

# New Horizons

Annual Report 2012





---

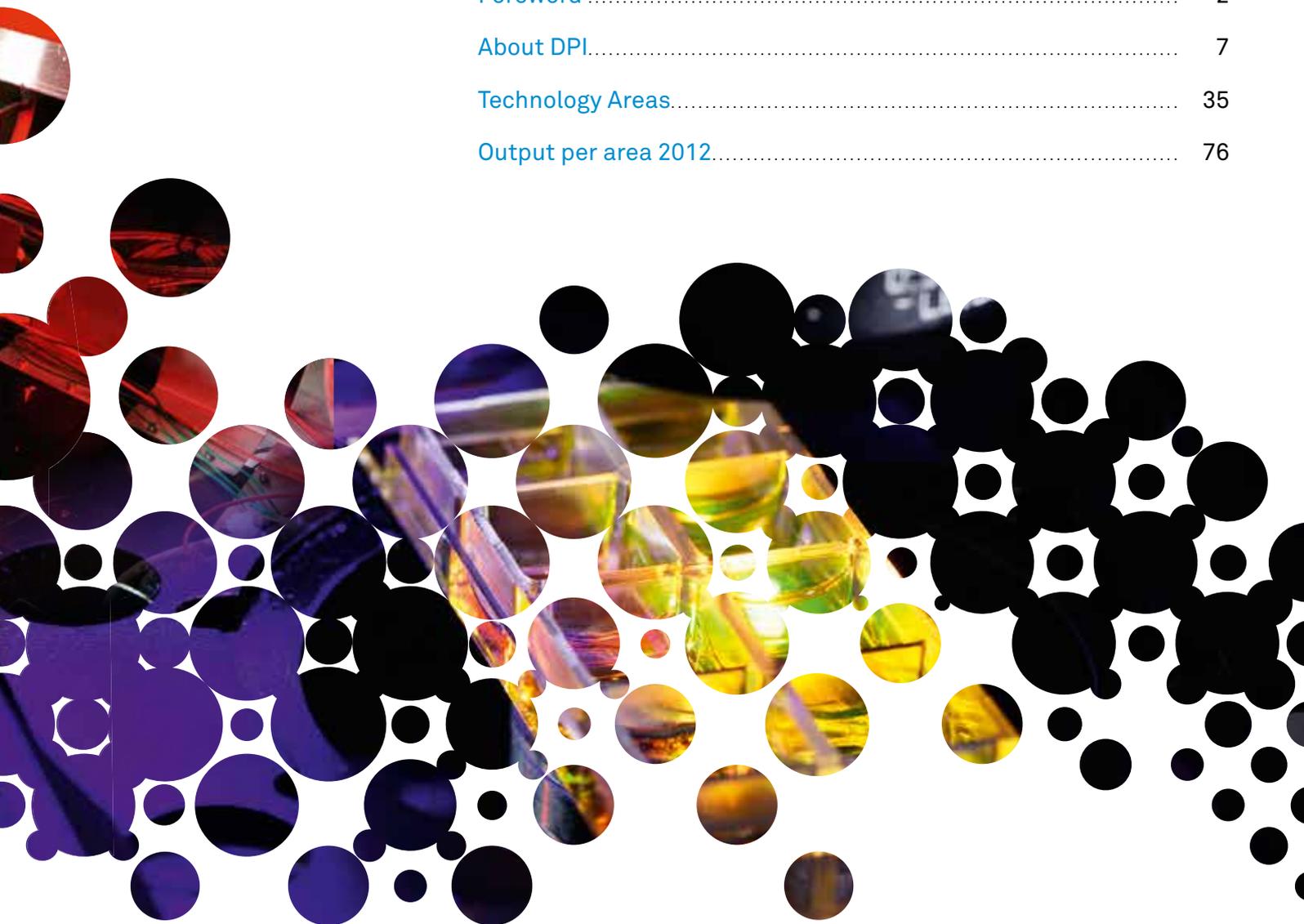
# The art of connecting

The polymer world is facing a number of challenges. There is a growth in market demand, the range and quality of technological options driven by modern science and technology are rapidly increasing. And there is strong pressure from society for sustainability and new technological solutions. The challenges are too broad and too complex to be addressed by a single party. The Dutch Polymer Institute truly addresses those challenges by organising polymer knowledge and connecting polymer technologists through the value chain.

---

## Contents

Foreword .....	2
About DPI.....	7
Technology Areas.....	35
Output per area 2012.....	76



---

# Foreword

## Reaching out

---

2012 marked the fifteenth anniversary of DPI (Dutch Polymer Institute). Did we have reason to celebrate? We believe we did. Over the past decade and a half, DPI has come to represent the best practice in collaborative research and innovation through public-private partnerships. DPI today is a widely acknowledged Centre of Excellence in polymer science and technology, firmly established in Europe and gradually reaching out to other parts of the world.

---

Scientific quality and industrial relevance: these are the mainstays of DPI's success. We specialise in bringing together stakeholders from academia and industry to enable world-class research that has clear industrial relevance. This is what we have been doing for the past fifteen years – and this is what we will continue to do in the future. It is our *raison d'être* – and our unique selling point.

The high reputation we enjoy is also the result of a consistent strategy. In growing our academic and industrial partner base and our project portfolio, we have all along been led by the two guiding principles of coherence and focus. We look for

partners who can strengthen our existing capabilities, or enable us to explore new combinations of scientific knowledge and industrial needs. Our aim is always to reinforce our core business, which is to carry out a world-class pre-competitive R&D programme that generates value for our stakeholders in the polymer value chain. This is also the rationale behind our taking up the coordination role for EU consortia and EU projects. In the years ahead, we will continue to pursue this strategy of coherence and focus, while at the same time exploring new areas of research and extending our partner base to exciting new regions.

### Recognised quality

With its research in the field of polymer science, DPI makes a significant contribution to the high ranking of the Netherlands globally in terms of national research output. The quality of our scientific work continues to improve as we continue to raise the bar. One indicator of our success is the consistently high Citation-Impact Factor we achieve for our scientific publications. In 2011, this was 2.04 – once again more than twice as high as the global average. The average Journal Impact Factor – a measure of the authority of the journals in which our researchers

publish – reached an impressive 4.99 in 2012.

In addition to the recognition that DPI as an institute gets for its achievements, individual DPI scientists are regularly honoured with international awards. For example, in 2012 Dr. Anurag Pandey won the Paul Schlack Man-made Fibres Prize 2012 for his thesis work in a DPI project, while Dr. Wilma Dierkes was granted the ACS Sparks Thomas Award for outstanding contributions and innovations in the field of elastomers by younger scientists, technologists and engineers.

Scientists who have completed their PhD research at DPI have valuable experience in fields that are relevant to industry. And having proved their mettle *vis-à-vis* highly demanding industrial partners at DPI, they have little difficulty finding jobs. Most of them end up being employed by DPI partners.

### Where science and business meet

In its role as a bridge between academia and industry, DPI regularly organises meetings to promote cross-fertilisation of ideas that will lead to new directions in research and innovation.

For example, each year in January we organise a one-day international workshop around a specific theme. Attracting industrial and academic participants from many different countries, the workshop provides a platform for forward-looking, cross-disciplinary discussions that provide insight into the latest developments in science, identify new challenges and point the way to future areas of research. In 2012, the workshop centred on polymer chemistry and synthesis.

