels production are by far the least mature. The ultimate goal of this cluster is to generate fuels using solar energy in sustainable processes that eventually can replace fossil fuels.



Several of the projects focus on the more modest goal of breaking up water into its elemental components: oxygen and hydrogen. This will be done by making use of sunlight or electrons, originating from for example wind turbines. The challenge here is to achieve overall energy efficiencies clearly above 10%, in a process that utilizes structured nanomaterials. This process is preferentially structured by self-assembly that also achieves separation of these gasses. Projects that aim to contribute to the other technological and scientific challenges, for instance those that focus on making use of light in new ways, are part of this cluster as well.

This project cluster will certainly gain from the expertise in other research clusters concerning self-assembly and materials structuring at different length scales, and the physics and chemistry that are related to gas production in the presence of a liquid.

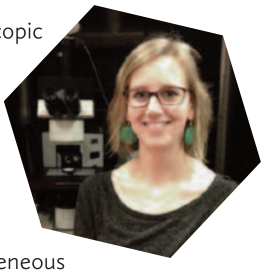
Catalyst particle-embedded luminescent nanoparticles for temperature sensing

Robin Geitenbeek (UU)

"Temperature is one of the most critical reaction parameters when it comes to the efficiency of a catalytic process. To accurately determine the local temperature in a catalytic reactor with micrometer resolution, we are investigating temperature dependent luminescence of rare-earth containing nanoparticles."

Single Particle Diagnostics: Integrating catalysis with optical spectroscopy within a microreactor device

Anne-Eva Nieuwelink (UU)



"Optical spectroscopic techniques like Raman and UV-vis will be used for characterizing inline the activity and properties of single heterogeneous catalyst particles for relevant reactions in the field of biomass-, photo- and solar catalysis."

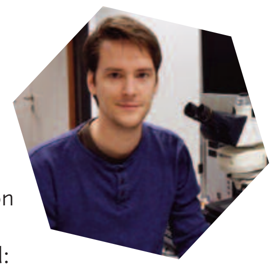
Thermodynamic and kinetic analysis of aqueous phase reforming by high pressure and temperature microfluidics

Renée Ripken (UT)

"In addition to a theoretical model, a high temperature and pressure microfluidic platform will be developed to study the thermodynamics and kinetics of aqueous phase reforming of biomass for hydrogen production."

From nanoscale (photo)electrolytic gas generation via microscale bubble nucleation to macroscale bubble transport

Peter van der Linde (UT)



"Solar hydrogen production, a zero-emission technology, can be optimized if bubble formation on electrodes is well understood: How do bubbles interact with electrode features, such as roughness, charge, etc., and how to apply the advances made?"

Self-assembled semiconductor nanorod membranes for photocatalytic water splitting

Christa van Oversteeg (UU)

"Membranes based on self-assembled chalcogenide semiconductor nanocrystals are studied for their use in photocatalytic water splitting. This approach uniquely allows to tune nanoscale properties of individual nanocrystals, while on the larger scale stable superstructures can be formed."

Towards a comprehensive description of photoelectrochemical processes on model photoelectrodes

Freddy Oropeza Palacio (TU/e)

"In this project, advanced X-ray photoelectron spectroscopies under both well-defined and in-situ conditions will be applied to investigate design parameters of model photoelectrodes for the production of CO_2 neutral solar fuels."

Fluidic Systems

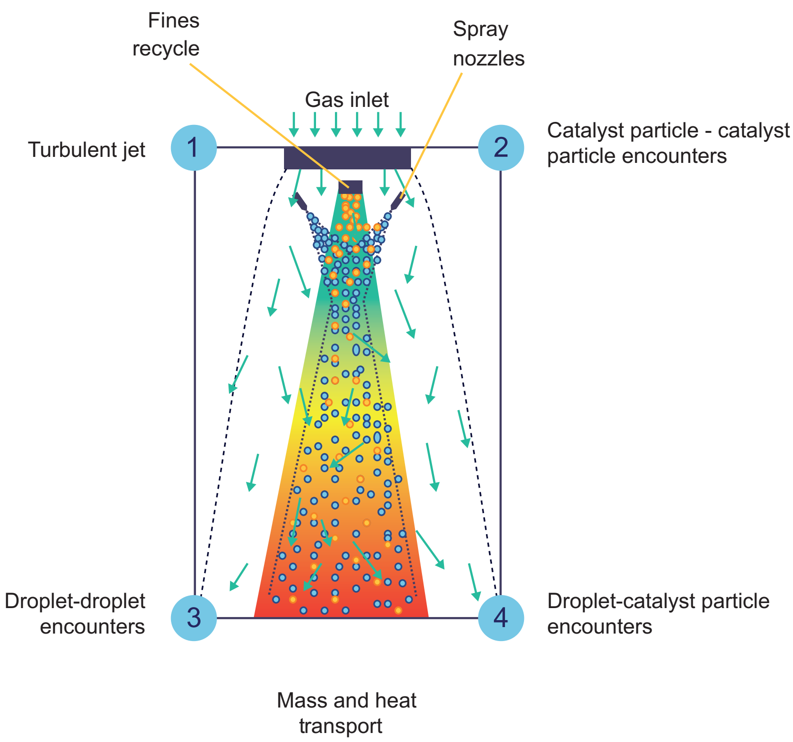
6 PROJECTS

Coordinated by Hans Kuipers & Detlef Lohse

A variety of large-scale manufacturing and transport processes encounter dispersed multiphase flows: flows with dispersed bubbles or particles. These in particular include flows in chemical plants and flows in which catalytic reactions may occur.

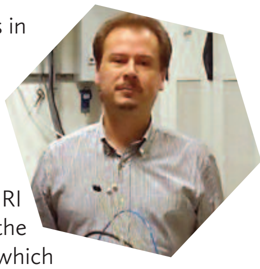
All these dispersed multiphase flows are not laminar, but turbulent. The questions we want to address are: How do bubbles affect mixing of reactants in such bubbly turbulent flows? How do bubbles change the mixing efficiency? What are the optimal parameters for the mixing of reactants? What is the interplay between the bubbles, the catalyst particles, and turbulent fluctuations on the mixing in turbulent multiphase flows?

To answer these fundamental questions, we will use both experimental methods, such as laser Doppler velocity and high-speed camera imaging, as well as computational fluid dynamics, such as front-tracking and immersed boundary techniques.



MRI flow imaging in dense gas-solid fluidized beds

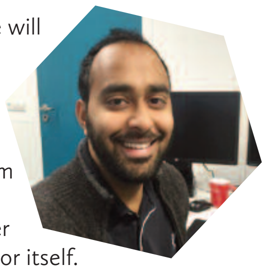
Paolo Lovreglio (TU/e)



"The flow systems in most chemical processes are multiphase flows and not transparent. By means of Flow MRI we can visualize the flow, something which cannot be done with optical (camera) techniques."

Open micro-structured random packing in gas-liquid solid reactors for Fischer-Tropsch catalysts: multiscale reactor modeling

Vishak Chandra (TU/e)



"In this project we will design a new reactor where the transport properties are fully resolved from the nanometer scale to the meter scale of the reactor itself. Latest Direct Numerical Simulation techniques like the Immersed Boundary Method will be used to study the transport phenomena at the particulate level."

Flow structure formation and evolution of gas-liquid solid reactive flows and coupling with turbulence

Maxim Masterov (TU/e)

"Our aim is to obtain a better understanding of the hydrodynamics and heat- and mass-transfer limitations, and the role of turbulence herein, in large scale slurry bubble columns using state-of-the-art computer simulations."

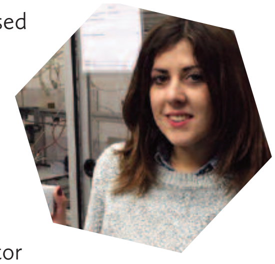
Chemical reactions & mixing in turbulent multiphase flow with active & passive catalytic particles

Peter Dung (UT)

"In this project we will study the mixing of passive scalar fields such as in reaction products out of a catalytic reaction (on floating microparticles) in a freely rising bubble swarm. In addition, we intend to investigate the effect of turbulence on the mixing, aiming to address the interplay between the bubbles, the catalytic particles and the turbulent fluctuations."

Open micro-structured random packing in gas-liquid solid reactors for Fischer-Tropsch catalysts: reactor development

Teresa de Martino (TU/e)



"Foam cobalt-based catalysts are synthetized and characterized to improve mass transfer in the Fischer-Tropsch reaction. A gas-liquid solid reactor suitable for the foam catalyst is designed."

Self-propelled particles to enhance catalysis

Ajoy Kandar (UU)

"We will study in detail the mechanisms of model systems of self-propelled particles, especially in the bubble-propulsion regime. Additionally we want to extend the study to 3D and quantitatively study its behavior on the single particle level as a function of concentration."