### New horizons

In today's rapidly globalising world, international collaboration is not only an economic necessity; increasingly, it is also proving to be a scientific advantage. We are making good progress in extending our international reach, both at the European level and in some high-growth economies such as China and Brazil.

---

DPI TEAM – Top row: John van Haare and Jan Stamhuis. Second row: Peter Kuppens, Jeanne van Asperdt, Renée Hoogers, Peter Nossin, Denka Hristova-Bogaerds and Marc Ruis. Third row: Christianne Bastiaens, Johan Tiesnitsch, Jacques Joosten, Monique Bruining and Martien Cohen Stuart. Fourth row: Shila de Vries, Thomas Manders, Annemarie Steinmann and Leo Robben.



## EU

The European Commission clearly sees DPI as a Centre of Excellence that has the all-round capabilities and the requisite scientific and industrial network to be able to take the lead in exploring and initiating European-level collaboration in polymers, for example under the EU's Seventh Framework Programme.

The Hybrid Materials Workshop organised in Luxembourg in 2010 jointly by DPI and SusChem (the European Technology Platform for Sustainable Chemistry) and sponsored by the European Commission paved the way for collaboration projects within the EU's Seventh Framework Programme, with scope for the participation of players from other non-EU countries, such as Russia. DPI will be coordinating several such projects.

So far, our EU funding proposals have enjoyed an exceptionally high rate of success. Of the two proposals we submitted to the EU, two – the COMPANOCOMP initiative and the SHINE project – were approved and granted funding. A noteworthy element of the COMPANOCOMP initiative is that it is a 50/50 partnership between an EU consortium and a Russian consortium.

In 2012, DPI and DPI Value Centre launched a new initiative: the Polymer Value Chain Projects. The set-up chosen will involve more and different players from the value chain, including SMEs, and will allow international participation under certain conditions.

## Beyond Europe

In order to achieve our ambition of becoming an International Centre of Excellence, it is crucial that we step up our efforts in teaming up with academic

and industrial partners in other countries, especially the high-growth economies of the world. In 2012, we further strengthened our networks in China and Brazil, the two countries that are currently the main focus of our internationalisation efforts, and also gained a stronger foothold in Russia.

In both China and Brazil, there is a growing interest in the DPI approach of promoting cooperation between companies and knowledge institutes. More and more, it is seen as a best practice that academic and industrial stakeholders in these countries could benefit from. And both countries are willing to make substantial financial contributions to joint projects.

In China, DPI has set up a collaboration with the Changchun Institute of Applied Chemistry (CIAC) of the Chinese Academy of Sciences. This is DPI's first academic partner in China. And in Brazil, we have started a collaboration with the National Council for Scientific and Technological Development (CNPq), in which the Eindhoven University of Technology is also participating.

## International talent pool

As a premier league player, it is vital for DPI to be able to attract top-notch scientists who can deliver on the DPI promise of world-class scientific quality in fields that are of relevance to our industrial partners.

International cooperation provides us with an opportunity to tap into the talent pools of other countries in research areas in which they are particularly strong or in which there is a shortage of suitable people in the Netherlands. DPI is increasingly attracting scientists from outside Europe, in particular China.

This not only benefits us but also the scientific communities in these countries. Working in a top-class research organisation like DPI offers these talented and ambitious young scientists an excellent opportunity to familiarise themselves with international scientific practices and conventions and become part of the international science community. DPI sees hosting and guiding foreign scientists as an important part of being an International Centre of Excellence.

## Social responsibility

While much of DPI's work is driven by industrial relevance, we see it as our corporate social responsibility to help address major global challenges that, at least initially, are more of a societal nature. DPI and DPI Value Centre set up a research programme to address Plastic Marine Litter, a complex and challenging problem that can only be solved through collaboration between scientists, industry, environmental organisations and governments.

## The way ahead

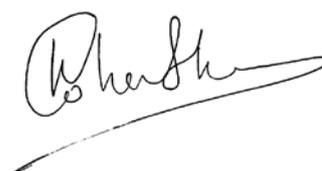
DPI intends to play an active role in initiating and setting up projects under the new Top Consortia for Knowledge and Innovation (TKI) structure introduced by the Dutch government to stimulate research and innovation in the ten top sectors designated for the Netherlands. In 2012, DPI and DPI Value Centre signed the first series of innovation contracts under this new structure and, in partnership with Food & Biobased Research (FBR) in Wageningen (Netherlands), set up the 'TKI Smart Polymeric Materials' (TKI SPM).

The Dutch government's current subsidy commitment to DPI extends until 2016. Although there is still a degree of uncertainty with regard to funding for the years after 2016, we firmly believe that with its past record and its current initiatives, both in the Netherlands and internationally, DPI has a very strong proposition as a key enabler of innovation. We are therefore hopeful that the government – which has always been a key stakeholder in DPI – will take a long-term view and show the same commitment to public-private collaboration and enterprise that DPI and its partners have shown during the past fifteen years.

**Jacques Joosten** – Managing Director



**Martien Cohen Stuart** – Scientific Director



DPI VALUE CENTRE TEAM – Top row:

Johan Tiesnitsch and Jos Lobée.

Second row: Eelco Rietveld, Peter Nossin, Bart van den Berg, Arie Brouwer and Louis Jetten.

Third row: Ineke Laeven, Judith Tesser, Martin van Dord, Peter Koppert, Gerrie Verhoeven and Coco Lenssen.



# Organisation 2012

## Supervisory Board

- **Dr. H.M.H. van Wechem**, *Chairman*
- **Dr. J.A. Roos**
- **Prof.dr. C.J. van Duijn**
- **Dr. F. Kuijpers**
- **Prof. K.C.A.M. Luyben**
- **Dr. M. Wubbolts**

## Council of Participants

- **Prof.dr. G. ten Brinke**  
*University of Groningen, Chairman*

## Scientific Reference Committee

- **Prof.dr. A.J. Schouten**  
*University of Groningen, Chairman*
- **Prof.dr. L. Leibler**  
*Ecole Supérieure Physique et Chimie Industrielles, Paris*
- **Prof.dr. H. Siringhaus**  
*University of Cambridge*
- **Prof.dr. B. Voit**  
*Institut für Polymerforschung, Dresden*

## Executive Board

- **Dr. J.G.H. Joosten**  
*Managing Director, Chairman*
- **Prof.dr. M.A. Cohen Stuart**  
*Scientific Director*

## Programme Area Coordinators

- **Dr. M.J. Bruining**  
*Corporate Research*
- **Dr. H. Gankema**  
*High-Throughput Experimentation, Coatings Technology*
- **Dr. J.A.E.H. van Haare**  
*Functional Polymer Systems, Large-Area Thin-Film Electronics*
- **Dr. P.M.M. Nossin**  
*Bio-Inspired Polymers*
- **Dr. J.E. Stamhuis**  
*Polyolefins, Performance Polymers, Enhanced Oil Recovery, Emerging Technologies*

## Scientific Programme Chairmen

- **Prof.dr. V. Busico**  
*Polyolefins*
- **Prof.dr. C. Creton**  
*Performance Polymers*
- **Prof.dr. F. de Schryver**  
*Functional Polymer Systems*
- **Prof.dr. C.D. Eisenbach**  
*Coatings Technology*
- **Prof.dr. U.S. Schubert**  
*High-Throughput Experimentation*
- **Prof.dr. G. Eggink**  
*Bio-Inspired Polymers*
- **Prof.dr. M.A. Cohen Stuart**  
*Corporate Research and Emerging Technologies*

## Organisation Staff

- **A.F.J. van Asperdt**  
*Financial Administration*
- **C.H.L.M. Bastiaens**  
*Communications*
- **Dr. M.J. Bruining**  
*General Affairs*
- **M.M.G. Heuvelmans**  
*Financial Administration*
- **R. Hoogers**  
*Secretariat*
- **Dr. D.G. Hristova-Bogaerds**  
*Project Manager COMPANOCOMP*
- **S.G. Koenders**  
*Project Administration*
- **P.J.J. Kuppens, AA**  
*Controlling*
- **A.M.G. Steinmann**  
*Project Administration*
- **S.K. de Vries, MSc**  
*Intellectual Property and Legal*

# About DPI



# DPI: International Centre of Excellence in Polymers

In the last few years DPI has transformed itself into an International Centre of Excellence in Polymers. To achieve that goal, the institute has expanded its pre-competitive research programme with projects focussing on pre-commercial and societal themes.