Nanoreactors

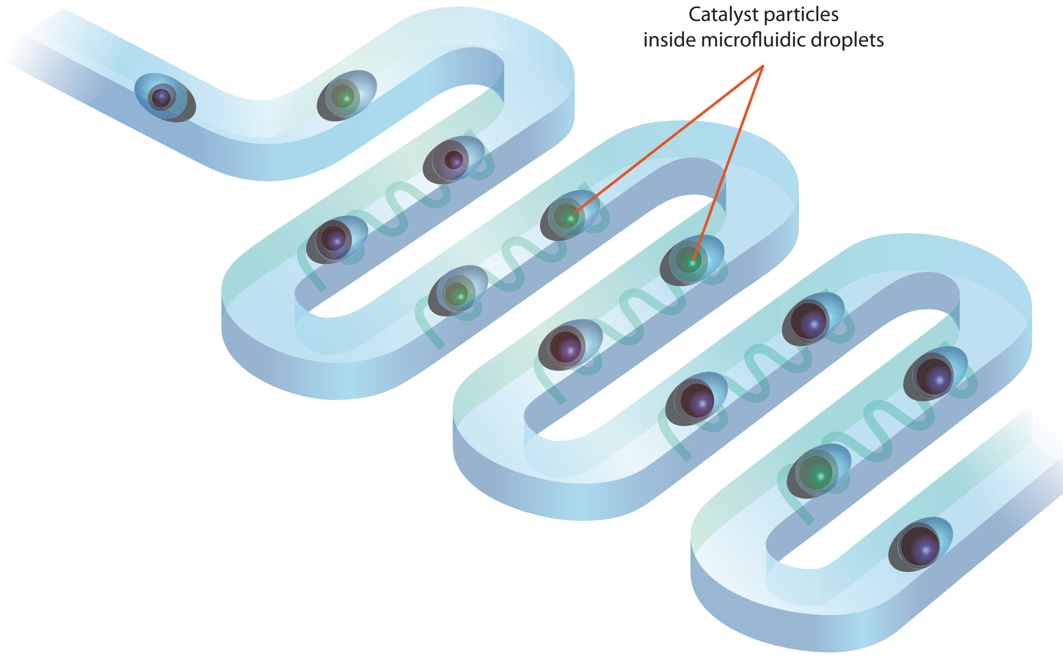
5 PROJECTS

Coordinated by Albert van den Berg & Bert Weckhuysen

A team of experts in the fields of nanoparticle synthesis and self-assembly, micro- and nanofluidics, nanosensing and spectroscopy, will work together in this project cluster to develop new strategies for catalyst optimization. Micro- and nanofabrication and micro/nanofluidic technologies will enable the realization of X-ray transparent nanoconfinements for in-situ spectroscopic nanoparticle analysis, while a microfluidic microdroplet platform will enable high-throughput creation of nanoliter environments with varying reaction conditions to study the performance of individual catalyst particles.

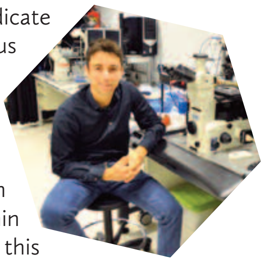
The use of micro- and nanofluidic technologies will be explored to synthesize and analyse both individual catalyst particles as well as self-assembled supra-particle aggregates. Integrated nanosensing structures will enable us to select those catalyst particles with the highest efficiency for further analysis. Based on this knowledge we hope to provide guidelines for the synthesis of new or improved catalyst materials with a better control over their physicochemical heterogeneities.

In addition, microfluidic structures will be designed and used to create locally well-defined conditions (e.g. shear forces, electrical and magnetic forces, temperature, chemical and/or pressure gradients) that determine the parameters of supraparticle self-assembly.



Single catalyst particle diagnostics: Integrating impedance sensing and sorting

Miguel Solsona (UT)



"Recent studies indicate that heterogeneous catalysts show tremendous variation in structure and performance, both between and within single particles. In this project, with the use of impedance spectroscopy and microfluidics a platform is developed to analyse single particle characteristics online."

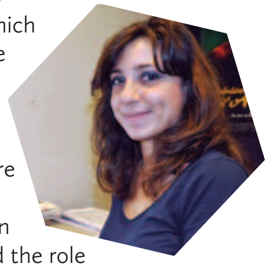
Supraparticles by microfluidics

Chris Kennedy (UU)

"The self-assembly of nanoparticles into spherical micro-structures (supraparticles) may enhance their ability to catalyze the photolysis of water. Microfluidics will be used here to reliably control supraparticle assembly and the resulting structures will be probed with electron tomography."

Hydrodynamics and interaction of self-assembly in droplet confinement

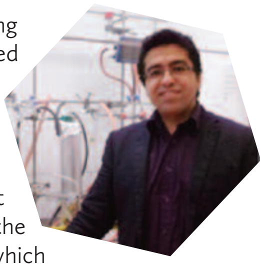
Giulia Fiorucci (UU)



"In hierarchical self-assembly (SA) atoms are arranged into nanoparticles, which can self-assemble and form micro-sized supraparticles. How the structure of these supraparticles can be optimized and the role of hydrodynamics in SA understood, can be obtained from numerical simulations by tuning the shape and interactions of the nanoparticles."

Nanoreactors for in-situ X-ray spectroscopy and microscopy

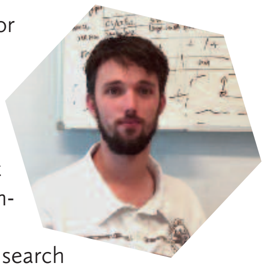
Ahmed Ismail (UU)



"We employ cutting edge time-resolved spectroscopy and state-of-the-art nanoreactors to answer important questions about the mechanisms by which solar fuel cells convert solar energy into chemical energy that is stored in hydrogen molecules via the water splitting process."

Single catalyst particle diagnostics: Droplet microreactor platform

Jeroen Vollenbroek (UT)



"There is a need for a single catalyst diagnostic platform to characterize single particles at low-cost and high-throughput, to enable a massive search to find and select the best catalyst particles and related synthesis formulation approaches."

Nanobubbles

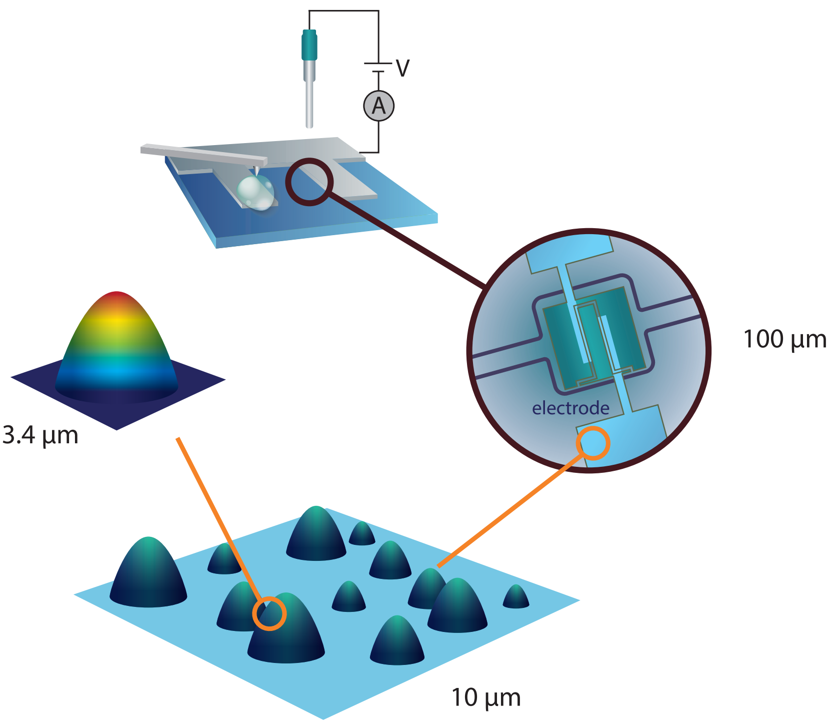
9 PROJECTS

Coordinated by Detlef Lohse & Bert Weckhuysen

In heterogeneous catalysis, gas bubbles often form at the catalyst surface, hindering its efficiency. In their smallest known form, the bubbles come as so-called surface nanobubbles. These bubbles are only a few femtoliters in volume and can stay at the interface as long as several hours or even days.

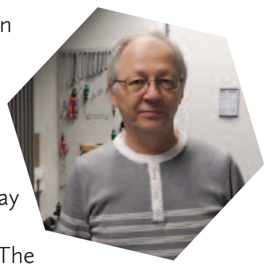
The formation of surface nanobubbles can occur not only through (catalytic) chemical reactions, but also through electrolysis, or when the interface experiences gas super-saturation due to a change of the solvent or in the temperature, or by pressure reduction. Very similar to surface nanobubbles are surface nanodroplets, which are liquid nanoscale domains on the solid surface in contact with an immiscible bulk liquid. These are also relevant in catalytic reactions that produce an oil phase in an aqueous environment or vice versa.

In this cluster we want to understand the fundamental properties and dynamics of surface nanobubbles and surface nanodroplets, using ultrafast imaging, atom force microscopy, and in-situ optical and vibrational spectroscopy. On the one hand, we aim to achieve single nanobubble and single nanodroplet spectroscopy. On the other hand, we want to understand collective effects of surface nanobubbles and surface nanodroplets, in particular the Ostwald ripening, which is related to their size distribution, surface coverage, and spatial arrangements. The ultimate aim is to find ways to reduce the disturbing effect of surface nanobubbles on the efficiency of catalytic reactions.