## PRE-COMPETITIVE PROGRAMME

DPI Rules & regulations apply to all projects				
Polyolefins	Performance Polymers	Functional Polymer Systems	Coatings Technology	High-Throughput Experimentation
<b>24 projects</b>	<b>22 projects</b>	<b>18 projects</b>	<b>11 projects</b>	<b>13 projects</b>
<b>Industry</b> <ul style="list-style-type: none"> <li>• Borealis</li> <li>• Braskem</li> <li>• Celanese</li> <li>• Dow Benelux</li> <li>• DSM</li> <li>• ExxonMobil</li> <li>• Freeslate</li> <li>• ITRI</li> <li>• Lanxess Elastomers</li> <li>• LyondellBasell</li> <li>• Petrobras</li> <li>• Sabic</li> <li>• Sinopec</li> <li>• Symyx</li> <li>• Teijin Aramid</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• AkzoNobel</li> <li>• BASF</li> <li>• Bayer</li> <li>• Bekaert</li> <li>• DSM</li> <li>• Lanxess Elastomers</li> <li>• Sabic</li> <li>• SKF</li> <li>• Teijin Aramid</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• BASF</li> <li>• DSM</li> <li>• ECN</li> <li>• Industrial Technology Research Institute</li> <li>• Philips</li> <li>• Rolic Technologies</li> <li>• Sabic</li> <li>• Solvay</li> <li>• TNO</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• AkzoNobel</li> <li>• Altana</li> <li>• DSM</li> <li>• Lawter</li> <li>• Saint Gobain</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• Chemspeed Technologies</li> <li>• Evonik</li> <li>• Forschungsgesellschaft Kunststoffe</li> <li>• Michelin</li> <li>• Microdrop Technologies</li> </ul>
<b>Academia</b> <ul style="list-style-type: none"> <li>• Fraunhofer Institute for Structural Durability and System Reliability LBF</li> <li>• Eindhoven University of Technology</li> <li>• ESCPE-Lyon</li> <li>• Japan Advanced Institute of Science and Technology</li> <li>• Loughborough University</li> <li>• Martin-Luther University of Halle-Wittenberg</li> <li>• Polymer Technology Group Eindhoven</li> <li>• Queens University</li> <li>• Radboud University Nijmegen</li> <li>• University of Antwerp</li> <li>• University of Amsterdam</li> <li>• University of Groningen</li> <li>• University of Manitoba</li> <li>• University of Naples Federico II</li> <li>• University of Ottawa</li> <li>• University of Perugia</li> <li>• University of Salerno</li> <li>• University of Udine</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• DWI an der RWTH Aachen</li> <li>• Eindhoven University of Technology</li> <li>• Fraunhofer Institute for Structural Durability and System Reliability LBF</li> <li>• Leibniz-Institut für Polymerforschung, Dresden</li> <li>• National Technical University of Athens</li> <li>• Queen Mary &amp; Westfield College, University of London</li> <li>• University of Amsterdam</li> <li>• University of Groningen</li> <li>• University of Twente</li> <li>• Wageningen University</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• ECN</li> <li>• Eindhoven University of Technology</li> <li>• Imperial College London</li> <li>• Nanoforce Technology</li> <li>• University of Cologne</li> <li>• University of Groningen</li> <li>• University of Wuppertal</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Eindhoven University of Technology</li> <li>• University of Groningen</li> <li>• University of Haute-Alsace</li> <li>• Wageningen University</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Fraunhofer Institute for Structural Durability and System Reliability LBF</li> <li>• Eindhoven University of Technology</li> <li>• Friedrich-Schiller University, Jena</li> <li>• Radboud University Nijmegen</li> </ul>
Expenditure € 2.69 million FTEs 28.8 (46 researchers)	Expenditure € 1.44 million FTEs 14 (26 researchers)	Expenditure € 1.65 million FTEs 16.4 (31 researchers)	Expenditure € 0.86 million FTEs 8.5 (12 researchers)	Expenditure €1.15 million FTEs 11.4 (21 researchers)

## Pre-competitive research programme

DPI's pre-competitive research programme currently embraces ten technology areas. Companies and knowledge institutes can participate in one or more of these areas, each of which encompasses a substantial number of projects. The participating companies jointly define the programmes for the specific technology areas in which they participate. PhD students and post-docs from our partner knowledge institutes perform their research in close

collaboration with scientists from our industrial partners. Shaping that collaboration between industry and academia is the key to building a coherent community that delivers the research results to the envisaged high standard and prepares our scientists for their future careers, in industry or elsewhere.

The interaction between academic researchers and industrial scientists takes various forms. Each project team submits quarterly reports to DPI, while twice a year every researcher also gives a presentation

for all of the partners in the specific technology area to highlight and explain its research results. This enables DPI to monitor, evaluate and steer the projects. The research results are shared within the technology area and all of the partners are free to use the knowledge that is acquired, with the exception of knowledge that is part of an invention. When an invention is reported and partners are interested in using that knowledge, DPI files a patent application and the industrial partners involved in that specific technology area have the first claim to it.

### DPI Rules & regulations apply to all projects

Bio-Inspired Polymers	Large-Area Thin-Film Electronics	Enhanced Oil Recovery	Emerging Technologies	Corporate Research
<b>11 projects</b>	<b>12 projects</b>	<b>3 projects</b>	<b>1 project</b>	<b>26 projects</b>
<b>Industry</b> <ul style="list-style-type: none"> <li>• Food and Biobased Research, Wageningen UR</li> <li>• FrieslandCampina</li> <li>• Petrobras</li> <li>• Sabic</li> <li>• Teijin Aramid</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• BASF</li> <li>• DSM</li> <li>• Philips</li> <li>• Solvay</li> <li>• TNO</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• Shell</li> <li>• SNF</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• DPI partners</li> <li>• M2i partners</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• All DPI partners take part in Corporate Research</li> </ul>
<b>Academia</b> <ul style="list-style-type: none"> <li>• Eindhoven University of Technology</li> <li>• Food and Biobased Research, Wageningen UR</li> <li>• Friedrich-Schiller-University, Jena</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Eindhoven University of Technology</li> <li>• Imperial College London</li> <li>• Max Planck Institute für Polymerforschung</li> <li>• University of Algarve</li> <li>• University of Cologne</li> <li>• University of Groningen</li> <li>• University of Twente</li> <li>• University of Wuppertal</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• University of Groningen</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• Fraunhofer Institute for Structural Durability and System Reliability LBF</li> <li>• Eindhoven University of Technology</li> <li>• ESRF, Grenoble</li> <li>• Foundation for fundamental research on matter (FOM)</li> <li>• Radboud University</li> <li>• TI Food and Nutrition (TIFN)</li> <li>• University of Groningen</li> <li>• University of Twente</li> <li>• Wageningen University</li> </ul>
Expenditure € 1.22 million FTEs 9.8 (19 researchers)	Expenditure € 1.09 million FTEs 11.7 (21 researchers)	Expenditure € 0.25 million FTEs 3.5 (4 researchers)	Expenditure € 0.01 million FTEs 0.3 (one researcher)	Expenditure € 1.86 million FTEs 15.9 (21 researchers)

## Industrial pre-commercial programme

The industrial pre-commercial programme consist of Value Chain projects and EU projects. The conditions for performing Value Chain projects are described below and those of EU projects are generally known and are available on the web.