Electrolytic gas production at catalytic surfaces

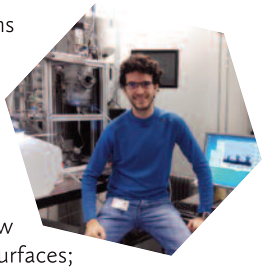
Vitaly Svetovoy (UT)



"Reaction between hydrogen and oxygen in nanobubbles is used to modify a catalytic surface in a controlled way with local nanoexplosions. The bubbles are produced by water decomposition as a result of short electrical pulses."

Transporting gas away from a catalyst surface

Alvaro Moreno Soto (UT)



“Catalytic reactions often happen on the surfaces of complex solid materials. During these reactions, bubbles may nucleate and grow on top of these surfaces; avoiding these reactions to occur. This gas settled on the catalyst surface must be transported away.”

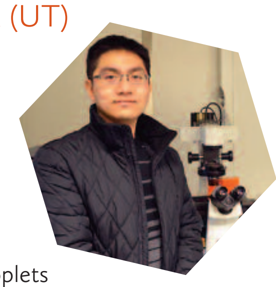
Metal nanoparticles, nanochannels and nanobubbles

Hai Le The (UT)

“An array of metal- (Pt, Au, Pd) nanoparticles embedded into a fused silica substrate is fabricated. Catalytic activity and mass transfer in closed-end nanopores are investigated for gas-phase catalytic reactions.”

Transporting gas away from a catalyst surface

Pengyu Lyu (UT)



“During the process of solvent shifting and solvent exchange, we study the evolution of micro/nano-droplets and micro/nano-bubbles in detail using 3D confocal microscopy to observe nucleation, growth, coalescence and so on.”

Theory and numerics for dynamics and collective effects

Ivan Devic (UT)

“Surface nanobubbles and nanodroplets are small gaseous/liquid domains that block the surface of catalyst, hence reducing its productivity. Goal of this theoretical research is to analyse fundamental properties of these domains and their interaction with the environment.”

Microscopic study of the initial stages of electrolytic gas production at catalytic surfaces

Edwin Dollekamp (UT)

“In this project, we will investigate the gas evolution under electrolytic conditions, with the primary aim to control the formation of bubbles and their release from a catalytically active surface. Electrochemical control of the catalytic surface allows optimization of its efficiency.”

Lattice Boltzmann numerics for dynamics and collective effects

Matteo Lulli (UT)

"Surface droplets and bubbles of nanometer dimensions might impact catalysts efficiency, therefore it is important to model the mechanisms for their formation and dissolution under flow. The Lattice Boltzmann technique offers a mesoscopic approach to tackle this problem without resorting to molecular dynamics simulations."

Surface nanobubbles and surface nanodroplets

José Encarnacion Escobar (UT)

“In this project we want to experimentally analyse and understand the properties and dynamics of surface nanobubbles and surface nanodroplets, using ultrafast imaging, AFM, and in-situ spectroscopic techniques.”

Surface nanobubbles during biomass catalysis on zeolite surfaces

Laurens Mandemaker (UU)

“In this project, we will develop a high-temperature, high-pressure Atomic Force Microscopy (AFM)-Vibrational Spectroscopy setup to investigate the one pot hydrogenation reaction of levulinic acid.”

Ivo Filot

Eindhoven University of Technology
MCEC tenure track
Assistant Professor Computational Catalysis

"If we truly understand catalysis to its core, we can start creating the next-generation catalysts that will be able to face the ongoing grand energy and environmental challenges. Therefore, we need to know exactly what the catalytic process goes through in every step, from the molecular level to that of the macroscale, and vice versa. We use simulations of catalytic processes to study this process.

But the existing simulation techniques are inadequate. For one thing, they are computationally very demanding. For another, the catalytic processes are in essence difficult to explore. To develop a full understanding of catalysis, we need to be able to connect the molecular information to any meso- or macroscopic simulation. Over the past five years, I have studied the possibility of connecting simulations that operate at fundamentally different length and timescales.

Within the MCEC program, I develop new computational methodologies that enable the simulation of mesoscale processes. With this I essentially bridge the gap between the catalytic simulations at the molecular and macroscopic level. This research is fundamental and can be applied to any catalytic process. Some simulations can even be readily validated at the molecular level (Hensen group) and the macroscopic level (Kuipers group).

The collective knowledge represented in MCEC School is crucial for the development of these new methodologies, as MCEC operates at the frontiers of scientific knowledge of catalysis and computational modeling."

Read Ivo Filot's entire contribution on his scientific research on page 44.

MCEC education

In order to succeed in their professional life, young researchers have to be able to look beyond the borders of their own domain, both academically and socially. If we want them to have a solid base for working in a multidisciplinary manner on the multiscale catalysis approach, we need to make sure that they a) gain insight into each other's expertise and background, b) have the opportunity to meet and discuss each other's work and c) actually put that in practice by working together on multidisciplinary projects. Our educational activities therefore focus on learning within the MCEC community, as a group together and from each other; always with respect to the individual development of each student.

MCEC finds it important to train its students broadly – in their academic competences, but also in their transferable skills, like communication, didactics and presentation. We encourage our students to, to name a few examples, join one of our teams (see page 9), present themselves at academic and/or public meetings, or organize a lab tour. All of these activities are not just extracurricular, but an integral part of the MCEC program. This especially holds for our own MCEC School.

Education plan

The education plan for all MCEC students consists of the following three elements:

1. Personal development, including scientific writing, project planning, ethic and research integrity and career orientation.
2. Scientific development in its own field of research.
3. Training in multidisciplinary and multiscale science approaches.

The educational program is set up and organized by the MCEC Education Committee:


Prof. Hans Kuipers
(Eindhoven University of Technology)
Chair


Prof. Rob Lammertink
(University of Twente)


Dr. Rosa Bulo
(Utrecht University)


Dr. Johan Padding
(Eindhoven University of Technology)

Within their graduate schools and programs, the three universities already offer excellent courses on personal and scientific development, symposia and summer and winter schools, on which the students can decide together with their supervisors. The participating graduate programs are:

Debye Institute for Nanomaterials Science

Where chemistry and physics meet to study the properties of materials at the nanoscale, with specific focus on catalysis, colloid science and nanophotonics.

Universiteit Utrecht

MESA+ Institute for Nanotechnology

Where researchers originating from the fields of chemistry, physics, materials science and engineering, focus on breakthroughs in nanotechnology.

UNIVERSITEIT TWENTE.

CE&E Chemical Engineering and Chemistry

Where chemists and chemical engineers work on e.g. molecular systems and materials chemistry, and chemical and process technology, including heterogeneous catalysis.

TU/e Technische Universiteit Eindhoven University of Technology

Whether a PhD student chooses to stay in academia or wants to proceed his or her career in industry, a governmental organization, or even start up a spin-off company: to be able to grow as a scientist, he or she will need to gain knowledge in a specific field of expertise. MCEC expects its PhD's and Postdocs to make use of the broad set of courses that have been developed in the framework of the three KNAW accredited interuniversity research schools NIOK, JMBC and OSPT. We will encourage our students to also sign up for courses from different disciplines in order to broaden their knowledge; with that, paving the way for multidisciplinary project collaborations.

J.M. Burgerscenter

The J.M. Burgerscenter (JMBC) is the Dutch research school for Fluid Mechanics. JMBC offers a multidisciplinary environment for advanced research in fluid mechanics and for the education of talented graduate and postgraduate students.

J.M.Burgerscentrum

Netherlands Research School in Process Technology

The Netherlands Research School in Process Technology (OSPT) is an interuniversity school in the area of chemical engineering and process technology. OSPT is part of the Innovation Academy of the Institute for Sustainable Process Technology (ISPT).

ISPT

Netherlands Institute for Catalysis Research

The Netherlands Institute for Catalysis Research (NIOK) is a virtual institute consisting of Dutch university research groups active in all areas of catalysis. It acts as the platform and sparring partner for national and international contacts on catalysis with academia, industry and government.

NIOK

MCEC school

To be able to work in the multidisciplinary consortium that MCEC is, PhD's need to obtain knowledge on more than just their field of expertise. The MCEC School aims to do just that. It's an integrated, five-day program with 6 ECTS (2 ECTS each yearly, with a certificate of attendance). The first MCEC School was held from October 12 to October 16, 2015 and will be followed by a second and third MCEC School in respectively October 2016 and October 2017. The program of the MCEC School is designed accordingly to the multidisciplinary approach of our research.

During the first School, introductory and advanced lectures were given by the six PI's and other members of the MCEC community in the fields of catalysis, fluid mechanics and process engineering. The MCEC research themes on solar fuels, biomass conversion and syngas conversion are certainly not familiar topics to everyone, which is why we had invited lecturers on those subjects.

To promote the interaction between PhD's with a different scientific background, the students were asked to work on a case study in a multidisciplinary team. The MCEC Education Committee composed the teams and the case studies in a way that challenged students to step outside of their comfort zone in terms of knowledge and collaboration. The results were presented on the last day. To stimulate the community building, MCEC together with the students had organized some informal and team building activities.

Afterwards, the PhD's received a survey to evaluate the first School and share their suggestions for the next one in 2016. The majority of the students reported that the lectures during the week provided a good balance between overview and specifics of the different fields. The setup of the sessions was coherent and provided new knowledge to everyone. The case studies were highly appreciated as they required teamwork and a true integration of knowledge. During the week, a foundation was laid for the PhD community and the further exchange of knowledge. Possibilities of setting up new collaborations were already discussed. According to the survey, getting to know one another in person and learning about the different projects others were involved in, was considered highly worthwhile.

Future plans

The suggestions mentioned in the evaluation have been taken into account for the second MCEC School. In order for our PhD's to bring multidisciplinary discussions and goal-oriented collaboration to the next level, we've changed some of the setups and added interesting new elements to the program. One of those, for example, is the 'PhD tutorial', in which our students teach about subjects they are passionate about and find useful for their fellow students with different backgrounds.

Furthermore, we would like to integrate science related subjects like research data management, science integrity, presentation to secondary school pupils, and general public outreach activities into MCEC Education. Although these subjects are, to some extent, already part of the programs of the three participating universities, we find it valuable to pay additional attention to these important matters in our own program.

Rosa Bulo

Assistant Professor
Simulation of Catalytic Reactions in Water
Member of the MCEC Education Committee

"The focus of my work is to understand the effect of water as a solvent on catalytic reactions, through the use of molecular simulation. I started out as a computational chemist, doing simulations on chemical reactions on the electronic scale. Now, I develop methods to combine these computations with those on the much larger multi-molecular scale, using methods from molecular physics.

As my research moved from single scale to multiscale, and from chemistry to physics, I had to learn a whole new scientific language to be able to communicate across these fields. Such interdisciplinary interactions have allowed me to apply established knowledge from one field, to solve outstanding problems in the other.

In the same manner, but on a much larger scale, the multidisciplinary and multiscale nature of MCEC can inspire completely new solutions; provided that the talented young MCEC researchers have the opportunity, the will, and the tools to communicate their needs and knowledge. By being part of the MCEC Education Committee and by teaching in the MCEC School, I hope to help create an environment in which this goal can be achieved."

Highlights

Outreach

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News sites
& platforms

19
Newspapers
& magazines

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5
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TEDx Binnenhof
Talk of Bert
Weckhuysen:
A city that runs on CO_2

18
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by MCEC PhD's
and PD's

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keynote lectures
at national and
international
conferences

63
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at universities
and industries

Personal grants

2
ERC
grants

1
NWO
VENI grant
Jovana Zecevic

1
NWO
VIDI grant
Pieter Bruijnincx

Albert van den Berg
receives ERC Advanced grant for the second time, to cultivate blood vessels on a chip, made from 'reprogrammed' human stem cells.

Petra de Jongh
receives ERC Consolidator grant for the development of catalysts for the sustainable production of fuels, synthetics and pharmaceuticals.

Scientific appointments

Marjolein Dijkstra
appointed as Scientific Director of the Debye Institute for Nanomaterials Science (DINS) at Utrecht University.

Detlef Lohse
appointed as Member of the Max Planck Gesellschaft and as an external member of the Göttingen Max Planck Institute for Dynamics and Self-Organization.

Albert van den Berg
appointed as Scientific Director of MIRA, the Institute for Biomedical Technology and Technical Medicine, at the University of Twente.

Academy memberschips and other recognitions

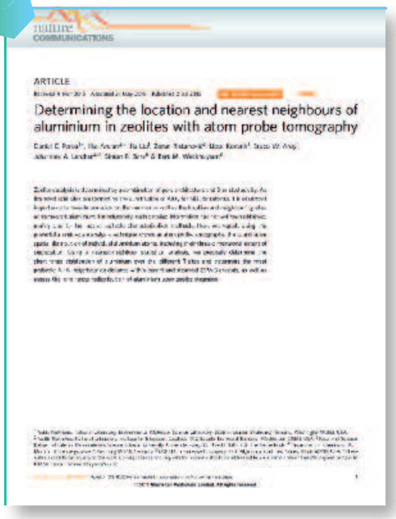
Hans Kuipers
Member of the
KNAW

Pieter Bruijnincx
Member of
the Young Academy
of the KNAW

Bert Weckhuysen
Member of the
KVAB

Bert Weckhuysen
Knight in the Order
of the Netherlands
Lion

Publications



TITLE
Determining the Location and Nearest Neighbours of Aluminium in Zeolites with Atom Probe Tomography

AUTHORS
D.E. Perea, I. Arslan, J. Liu, Z. Ristanović, L. Kovarik, B.W. Arey, J.A. Lercher, S.R. Bare, and B.M. Weckhuysen

JOURNAL
Nat. Commun. 2015, 6, 7589.

TITLE
Quantitative 3D Fluorescence Imaging of Single Catalytic Turnovers Reveals Spatiotemporal Gradients in Reactivity of Zeolite H-ZSM-5 Crystals upon Steaming

AUTHORS
Z. Ristanović, J.P. Hofmann, G. De Cremer, A.V. Kubarev, M. Rohnke, F. Meirer, J. Hofkens, M.B.J. Roeffaers, and B.M. Weckhuysen

JOURNAL
J. Am. Chem. Soc. 2015, 137, 6559–6568.

TITLE
Life and Death of a Single Catalytic Cracking Particle

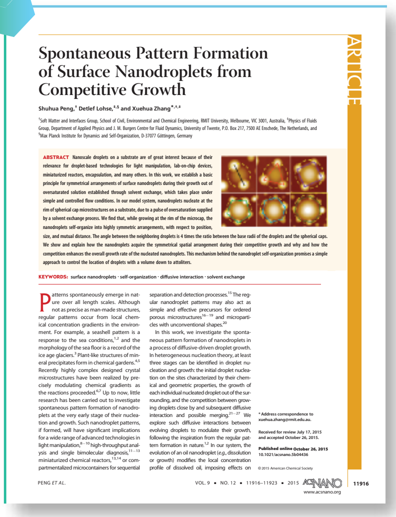
AUTHORS
F. Meirer, S. Kalirai, D. Morris, S. Soparawalla, Y. Liu, G. Mesu, J. C. Andrews, and B. M. Weckhuysen

JOURNAL
Science Advances 2015, 1, e1400199.

TITLE
Formation of Surface Nanodroplets under Controlled Flow Conditions

AUTHORS
X. Zhang, Z. Lu, H. Tan, L. Bao, Y. He, C. Sun, and D. Lohse

JOURNAL
Proc. Nat. Acad. Sci. 2015, 112, 9253-9257.

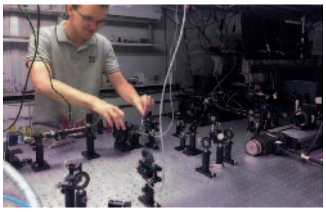


TITLE
Spontaneous Pattern Formation of Surface Nanodroplets from Competitive Growth

AUTHORS
S. Peng, D. Lohse, and X. Zhang

JOURNAL
ACS Nano 2015, 9, 11916-11923.

Scientific research
Freddy Rabouw



Freddy Rabouw (1988)

Utrecht University

MCEC tenure track

Assistant Professor Multiscale Science on Heterogeneous Catalysis

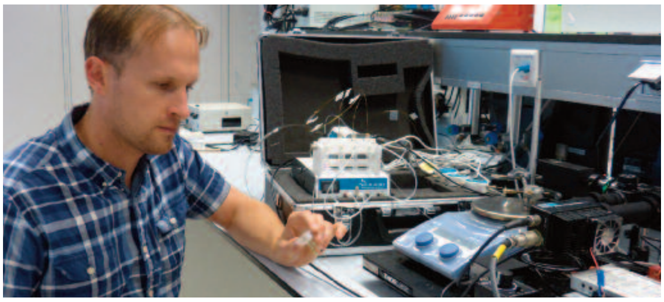
My expertise has been the study and characterization of nanomaterials. Using time-resolved optical spectroscopy, I have investigated the excited state dynamics of semiconductor and insulator nanoparticles over more than twelve orders of magnitude in time. The fastest timescale that I have studied is sub-picosecond, using ultra-fast pump-probe spectroscopy. This is the timescale on which, following light absorption, electrons and holes lose their excess energy as they relax to the band edge (i.e., to the HOMO-LUMO states). The longest timescale is the second to minute timescale on which nanoparticles undergo structural and/or electronic changes.

The most pronounced effect of such changes is the phenomenon of "blinking" in semiconductor nanocrystals: they randomly switch from a brightly emitting state to a dark state over timescales of milliseconds to minutes. In addition to optical spectroscopy of excited state dynamics, I also used diffraction techniques to learn about the structural properties of nanomaterials. With small-angle X-ray scattering at the ESRF synchrotron in Grenoble (France), I have followed the self-assembly of nanoparticles in micrometers large superstructures in-situ, as well as the synthesis of nano- and micrometer sized crystals from molecular precursors. Furthermore, I have determined the crystal structures, and the size and orientation of nanocrystals, using X-ray and electron diffraction with two-dimensional detectors.