The Value Chain projects offer companies and/or research institutes the opportunity to establish consortia for innovation projects, in which they collaborate within the value chain. Every partner plays an active role in the project, which must be aimed at further development of the innovation. The projects are intended to

generate economic activity within the foreseeable future (i.e., no later than two to five years after completion of the project).

DPI's role is to actively assist in establishing the collaboration between the partners and to coordinate the project. DPI can also act as coordinator of a project. Particularly when SMEs are involved, DPI works together with the DPI Value Centre.

DPI provides a model framework for the collaboration, but the detailed rules are agreed between the members of the consortium. As regards intellectual property, the basic principle is that the knowledge created during the course of

the project (foreground knowledge) is the property of the inventing partner, and any background knowledge contributed to the project remains the property of the partner that provided it. Other partners have free access to the knowledge contributed to and/or generated during the project, but only to the extent necessary for developments in the project. Specific agreements are made to enable access to another partner's IP for commercial application of the knowledge outside the project.

### PRE-COMMERCIAL PROGRAMME

Model framework for collaboration		
Rules and regulations set by involved partners	Rules and regulations set by involved partners	Rules and regulations set by involved partners
<b>CompNano Comp</b> (1-10-2011/ 30-9-2014)	<b>SHINE</b> (1-2-2013/31-7-2016)	<b>Value Chain projects</b>
<b>Partners</b> <ul style="list-style-type: none"> <li>• DPI</li> <li>• Rhodia</li> <li>• National Technical University of Athens</li> <li>• Eindhoven University of Technology</li> <li>• Centre National de la Recherche Scientifique - Laboratoire Polymères et Matériaux Avancés</li> <li>• General Electric</li> <li>• European Centre for Nanostructured Polymers</li> <li>• University of Ulm</li> <li>• Lomonosov Moscow State University</li> <li>• Institute of Macromolecular Compounds St. Petersburg</li> <li>• National Research Centre Kurchatov Institute</li> <li>• Phys Chem Ltd</li> </ul>	<b>Partners</b> <ul style="list-style-type: none"> <li>• DPI</li> <li>• Acciona Infraestructuras</li> <li>• Arkema</li> <li>• BIWI SA</li> <li>• Cidetec</li> <li>• Critical Materials</li> <li>• ESPCI ParisTech</li> <li>• Forschungszentrum Jülich</li> <li>• Fraunhofer UMSICHT</li> <li>• MTA-TTK</li> <li>• SKF Engineering &amp; Research Centre</li> <li>• Teijin Aramid</li> <li>• Delft University of Technology</li> </ul>	<a href="#">For details, see page 26</a>
Budget €2.2 million (€1.5 million EU subsidy)	Budget €6.4 million (€4.0 million EU subsidy)	

## Projects driven by societal themes

DPI is confronted with new demands from society in relation to scientific research into polymers. A major international issue is that of 'plastic soup', the vast volumes of plastic waste that accumulate in certain areas of the oceans and seas and harm the ecosystem. DPI has become increasingly aware in recent years that companies, knowledge institutions and the government are not its only stakeholders. Society at large can also benefit from the knowledge and expertise generated by the DPI community as a source of possible solutions for societal issues such as 'plastic soup'.

### SOCIETAL PROGRAMME

#### Plastic Marine Litter (to prevent plastic from ending up in the oceans)

Start date 1-9-2012

##### Partners

- DPI
- DPI Value Centre
- IMSA
- Stichting De Noordzee
- University Utrecht
- Kruidenier Foodservices
- SABIC
- Van Gansewinkel

**DPI achieved several milestones in pursuit of its ambition of becoming an International Centre of Excellence in Polymers in 2012. The principal achievements were its further internationalisation, the start of 13 Value Chain projects and the approval and funding of a European project.**

#### Internationalisation

When DPI updated its strategy in 2010, one of the plans it announced was the intention to intensify international collaboration, particularly with partners in the emerging economies of Brazil and China. DPI had established its first contacts with Brazilian institutes in 2008. In last year's Annual Report, we announced the news that DPI, Eindhoven University of Technology, and Brazil's CNPq (National Council for Scientific and Technological Development) had signed a Letter of Understanding for a collaboration agreement. The three partners worked out the details of the collaboration in 2012 and five projects started in January 2013. The research in these five studies, which will focus on developing and finding applications for biopolymers and polyolefins, will be carried out by eleven PhD students and two post-docs as part of a transatlantic exchange programme.

DPI has also built up strong relationships with Chinese companies and knowledge institutes in the last few years. DPI had the pleasure of welcoming Sinopec as its first Chinese industrial partner in 2011, and in

2012 the Changchun Institute of Applied Chemistry (CIAC) was awarded a project, which started in January 2013. The CIAC, DPI's first academic partner in China, is joining DPI's Coatings Technology programme. Over the next five years, between five and ten PhDs and post-docs will be working on the 'Preparation and Characterisation of Model Waterborne Clearcoats' project under the supervision of Professor Yongfeng Men. The aim of the project is to develop new methods of preparing waterborne resins, as well as methods of monitoring and characterising the drying process.

#### Value Chain Projects

Another component of DPI's strategy was to set up a pre-commercial programme with projects along the knowledge chain or along the value chain. At the beginning of 2012, DPI and DPI Value Centre opened a call for proposals for these kinds of projects. For each proposal, there must be at least four parties involved, including at least one SME, and the aim of the project has to be the development of an innovation. Projects should also generate economic activity within the foreseeable future (i.e., no later than two to five years after completion of the project).

The first thirteen proposals were approved in April and the first projects started in May. In September DPI and DPI Value Centre organised a kick-off meeting where presentations were given about the pro-

jects. The participants were all very positive about the set-up of the projects and expect them to produce valuable results.