What has interested me most over the past few years is to measure the dynamics of a material, such as luminescent nanoparticles, and then build a model to understand the physics on a microscopic scale. My first project within the MCEC program will be to develop a microscopic technique to study individual chemical reactions taking place on an individual catalytic nanoparticle. We will work with a model reaction system, where a semiconductor catalyst photo-catalytically converts a red-emitting dye molecule to a green-emitting dye. While illuminating, a microscope objective will collect the light emitted by the dye molecules as they undergo the conversion rates, where the red and green emission goes to two separate detectors. By cross-correlating the signal recorded by the detectors, we will be able to quantify the rates of the different steps involved in the catalytic process; i.e., diffusion, adsorption and desorption, and chemical reaction. We will search for differences in rates between different nominally identical catalyst particles, or temporal variations in the rates for a single particle. Such inter- and intraparticle heterogeneities will then be correlated to the structure of the catalyst particles (e.g., crystal structure and facetting). The eventual dream is to study not only a model conversion reaction of organic dyes, but individual catalyst particles performing more relevant reactions, involving non-fluorescent molecules, with a clear connection to energy challenges.

The above-described research project will benefit from the knowledge and people present within the MCEC consortium, such as knowledge on the synthesis of nanoparticles (chemical or lithographic), high-resolution micro-spectroscopy and heterogeneous catalysis. On the other hand, I hope that the microscopic photon-correlation technique that we aim to develop will contribute to ongoing studies into fluid dynamics in complex structures or bubble formation and will ultimately lead to an increased fundamental knowledge in the field of heterogeneous catalysis.

Scientific research
Mathieu Odijk



Mathieu Odijk (1981)

University of Twente

MCEC tenure track

Assistant Professor Micro- and Nanodevices for Chemical Analysis

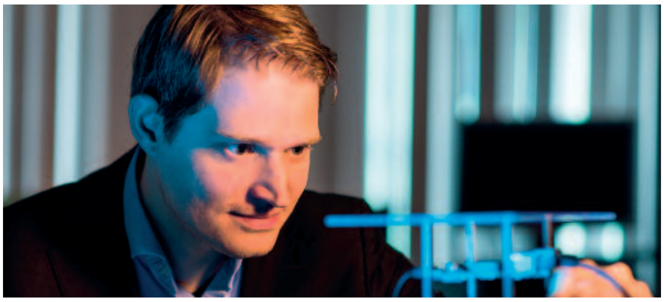
During my PhD I worked on the design and fabrication of an electrochemical microreactor to study drug metabolism reactions, normally catalyzed by enzymes of the cytochrome P450 family present in the liver. That research combined the fields of microfluidics and microfabrication, and the field of analytical chemistry. Although I have continued working on this topic, currently running research projects also include the use of microdroplets, electrochemical sensing, and capacitive deionization inside a microfluidic environment.

My main interests are to use the advantages offered by advanced micro- and nanofabrication to push boundaries to enable to drive chemical reactions in unique conditions or to sense molecules in a more sensitive, precise or more localized environment. In the future I would like to apply (optical) spectroscopy techniques, such as Surface Enhanced Raman Spectroscopy (SERS) and Surface Enhanced Infrared Spectroscopy (SEIRAS) to microfluidic chips and/or electrodes to study (electrochemical) reactions. As an example, I initiated a research project within the MCEC program where SERS and SEIRAS are combined to study reactions in biomass conversions. In the future the devices developed within this project might also be of use in the field of solar fuels.

Another advantage offered by miniaturization is to do high-throughput screening of a variety of reaction conditions or single catalyst particles using droplet microfluidics, as droplets can be generated at speeds of 10-1000 droplets per second. Within the MCEC program droplet microfluidics is currently used to screen single catalyst particles with high-throughput using Raman, fluorescence, or impedance spectroscopy. I provide input to three PhD students within the MCEC program working on this particle diagnostic platform, solving challenges in particle encapsulation, chemical analysis and microreactor design. Adding a gradient generator in the future to this work would also allow to use these microdroplets to screen for optimal reaction conditions, or to screen for a wide variety of compositions to fabricate catalyst particles with optimal properties.

Recently more substantial collaborations within the MCEC program have started to develop, enabled by the ongoing contacts at the various MCEC events. Examples where MCEC has stimulated collaboration include the project of Peter van der Linde (supervised by Dr. Fernandez Rivas and Prof. Gardeniers) where oxygen or hydrogen gas bubbles are electrocatalytically generated. As a second example, we have also noticed that in one of our heated microreactors gas bubbles in a multiphase flow microenvironment tend to follow the locations of highest temperatures. We are working on an explanation of this interesting phenomenon in close collaboration with the Physics of Fluids group of Prof. Lohse. Lastly, we recently started a collaboration with PhD student Ahmed Ismail of Utrecht University (supervised by Profs. De Groot and Weckhuysen) to study catalysts for water splitting using X-ray spectroscopy. I'm very enthusiastic about these collaborations, which would most likely not have been initiated without the MCEC program.

Scientific research
Ivo Filot



Ivo Filot (1985)

Eindhoven University of Technology

MCEC tenure track

Assistant Professor Computational Catalysis

Catalysis is at its core a multiscale phenomenon. At the molecular level, the composition and chemical structure of the catalyst determine the possible reaction pathways. Such pathways allow us to convert reactants towards desired products, which are in the absence of a catalyst sometimes very difficult to synthesize. The reaction networks are determined by the quantum chemical laws of nature and are fundamentally difficult to explore and computationally very demanding to simulate.

To develop an (idealized) holistic understanding of catalysis, we need to be able to connect the molecular information to any meso- or macroscopic simulation. For this, new computational routines need to be developed that reduce the computational costs originating from both the complexity that quantum systems entail and the combinatorial complexity that arises by the number of chemical interactions when upscaling to larger length scales. The focus of my research is to develop such routines and use them to develop a broad yet comprehensive picture of those catalytic processes that are currently crucial to solve the energy and environmental grand challenges our world faces.

Over the past five years, I have studied the possibility of connecting simulations that operate at fundamentally different length and timescales. Though such connections are technically possible and proven to be insightful, they are limited in their applicability due to the underlying assumptions that need to be made to reduce the computational costs of such simulations. My focus within the MCEC program is to expand on this knowledge and develop routines that are able to model catalytic processes at much higher level of detail. Furthermore, we aim for a broader scope than what is currently available and remove as many assumptions as possible that limit the applicability of these simulations. This research endeavour is fundamental in nature and is readily applicable to the three research topics defined within the MCEC program.

As a stepping stone towards more advanced routines, we are currently developing a reactive force field to describe the Fischer-Tropsch synthesis process. This force field should enable us to study this important catalytic reaction at the mesoscopic scale. Simulations at this level can be readily validated by already existing experimental data at the molecular level (Hensen group) and the macroscopic level (Kuipers group). This first research step will answer fundamental questions as to what parameters and data are required at both the molecular and macroscopic level to construct mesoscale simulations and how we should fit and validate simulation routines.

The long-term goal is to look beyond force fields. Despite the flexibility offered by the parametrization of the force field, any force field places at least some constraints on its calculations due to the underlying mathematical functions and computational routines. The next step is to develop a force field which is able to train itself, not only in terms of the underlying parameters, but even at which functions and routines to use. Such kind of full dynamical force fields may be able to model the most complex of catalytic reactions at only a fraction of the cost of a conventional quantum chemical calculation, enabling us to simulate heterogeneous catalysis at the mesoscopic scale.

List of abbreviations

ARC CBBC	Advanced Research Center Chemical Building Blocks Consortium
FMS	Research Center for Functional Molecular Systems
JMBC	J.M. Burgerscenter
ISPT	Netherlands Research School in Process Technology
MT	Management Team
NIOK	Netherlands Institute for Catalysis Research
NWO	Netherlands Organization for Scientific Research
OCW	Dutch Ministry of Education, Culture and Science
PD	Postdoc
PI	Principal Investigator
SAB	Scientific Advisory Board
SB	Supervisory Board
TU/e	Eindhoven University of Technology
UT	University of Twente
UU	Utrecht University

Appendix

Appendix I: Abstract of the MCEC program application

Research teams from the fields of Chemistry, Physics and Engineering at the universities of Utrecht, Eindhoven, and Twente propose an ambitious research program on Multiscale Catalytic Energy Conversion to jointly address one of the Grand Challenges our society faces today, i.e. sustainable energy conversion. The current inefficient use of fossil resources as well as the gradual shift to new, more sustainable resources demand that our traditional chemical conversion processes are redesigned. More efficient and sustainable production of fuels and chemicals requires the development of smart catalyst-reactor combinations with optimal transport of heat and mass at every length scale, i.e. from the atomic level to the level of the actual reactor. The ultimate program aim is to develop radically improved catalytic energy conversion processes through full control over the structural complexity of catalyst materials and reactors and that are capable of efficiently converting the feedstocks of today and tomorrow.

The six main applicants are internationally leading scientists in the diverse fields of catalysis, soft condensed matter, multiscale modeling & theory, physics of fluids, chemical reactor engineering and nano- and microfluidics. Together, these disciplines span all relevant length scales of catalytic conversion processes. This program allows them to join forces and combine their expertise in the Netherlands Center for Multiscale Catalytic Energy Conversion (MCEC). This interdisciplinary center will provide a solid organizational basis that allows the multi-facetted frontiers of catalytic complexity to be tackled for the first time in an integrated manner. MCEC brings together a group of 30 scientists, both established, internationally renowned senior scientists and young, up-and-coming talent. Indeed, in addition to doing frontier research, an important objective of MCEC is to attract, educate, and foster talent and to train them in the multidisciplinary approach that the complex, multiscale systems at hand require.

We seek to make step changes in our ability (i) to make complex catalyst materials that are hierarchically structured up to the mesoscale, for instance by controlled self-organization, and combine these novel materials with innovative reactor concepts, such as micro-structured/high gravity multiphase reactors, (ii) to develop theoretical models that predict from first principles the activity, dynamics and accessibility of the active sites within complex catalyst particles and combine these with quantitative models on mass and heat transport phenomena within complex, structured reactors, and (iii) to measure what happens during catalytic processes by developing spectroscopic and microscopic tools to study catalytic activity, to validate the developed synthesis methods for the catalyst particles, and to validate new quantitative models for multiscale modeling of multiphase flows in reactors.

Three Scientific Challenges have been defined: (i) Mastering catalytic events; (ii) Mastering complex multiscale structures and (iii) Mastering mass & heat flow. Each challenge focuses on the fundamental questions of the nanoscopic, mesoscopic and macroscopic worlds of a catalytic process. Together they cover all length scales. This multiscale approach is expected to result in a thorough understanding of a) the emergence of collective properties, e.g. meta-materials of which the activity/selectivity of the sum exceeds that of the individual parts, b) cooperativity/communication between seemingly disparate chemical and physical phenomena, and c) the effects of defects and interfaces, i.e. sites that can be the actual active site, but also a transport barrier or the origin or location of physicochemical phenomena, such as surface nanobubbles.

All the knowledge, experimental tools and theoretical models developed within these Scientific Challenges will be integrated in three Technological Challenges. These Technological Challenges thus cover all length scales of a catalytic process and fully integrate the different disciplines. The Technological Challenges each focus on a resource (i.e., methane/synthesis gas, biomass, and solar energy), representing the gradual shift in composition of our energy mix from one based mostly on fossil resources to a more and more sustainable one. The research efforts will ultimately culminate in three devices for energy-efficient production of the current and future fuels and chemicals. The devices serve as a showcase how the combination of highly structured, hierarchical catalyst materials with innovative reactor concepts will result in step changes in energy-efficiency by addressing each of the length scales involved.

Catalysis is at the very heart of the Dutch chemical industry, with all fuels and most chemicals going through a catalytic conversion step in their production. The novel catalyst-reactor combinations, as well as the models and spectroscopic and microscopic tools developed in this program are therefore expected to make a large impact on the current energy conversion processes and guide the way for future ones. Moreover, the developed knowledge and methods are not limited to the field of catalysis as they are also highly relevant and equally applicable to other important functional materials, such as batteries, fuel cells, diagnostic devices, photonic devices, electronics and drug delivery systems. Thus, we expect that our research program will certainly impact other fields of science.

Appendix II: Composition of governing bodies

Management Team

Members	Affiliation
Prof. Bert Weckhuysen ***Scientific Director***	Utrecht University
Prof. Alfons van Blaaderen	Utrecht University
Prof. Rutger van Santen	Eindhoven University of Technology
Prof. Hans Kuipers	Eindhoven University of Technology
Prof. Detlef Lohse	University of Twente
Prof. Albert van den Berg	University of Twente
Prof. Emiel Hensen	Eindhoven University of Technology ** as of 2016 new member*

Supervisory Board

Members	Affiliation
Prof. Gerrit van Meer	Utrecht University, Dean Faculty of Science
Prof. Frank Baaijens	Eindhoven University of Technology, Rector Magnificus ** as of May 1, 2015*
Prof. Dave Blank	University of Twente, former Director of MESA+ Institute for Nanotechnology, Chief Scientific Ambassador ** as of September 1, 2015*

Scientific Advisory Board

Members	Affiliation
Prof. Gert-Jan van Heijst ***Chairman***	Eindhoven University of Technology
Prof. Klavs Jensen ***Vice-chairman***	Massachusetts Institute of Technology
Prof. Daan Frenkel	University of Cambridge
Prof. Lynn Gladden	University of Cambridge
Prof. Jacques Magnaudet	Institut de Mécanique des Fluides de Toulouse
Prof. Jens Nørskov	Stanford University
Prof. Robert Schlögl	Fritz Haber Institute of the Max Planck Society
Prof. Unni Olsbye	University of Oslo ** as of 2016 new member*

Team Education Committee

Members	Affiliation
Prof. Hans Kuipers ***Chairman***	TU/e
Dr. Rosa Bulo	UU
Prof. Rob Lammertink	UT
Dr. Johan Padding	TU/e

Team Community

Members	Affiliation
Dr. Mathieu Odijk ***Chairman***	UT
Ivan Devic (MSc)	UT
Robin Geitenbeek (MSc)	UU
Teresa de Martino (MSc)	TU/e
Anne-Eva Nieuwelink (MSc) ***Student representative***	UU
Aditya Sengar (MSc) ***Student representative***	TU/e
Miguel Solsona (MSc)	UT
Lennart Weber (MSc)	UU

Team Events

Members	Affiliation
Dr. Pieter Bruijnincx	UU
Prof. Niels Deen	TU/e
Prof. Han Gardeniers	UT

Team Outreach **** Established in 2016***

Members	Affiliation
Dr. Ivo Filot ***Chairman***	TU/e
Robin Broos (MSc)	TU/e
Hai Le The (MSc)	UT
Aura Visan (MSc)	UT

Team Fostering talent **** Established in 2016***

Members	Affiliation
Prof. Albert van den Berg ***Chairman***	UT
Dr. Rosa Bulo	UU
Dr. Ivo Filot	TU/e
Prof. Han Gardeniers	UT

MCEC office

Members	Affiliation
Emke Molnar ***Managing Director***	UU
Christine Geense ***Communication Officer***	UU
Pieter Thijssen ***Financial Officer***	UU

Appendix III: MCEC community

Appendix III: MCEC community

List of the co-applicants according to MCEC program application

	Members	Affiliation
Chemistry	Dr. Monica Barroso	UU
	Dr. Pieter Bruijnincx	UU
	Prof. Frank de Groot	UU
	Prof. Emiel Hensen	TU/e
	Prof. Krijn de Jong	UU
	Prof. Petra de Jongh	UU
	Prof. Andries Meijerink	UU
	Dr. Evgeny Pidko	TU/e
	Prof. Nico Sommerdijk	TU/e
Physics	Prof. Marjolein Dijkstra	UU
	Dr. Marijn van Huis	UU
	Prof. Rob Lammertink	UT
	Prof. Devaraj van der Meer	UT
	Prof. Andrea Prosperetti	UT
	Dr. Jacco Snoeijer	UT
	Prof. Harold Zandvliet	UT
Engineering	Prof. Niels Deen	TU/e
	Prof. Jan Eijkel	UT
	Dr. Séverine le Gac	UT
	Prof. Han Gardeniers	UT
	Prof. Volker Hessel	TU/e
	Dr. Xander Nijhuis	TU/e ** as of March 1, 2015 new position at SABIC*
	Prof. Jaap Schouten	TU/e
	Prof. Martin van Sint Annaland	TU/e

List of scientists additionally involved in supervising MCEC projects

	Members	Affiliation
Chemistry	Dr. Rosa Bulo	UU
	Dr. Ivo Filot ***MCEC Assistant Professor***	TU/e
	Dr. Jan Philipp Hofmann	TU/e
	Dr. Celso de Mello Donega	UU
	Dr. Jovana Zecevic	UU
Physics	Dr. Laura Filion	UU
	Dr. Arnout Imhof	UU
	Dr. Stefan Kooij	UT
	Dr. Mathieu Odijk ***MCEC Assistant Professor***	UT
	Dr. Wouter Olthuis	UT
	Dr. Leo Pel	TU/e
	Dr. Freddy Rabouw ***MCEC Assistant Professor***	UU ** as of January 1, 2017*
	Prof. Frederico Toschi	TU/e
	Prof. Roberto Verzicco ***MCEC Professor***	UT
	Prof. Xuehua Zhang ***MCEC Professor***	UT
Engineering	Dr. David Fernandez Rivas	UT
	Dr. Fausto Gallucci	TU/e
	Prof. Gunther Kolb	TU/e
	Dr. Johan Padding	TU/e
	Dr. Frank Peters	TU/e
	Dr. Chao Sun	UT