#### European success

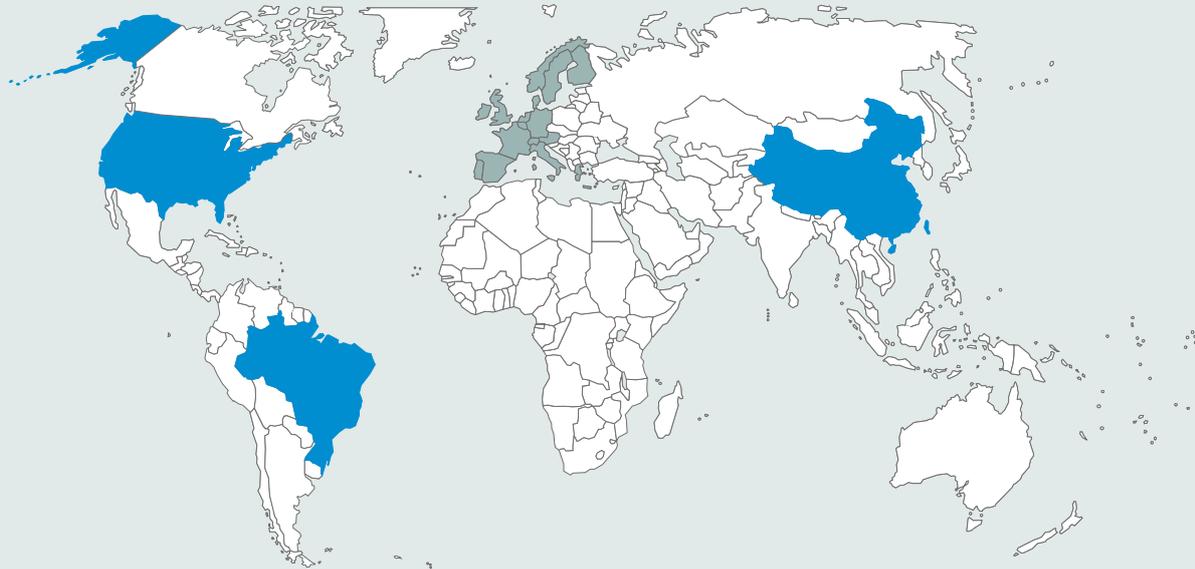
In June of 2012 we received the news that the SHINE project, our second proposal under the Seventh Framework Programme of the European Commission, had been approved. After some negotiations, funding was also secured and the project was ready to start in February 2013. The aim of the SHINE project is to develop self-healing elastomers for dynamic seals and vibration and noise abatement systems. The overall impact of the project could be enormous because of the anticipated effects in three domains:

- economic impact: long-lasting and cost-saving seals for vehicles, heavy-duty seals for wind turbines, vibration abatement systems for roads and bridges, noise abatement systems, asphalt mixtures;
- social impact: increased reliability, enhanced safety, fewer accidents;
- environmental impact: reduction of maintenance costs, energy savings, cuts in pollutants.

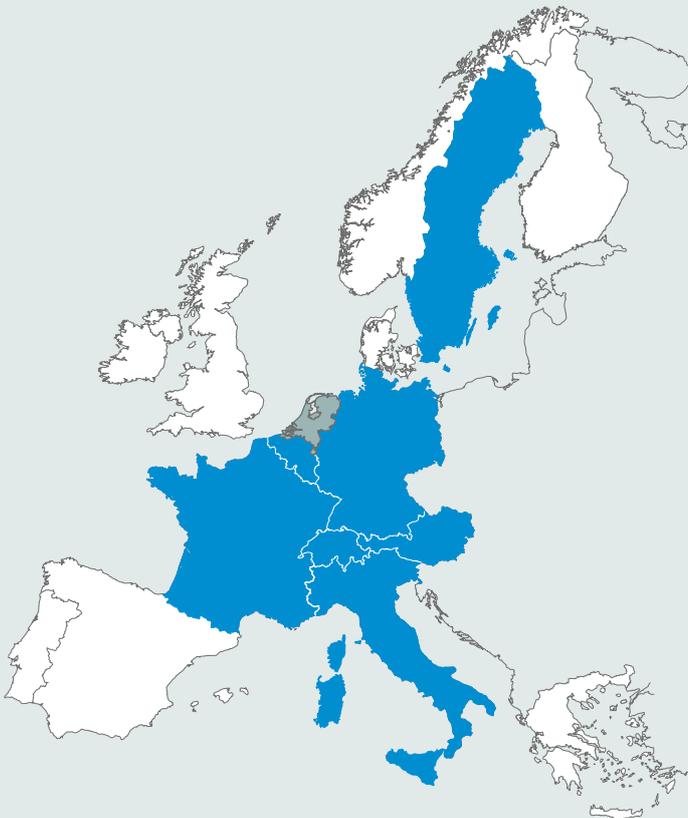
The consortium carrying out the project consists of two universities, four research centres, five large companies and one SME. The total budget is € 6.4 million, including an EU subsidy of € 4.0 million.

# Partners Industry 2012

## North and South America, Asia



## Europe



	Altana
	BASF
	Bayer
	Bekaert
	Borealis
	Celanese
	Chemspeed Technologies
	Evonik
	Forschungsgesellschaft Kunststoffe



**Braskem**

Braskem

**ExxonMobil**

ExxonMobil

**ITRI**  
Industrial Technology  
Research Institute

Industrial Technology Research  
Institute Taiwan

**freeslate**

Freeslate (new per 2012)

**PETROBRAS**

Petrobras

**SINOPEC**

Sinopec

**Symyx**

Symyx

## The Netherlands



**AkzoNobel**

AkzoNobel

**Dow**

Dow Benelux

**DSM**  
FOOD & BIOMASS RESEARCH  
WAGeningen UR

DSM

**ECN**  
Energy Research Centre of the Netherlands

ECN

**FOOD & BIOMASS RESEARCH**  
WAGeningen UR

Food and Biobased Research  
Wageningen UR

**FrieslandCampina**

FrieslandCampina

**LANXESS**  
Empowering Chemistry

Lanxess Elastomers

**LAWTER**

Lawter (new per 2012)

**PHILIPS**

Philips

**سابك**  
sabic

Sabic

**SHELL**

Shell

**TEIJIN**  
Human Chemistry. Human Solutions

Teijin Aramid

**TNO** innovation  
for life

TNO

**lyondellbasell**

LyondellBasell

**MICHELIN**

Michelin

**microdrop**  
TECHNOLOGIES

Microdrop Technologies

**ROLIC**

Rolic Technologies (new per 2012)