Appendix IV: Overview MCEC projects organized by project clusters

Biomass Conversion

Coordinated by Pieter Bruijnincx & Niels Deen

Project	Position	University	Project leader / first supervisor	Candidate	Start
Bio-oil to chemicals and fuels: (in-situ) catalyst deactivation studies at multiple length scales	PhD	UU	Prof. Bert Weckhuysen	Beatriz Luna Murillo	1-11-2015
Integrated and structured Fluid Catalytic Cracking reactor: Gas-(liquid)-solid multiscale modeling of a riser reactor with draft tube for intensified and uniform phase contacting	PhD	TU/e	Prof. Niels Deen	Lijing Mu	15-10-2014
Catalytic biomass conversion by porous oxides	PhD	TU/e	Prof. Emiel Hensen	Evgeny Uslamin	5-1-2015
Theory of Lewis acid zeolite catalysis for biomass conversion	PhD	TU/e	Prof. Emiel Hensen	Roderigh Rohling	1-1-2015
Polyalcohol reforming to synthesis gas as logistic fuel for mobile fuel cell applications	PD 2y	TU/e	Prof. Gunther Kolb	Vetrivel Shanmugam	30-4-2015
Surface heterogeneity and interfacial transport	PhD	UT	Prof. Rob Lammertink	Aura Visan	1-8-2014
Acidic water in zeolite pores: Multiscale modeling of water-active site interactions *	PhD	UU	Prof. Bert Weckhuysen	Katarina Stanciakova	1-9-2015
In-situ studies porous materials synthesis	PhD	TU/e	Prof. Emiel Hensen	Jan Wiesfeld	1-10-2014
Surface enhanced spectroscopy in a flow-through microfluidic chip	PhD	UT	Dr. Mathieu Odijk *MCEC Assistant Professor*	*New project in 2016*	

*** Strong collaboration with project cluster Nanobubbles**

Syngas Conversion

Coordinated by Hans Kuipers & Rutger van Santen

Project	Position	University	Project leader / first supervisor	Candidate	Start
Direct conversion of synthesis gas to aromatics	PhD	UU	Prof. Krijn de Jong	Lennart Weber	1-1-2015
Kinetics and mechanism of syngas chemistry	PhD	TU/e	Prof. Emiel Hensen	Robin Broos	19-1-2015
Realistic systems: Multi-component intra-particle transport + catalytic conversion and coupling of multi-component particle model to MC-DNS-boundary Layer effects in catalytic conversion: MC-DNS study of coupled heat and mass transfer with catalytic surface reaction	PhD	TU/e	Prof. Hans Kuipers	Jiangtao Lu	1-9-2014
Influence of wall corrugation on mass transfer in liquid catalytic reactors	PhD	TU/e	Dr. Johan Padding	Aditya Sengar	1-7-2015
Supraparticles for catalysis	PhD	UU	Prof. Alfons van Blaaderen	Ramakrishna Kotni	15-1-2016
Liquid-phase TEM and cryo-TEM of fundamentals of catalyst assembly	PhD	UU	Prof. Krijn de Jong	Petra Keijzer	1-10-2016
Mesoscale modeling in catalysis	PhD	TU/e	Dr. Ivo Filot *MCEC Assistant Professor*	*New project in 2016*	

Future Methodologies in Catalysis & Solar Fuels

Coordinated by Alfons van Blaaderen & Emiel Hensen

Project	Position	University	Project leader / first supervisor	Candidate	Start
Catalyst particle-embedded luminescent nanoparticles for temperature sensing	PhD	UU	Prof. Andries Meijerink	Robin Geitenbeek	15-11-2014
XPS double feature: Towards a comprehensive description of photoelectrochemical processes on model photoelectrodes under in-situ conditions	PD 3y	TU/e	Prof. Emiel Hensen	Freddy Oropeza Palacio	1-09-2016
Single catalyst particle diagnostics: Integrating biomass and solar catalysis with optical spectroscopy within a microreactor device *	PhD	UU	Prof. Bert Weckhuysen	Anne-Eva Nieuwelink	1-10-2015
Thermodynamic and kinetic analysis of anqueous phase reforming by high pressure and temperature microfluidics	PhD	UT	Dr. Séverine Le Gac	Renée Ripken	1-4-2015
From nanoscale (photo)electrolytic gas generation via microscale bubble nucleation to macroscale bubble transport *	PhD	UT	Prof. Han Gardeniers	Peter van der Linde	1-1-2015
Self-assembled semiconductor nanorod membranes for photocatalytic water splitting *	PhD	UU	Dr. Celso De Mello Donega	Christa van Oversteeg	1-10-2015
Single catalytic conversion events using fluorescence correlation spectroscopy	PhD	UU	Dr. Freddy Rabouw ***MCEC Assistant Professor***	Stijn Hinterding *New project in 2016*	1-11-2016

*** Strong collaboration with project cluster Nanobubbles**

Fluidic Systems

Coordinated by Hans Kuipers & Detlef Lohse

Project	Position	University	Project leader / first supervisor	Candidate	Start
Flow structure formation and evolution of gas-liquid solid reactive flows and coupling with turbulence	PhD	TU/e	Dr. Johan Padding	Maxim Masterov	1-2-2015
Chemical reactions & mixing in turbulent multiphase flow with active & passive catalytic particles	PhD	UT	Prof. Detlef Lohse	Peter Dung	1-8-2016
Self-propelled particles to enhance catalysis *	PD 2y	UU	Prof. Alfons van Blaaderen	Ajoy Kandar	11-4-2016
Open micro-structured random packing in gas-liquid solid reactors for Fischer-Tropsch catalyst: reactor development (proof of principle)	PhD	TU/e	Prof. Jaap Schouten	Teresa De Martino	7-1-2015
Open micro-structured random packing in gas-liquid solid reactors for Fischer-Tropsch catalyst: multiscale reactor modeling	PhD	TU/e	Prof. Hans Kuipers	Vishak Chandra	1-10-2015
MRI flow imaging in dense gas-solid fluidized beds	PhD	TU/e	Prof. Hans Kuipers	Paolo Lovreglio	1-9-2014

*** Strong collaboration with project cluster Nanobubbles**

Nanoreactors

Coordinated by Albert van den Berg & Bert Weckhuysen

Project	Position	University	Project leader / first supervisor	Candidate	Start
Nanoreactors for in-situ X-ray spectroscopy and microscopy	PhD	UU	Prof. Frank de Groot	Ahmed Mohammed Ismail	1-9-2015
Single catalyst particle diagnostics: Droplet microreactor platform	PhD	UT	Prof. Albert van den Berg	Jeroen Vollenbroek	15-7-2016
Single catalyst particle diagnostics: Integrating impedance sensing & sorting	PhD	UT	Prof. Albert van den Berg	Miguel Solsona	1-3-2015
Supraparticles by microfluidics	PhD	UU	Prof. Alfons van Blaaderen	Chris Kennedy	1-9-2015
Hydrodynamics and interaction of self-assembly in droplet confinement	PhD	UU	Prof. Marjolein Dijkstra	Giulia Fiorucci	1-4-2015

Nanobubbles

Coordinated by Detlef Lohse & Bert Weckhuysen

Project	Position	University	Project leader / first supervisor	Candidate	Start
Can we observe surface nanobubbles during biomass catalysis on zeolite surfaces? An Operando AFM-Vibrational Spectroscopy study	PhD	UU	Prof. Bert Weckhuysen	Laurens Mandemaker	1-9-2016
Metal nanoparticles, nanochannels and nanobubbles	PhD	UT	Prof. Jan Eijkel	Hai Le The	1-4-2015
Transporting gas away from a catalyst surface	PhD	UT	Prof. Devaraj van der Meer	Alvaro Moreno Soto	1-4-2015
Idem project: Transporting gas away from a catalyst surface	PD 1y	UT	Prof. Devaraj van der Meer	Pengyu Lyu	1-9-2015
Surface nanobubbles and surface nanodroplets: Theory and numerics for dynamics and collective effects *	PhD	UT	Prof. Detlef Lohse	Ivan Devic	1-11-2014
Surface nanobubbles and surface nanodroplets *	PhD	UT	Prof. Detlef Lohse	José Encarnacion Escobar	1-3-2016
Surface nanobubbles and surface nanodroplets: Lattice Boltzmann numerics for dynamics and collective effects	PD 1y	UT	Prof. Detlef Lohse	Matteo Lulli	1-1-2015
Microscopic study of the initial stages of electrolytic gas production at catalytic surfaces	PhD	UT	Prof. Harold Zandvliet	Edwin Dollekamp	15-1-2015
Electrolytic gas production at catalytic surfaces with alternate current and the resulting chemical reactions	PD 3y	UT	Prof. Detlef Lohse	Vitaly Svetovoy	1-10-2014

*** Strong collaboration with project cluster Future Methodologies in Catalysis & Solar Fuels**

Appendix V: MCEC School 2015 program

Appendix V: MCEC School 2015 program

	Monday	Tuesday	Wednesday	Thursday	Friday
Morning (1^{st} half)	Energy challenge By: Hans Kuipers and Bert Weckhuysen	Microreactors, microfluidics By: Albert van den Berg and Bert Weckhuysen	Single phase flow By: Detlef Lohse	Solar fuels By: Thomas Jaramillo (Stanford University)	**Case study**
Morning (2^{nd} half)	Heterogeneous catalysis: principles and practice By: Bert Weckhuysen	**Outdoor activity**	Multiphase flow & reactors By: Hans Kuipers and Detlef Lohse	Biomass By: Pieter Bruijnincx and Ruud van Ommen (Delft University of Technology) Solar fuels By: Monica Barroso	Syngas production & conversion By: Emiel Hensen and Krijn de Jong
Afternoon (1^{st} half)	Concepts of heterogeneous catalysis By: Rutger van Santen	Structuring by self-assembly By: Alfons van Blaaderen and Marjolein Dijkstra	Expt. & comp. multiphase flow By: Niels Deen and Hans Kuipers	Discussion: Community building	**Presentation case studies**
Afternoon (2^{nd} half)	Introduction case study By: Rosa Bulo, Rob Lammertink and Johan Padding	Structuring by self-assembly By: Alfons van Blaaderen and Marjolein Dijkstra	**Outdoor activity**	**Case study**	Closure
Evening	**Case study**	**Case study**	**Case study**	**Case study**	

Appendix VI: MCEC key publications

Title: Breakthroughs in Hard X-ray Diffraction: Towards a Multiscale Science Approach in Heterogeneous Catalysis
Authors: Z. Ristanović and B.M. Weckhuysen
Journal: Angew. Chem. Int. Ed. **2014**, *53*, 8556-8558.
DOI:10.1002/anie.201404463
** Open access*

Title: A Radical Twist to the Versatile Behavior of Iron in Selective Methane Activation
Authors: M. Ruitenbeek and B.M. Weckhuysen
Journal: Angew. Chem. Int. Ed. **2014**, *53*, 11137–11139.
DOI:10.1002/anie.201407109
** Open access*

Title: X-ray Fluorescence Tomography of Aged Fluid-Catalytic-Cracking Catalyst Particles Reveals Insight into Metal Deposition Processes
Authors: S. Kalirai, U. Boesenberg, G. Falkenberg, F. Meirer, and B.M. Weckhuysen
Journal: ChemCatChem **2015**, *7*, 3674-3682.
DOI:10.1002/cctc.201500710
** Open access*

Title: Determining the Location and Nearest Neighbours of Aluminium in Zeolites with Atom Probe Tomography
Authors: D.E. Perea, I. Arslan, J. Liu, Z. Ristanović, L. Kovarik, B.W. Arey, J.A. Lercher, S.R. Bare, and B.M. Weckhuysen
Journal: Nat. Commun. **2015**, *6*, 7589.
DOI:10.1038/ncomms8589
** Open access*

Title: Quantitative 3D Fluorescence Imaging of Single Catalytic Turnovers Reveals Spatiotemporal Gradients in Reactivity of Zeolite H-ZSM-5 Crystals upon Steaming
Authors: Z. Ristanović, J.P. Hofmann, G. De Cremer, A.V. Kubarev, M. Rohnke, F. Meirer, J. Hofkens, M.B.J. Roeffaers, and B.M. Weckhuysen
Journal: J. Am. Chem. Soc. **2015**, *137*, 6559–6568.
DOI:10.1021/jacs.5b01698
** Open access*

Title: High-Resolution Single-Molecule Fluorescence Imaging of Zeolite Aggregates within Real-Life Fluid Catalytic Cracking Particles
Authors: Z. Ristanović, M. M. Kerssens, A. V. Kubarev, F. C. Hendriks, P. Dedecker, J. Hofkens, M. B. J. Roeffaers, and B. M. Weckhuysen
Journal: Angew. Chem. Int. Ed. **2015**, *54*, 1836-1840.
DOI:10.1002/anie.201410236
** Open access*

Title: Fluid Catalytic Cracking: Recent Developments on the Grand Old Lady of Zeolite Catalysis
Authors: E.T.C. Vogt and B.M. Weckhuysen
Journal: Chem. Soc. Rev. **2015**, *44*, 7342-7370.
DOI:10.1039/C5CS00376H
** Open access*

Title: Life and Death of a Single Catalytic Cracking Particle
Authors: F. Meirer, S. Kalirai, D. Morris, S. Soparawalla, Y. Liu, G. Mesu, J. C. Andrews, and B. M. Weckhuysen
Journal: Science Advances **2015**, *1*, e1400199.
DOI:10.1126/sciadv.1400199
** Open access*

Title: Surface Nanobubbles and Nanodroplets
Authors: D. Lohse and X. Zhang
Journal: Rev. Mod. Phys. **2015**, *87*, 981-1035.
DOI: 10.1103/RevModPhys.87.981

Title: Formation of Surface Nanodroplets under Controlled Flow Conditions
Authors: X. Zhang, Z. Lu, H. Tan, L. Bao, Y. He, C. Sun, and D. Lohse
Journal: Proc. Nat. Acad. Sci. **2015**, *112*, 9253-9257.
DOI: 10.1073/pnas.1506071112
** Open access*

Title: Spontaneous Pattern Formation of Surface Nanodroplets from Competitive Growth
Authors: S. Peng, D. Lohse, and X. Zhang
Journal: ACS Nano **2015**, *9*, 11916-11923.
DOI: 10.1021/acsnano.5b04436

Title: Pinning and Gas Oversaturation imply Stable Single Surface Nanobubbles: An Exact Calculation
Authors: D. Lohse and X. Zhang
Journal: Phys. Rev. E **2015**, *91*, 031003.
DOI: 10.1103/PhysRevE.91.031003

Title: Stick-jump Mode in Surface Droplet Dissolution
Authors: E. Dietrich, E.S. Kooij, X. Zhang, H.J.W. Zandvliet, and D. Lohse
Journal: Langmuir **2015**, *31*, 4696-4703.
DOI: 10.1021/acs.langmuir.5b00653

Title: Gravitational Effect on the Formation of Surface Nanodroplets
Authors: H. Yu, Z. Lu, D. Lohse, and X. Zhang
Journal: Langmuir **2015**, *31*, 12628-12634.
DOI: 10.1021/acs.langmuir.5b03464

Title: Stability of Micro-Cassie States on Rough Substrates
Authors: Z. Guo, Y. Liu, D. Lohse, X. Zhang, and X. Zhang
Journal: J. Chem. Phys. **2015**, *142*, 244704.
DOI: http://dx.doi.org/10.1063/1.4922905

Appendix VII: MCEC awards, prizes and recognitions

Name	Affiliation	Award/Prize/Recognition	Year
Prof. Albert van den Berg	*UT*	Appointed as Scientific Director of the Research Institute for Biomedical Technology and Technical Medicine (MIRA) of the University of Twente	2014
Prof. Detlef Lohse	*UT*	Winning entry at the Gallery of Fluid Motion of the American Physical Society (APS) "Laser impact on a drop" (Van Dyke Prize)	2014
Prof. Bert Weckhuysen	*UU*	Fellow of the American Association for Advancement of Science (AAAS)	2014
Prof. Bert Weckhuysen	*UU*	Appointed as Visiting Professor in the Department of Chemistry of University College London (UCL)	2014
Prof. Bert Weckhuysen	*UU*	Member of the International Advisory Board of the State Key Laboratory of Catalysis (SKLC) of the Dalian Institute of Chemical Physics	2014
Dr. Pieter Bruijnincx	*UU*	Member of The Young Academy of the Royal Netherlands Academy of Arts and Sciences (KNAW)	2015
Prof. Marjolein Dijkstra	*UU*	Appointed as Scientific Director of the Debye Institute for Nanomaterials Science (DINS) of Utrecht University	2015
Prof. Krijn de Jong	*UU*	Member of Academia Europaea	2015
Prof. Hans Kuipers	*TU/e*	Member of the Royal Netherlands Academy of Arts and Sciences (KNAW)	2015
Prof. Detlef Lohse	*UT*	Member of the Max Planck Gesellschaft and External Member of the Max Planck Institute for Dynamics and Self-Organization at Göttingen	2015
Prof. Nico Sommerdijk	*TU/e*	Winner of the Soft Matter and Biophysical Chemistry Award 2015	2015
Prof. Bert Weckhuysen	*UU*	Knight in the Order of the Netherlands Lion	2015

Prof. Bert Weckhuysen	*UU*	Member of the Royal Flemish Academy of Belgium for Science and the Arts (KVAB)	2015
Prof. Bert Weckhuysen	*UU*	“Captain of Science” of the Topteam Chemistry as appointed by Minister Kamp of Economic Affairs	2015
Prof. Bert Weckhuysen	*UU*	Fellow of Chemical Publishing Society Europe	2015

MCEC Office
Universiteitsweg 99
3584 CG Utrecht
The Netherlands

Contact details

Prof.dr.ir. B. M. Weckhuysen
Utrecht University, Scientific Director
T. +31 (0)30 253 4328
b.m.weckhuysen@uu.nl

Mrs. E. Molnar
Utrecht University, Managing Director
T. +31 (0)6 288 344 76
science.mcecoffice@uu.nl

www.mcec-researchcenter.nl

Composed by MCEC Office,
in particular Emke Molnar and Christine Geense
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Netherlands Center for Multiscale Catalytic Energy Conversion (MCEC) addresses one of the grand challenges our society faces today: sustainable energy conversion. This NWO Gravitation Program involves researchers from Utrecht University, University of Twente and Eindhoven University of Technology.

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