**SAINT-GOBAIN**

Saint-Gobain

**SKF**

SKF

**SNF FLOERGER**

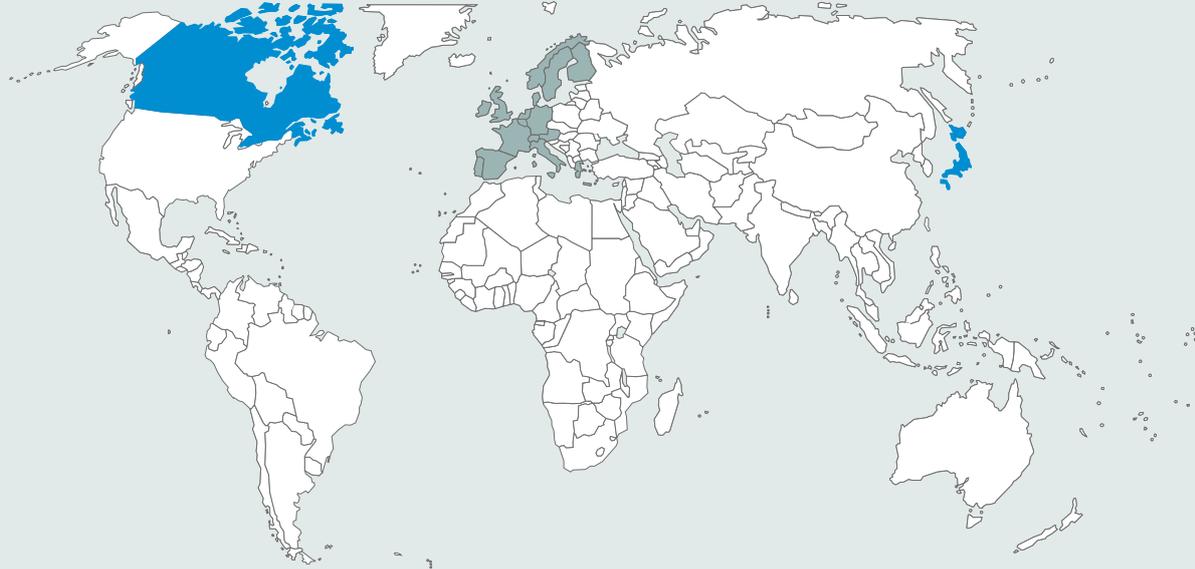
SNF Floerger

**SOLVAY**  
making water "feel different"

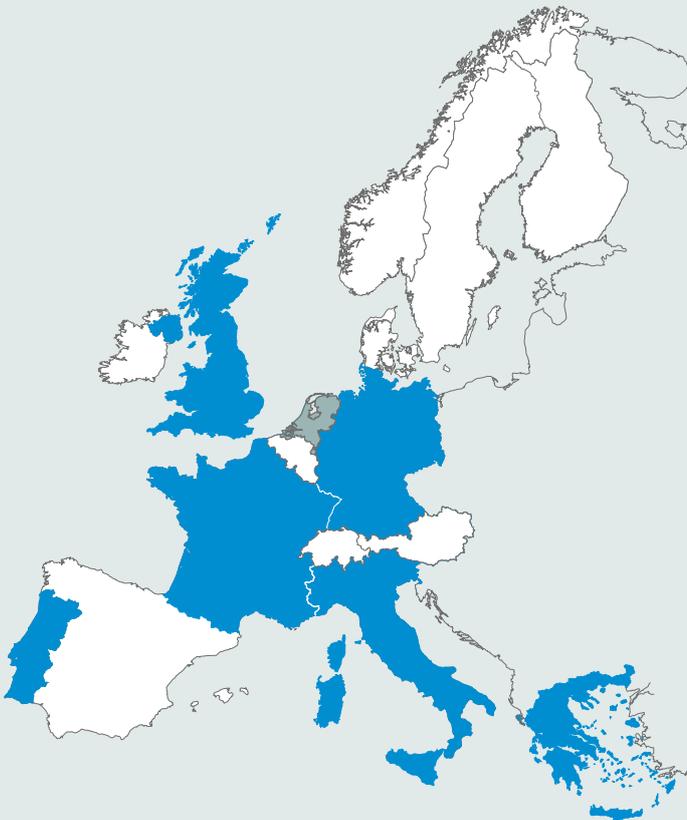
Solvay

# Partners Knowledge institutes 2012

## North America, Africa and Asia



## Europe



	DWI an der RWTH Aachen (new in 2012)
	ESCPE-Lyon
	ESPCI (no research projects in 2012)
	Forschungsinstitut für Pigmente und Lacke (no research projects in 2012)
	Fraunhofer Institute for Structural Durability and System Reliability LBF
	Friedrich-Schiller-University, Jena
	Imperial College London
	Innovent (no research projects in 2012)
	Leibniz-Institut für Polymerforschung Dresden
	Loughborough University
	Martin-Luther-University Halle-Wittenberg
	Max-Planck Institute für Polymer Forschung
	Nanoforce Technology
	National Technical University of Athens



	Japan Advanced Institute of Science and Technology
	Queens University
	University of Manitoba
	University of Ottawa

## The Netherlands



	Queen Mary & Westfield College, University of London
	University of Algarve
	University of Antwerp (new in 2012)
	University of Bayreuth (no research projects in 2012)
	University of Cologne
	University of Duisburg-Essen (no research projects in 2012)
	University of Haute-Alsace
	University of Leeds (no research projects in 2012)
	University of Naples Federico II
	University of Perugia
	University of Salerno
	University of Udine (new in 2012)
	University of Wuppertal

	Delft University of Technology
	ECN
	Eindhoven University of Technology
	Food and Biobased Research Wageningen UR
	NWO
	Polymer Technology Group Eindhoven
	Radboud University Nijmegen
	University Maastricht (no research projects in 2012)
	University of Amsterdam
	University of Groningen
	University of Twente
	Wageningen University

# Summary of financial data 2012

## Income

	(x EUR million)	%
Contributions from industrial partners	3.87	13.3
In-kind contributions from industrial partners	10.57	36.5
Revenue Patents	0.05	0.2
Revenue DPI Value Centre	0.44	1.5
Contributions from knowledge institutes	3.19	11.0
Contributions from Ministry of EA	9.00	31.0
EU FP7 projects	0.78	2.7
Industrial pre-commercial research programme Value Chain	1.10	3.8
<b>Total income</b>	<b>29.00</b>	<b>100</b>

## Expenditure

	(x EUR million)	%
<b>By nature</b>		
Personnel costs	12.40	44.8
Depreciation	0.38	1.4
Other costs	1.75	6.3
In-kind contribution	10.73	38.8
EU FP7 projects	0.79	2.9
Industrial pre-commercial research programme Value Chain	1.60	5.8
<b>Total expenditure</b>	<b>27.65</b>	<b>100</b>

### By Technology Area

Polyolefins	2.69	22.0	
Performance Polymers	1.44	11.8	
Functional Polymer Systems	1.65	13.5	
Coatings Technology	0.86	7.0	
High-Throughput Experimentation	1.15	9.4	
Bio-Inspired Polymers	1.22	10.0	
Large-Area Thin-Film Electronics	1.09	8.9	
Enhanced Oil Recovery	0.25	2.1	
Emerging Technologies	0.01	0.1	
Corporate Research	1.86	15.2	
<b>Sub total</b>	<b>12.22</b>	<b>100</b>	

Knowledge Workers Scheme	0.23
Knowledge Transfer	0.48
Organisation and support	1.14
Support to DPI Value Centre	0.44
In-kind contribution	10.73
EU FP7 projects	0.79
Industrial pre-commercial research programme Value Chain	1.60
Societal theme	0.02

<b>Total expenditure</b>	<b>27.65</b>
--------------------------	--------------

# Key Performance Indicators 2012

## Number of industrial partners



## European governmental funding (% of total funding)



## Number of partner knowledge institutes (universities, etc.)



## Participation of foreign knowledge institutes as % of total expenditure



## Industrial contribution (cash and in-kind) as % of total income



## Overhead costs as % of total expenditure



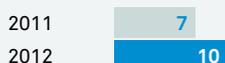
## Contribution Ministry of Economic Affairs as % of total income



## Expenditure for knowledge transfer



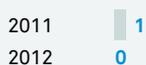
## Number of patents filed by DPI



## Track record DPI researchers

Left in total	60
Employed by partner knowledge institute	20
Employed by non-partner knowledge institute	7
Employed by partner industrial company	12
Employed by non-partner industrial company or start-up	10
Unknown	11

## Number of patents licensed or transferred to industrial partners and DPI Value Centre



## Research output

	2011	2012
Scientific publications	157	159
PhD theses	14	37

Interest shown by industrial partners	8
Interest shown by university partners	0
Interest shown by DPI Value Centre	0

Number of patents to be transferred 8

# DPI Value Centre stretches its boundaries...

In its first five years, DPI Value Centre has established a reputation as the centre of expertise for businesses in any way involved in innovation in relation to polymers and their application.

Small and medium-sized enterprises (SMEs) are curious about the latest developments. They are active participants in our projects and share knowledge at the meetings we organise. Centres of Open Chemical Innovation (COICs), innovation campuses and regional development companies turn to DPI Value Centre for advice on strategies to create new business. We are also cooperating with organisations in Belgium and Germany to involve SMEs in cross border activities and projects. These activities, in which sustainability is a priority, have enormous economic importance.

Companies are constantly searching for new market opportunities. One trend is the search for alternative – sustainable – products and processes. Renewable biobased raw materials, and circular economy are hot topics. The market demands less use of oil-based polymers, so there is growing interest in the application of biopolymers, e.g. biocomposites. In association with NRK, the trade association of the Dutch rubber and plastics industry, and Wageningen University and Research Centre, DPI Value Centre published a booklet on the potential of biobased composites. The first market day on this theme, was well attended. There are not many producers of biocomposites in the Netherlands yet, however, the booklet has attracted a lot of interest.

We collaborate intensively with other institutions in pursuit of innovations in processes, as well as developing biobased and new chemicals, in the top sector Chemicals, a sector that overlaps with other top sectors, including energy, the creative industry, agro&food, and life

**CROSS-BORDER EVENT ON  
ADVANCED MATERIALS**  
14 June 2012



sciences. By expanding our engagement with research into materials to other industries, such as textiles, these activities directly benefit the companies in our network. Our collaboration with Modint, the trade association for the textile industry, led to the appointment of a joint innovation coach and the organisation of a first market day for (bio)fibres. New projects are being developed in areas at the interface of textiles and polymers, such as the production of smart textiles.

New regional, chemical-related business activities are being encouraged in the Netherlands, and DPI Value Centre is closely involved in these efforts, which will enhance opportunities for companies in our sector. DPI Value Centre's know-how makes it easier to select promising ideas

with the prospect of further development into technologies with commercial potential. Established at the Chemelot campus in Geleen (DSM, Sabic, the regional development company Liof), which is attracting a growing number of companies, DPI Value Centre promotes new business at the location, helps to coach companies in innovation, supports start-ups and inspires companies to apply new technologies. In Bergen op Zoom, most of the companies located on the green campus are businesses that use biobased polymers. Major players include Dow, Sabic, Nuplex and the regional-development company Rewin. There are also initiatives to stimulate regional development in the north of the country (Groningen, Emmen and Zwolle), where there has traditionally been a strong textile industry. New

developments focus on applications for (bio)fibres, and there is a growing cooperation with Windesheim University of Applied Sciences and the new Polymer Science Park in Zwolle. In Eindhoven, the cooperation with TU Eindhoven focuses on valorisation of intellectual property.

ARIE BROUWER:

*"Our point of departure is still innovation in polymers. By building an interface with regional partners, we can do more for companies in our target group. We are searching for crossovers with other sectors and exploring the opportunities they offer. Our approach and extensive network are highly valued and generate challenging projects with high economic impact."*

## FIRST CROSS-BORDER EVENT ON ADVANCED MATERIALS

### **Innovate with your neighbours**

As experts will tell you, North-West Europe is a region at the forefront of advanced materials and the development of highly innovative products and processes. The region offers tremendous opportunities and potential for successful cooperation, primarily in the fields of materials, products and processes, but also in tooling and simulation. A benchmarking study has shown that business prospects are further enhanced by transnational cooperation. These factors formed the background to the first Cross-border Event on Advanced Materials, held in Maastricht on 14 June 2012.

The event gave companies and institutes from Belgium, France, the Netherlands and the German federal state of North Rhine-Westphalia an opportunity to meet potential partners for new industrial activities and R&D. The objective was to encourage international partners to work together to stimulate cross-border business cooperation oriented towards innovation

in areas such as technology transfer, market access and network creation.

### **Added value of transnational cooperation**

Politicians also recognise the added value of cross-border cooperation. Mark Verheijen (a member of the Dutch parliament) and Harald Cremer (the director of Cluster NanoMikro\_Werkstoffe NRW in Germany) stressed the economic importance of transnational cooperation. During a debate with executives from the participating organisations: Umberto Baraldi of Sirris (Belgium), Jacques Joosten of DPI (Netherlands), Maudez Le Dantec of Plastipolis (France) and Bärbel Naderer of Cluster Kunststoff NRW (Germany) the opportunities in terms of job creation were also highlighted.

### **Cooperation in the value chain**

Transnational cooperation generates added value for every target group, from large companies and start-ups to suppliers and knowledge institutes. Representatives from each country

discussed part of the chain on the basis of a specific application of their own. As Rolf Scherrenberg from Sabic said, "Cooperation and diversity is key. Success in innovation lies in cooperation with the right partners at the right time."

In two parallel workshop sessions, during which the participants discussed emerging trends, ideas and business opportunities in small groups, each participant had the chance to make contact with potential business partners. This gave them the opportunity to identify new unique selling propositions, generate challenging business ideas and secure support for business development and possible funding. The sessions also produced ideas for a number of projects.

Arie Brouwer, who chaired the meeting, said, "Based on the positive energy, results and reactions of the participants, I'm sure this has been important stepping stone towards closer cooperation in this EUregion. We agreed to organise a second event in 2013 with the international partners."

# IP results 2012

In 2012, DPI filed 10 patent applications on the basis of 22 reported inventions.

The highest number of inventions and subsequent priority filings were produced in the Performance Polymers technology area. The Corporate Research technology area also generated a number of inventions and patent applications that were of interest to our partner companies.

The programme of the Corporate Research technology area serves the DPI community in general, with all of DPI's partner companies participating indirectly in it. By contrast with DPI's other technology areas, however, rather than being steered directly by representatives of the industry partners, the Corporate Research technology area is steered by a programme committee comprising the scientific chairs of the other technology areas. The programme hosts both enabling and conceptual new projects, which makes it all the more remarkable, and gratifying,

that the projects in this area are successful in generating inventions of interest to DPI's partners.

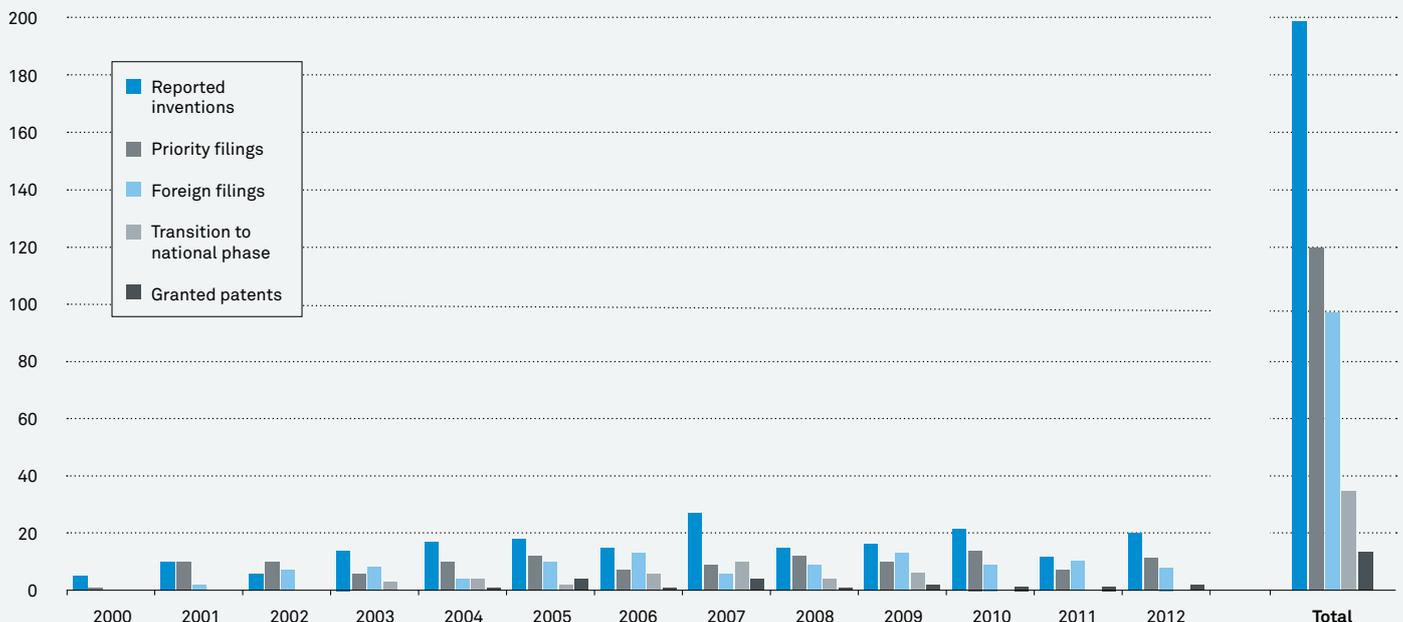
To honour the researchers whose inventions proved to be of interest to our partners and led to the filing of patent applications, we granted Certificates of Invention.

At our Annual Meeting in 2012, we awarded 23 Certificates of Invention to the inventors of six patent applications filed during the academic year 2011-2012.

## Valorisation of IP

The research taking place within the pre-competitive programme of DPI (i.e., the research taking place in the technology areas) is by nature relatively fundamental and is positioned at the front end of the innovation funnel. Needless to say, the resulting inventions and patent applications are related to the early stages of a process, which, within our sector, generally means that another five to ten years of research, and a relatively large, high-risk investment, will be required to reach the end of the innovation funnel. This is one of the reasons why the transfer of our patent applications to interested partners and third parties remains a challenge. In order

## DPI patents 2000-2012



to maximise applicability and future business options, we therefore emphasise the importance of the active involvement of contact persons from industry during the project itself, as well as during the process of patent filing.

In this context, we also stress the importance of the activities of the DPI Value Centre in this process. In the case of transfers to third parties, the DPI Value Centre endeavours to set up proof-of-concept projects in order to provide a more attractive technology package for companies to pick up and develop further and commercialise. These activities of the DPI Value Centre are of great value to the valorisation of DPI's patent portfolio.

#### New programmes, new challenges

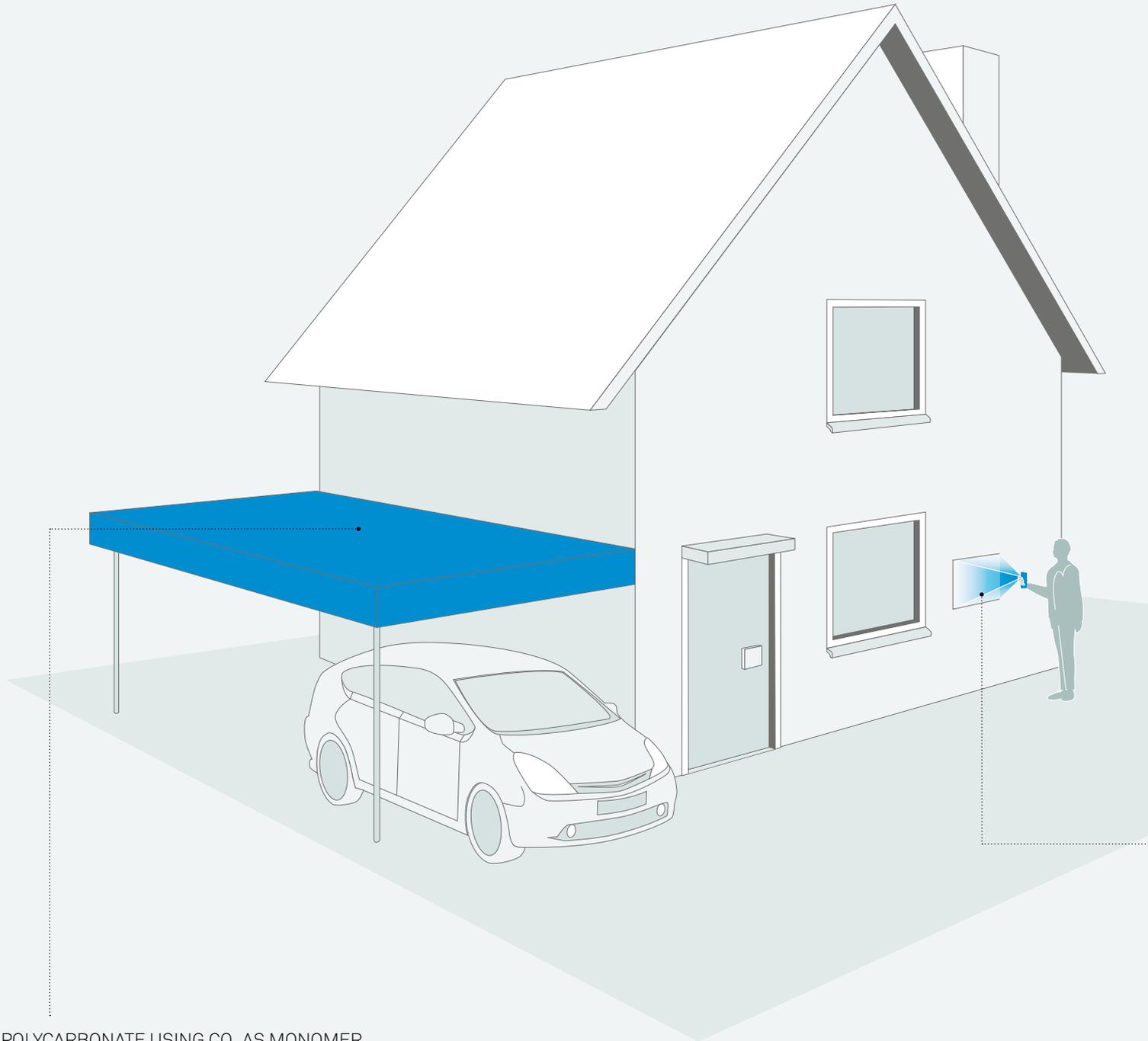
A few years ago, DPI developed a pre-commercial programme that consists mainly of projects in which a consortium of partners all play an active role. This requires a different IP structure, which, in principle, is determined by the project partners. DPI provides a model framework based on general best practices in consortium agreements.

Within the pre-competitive programme the research results are owned by DPI and shared amongst the partners that participate in that particular technology area. All of the partners are free to use the knowledge that is acquired, with the exception of knowledge that is part of an invention. When an invention is reported and partners are interested in using that knowledge, DPI files a patent application and the industrial partners involved in that specific technology area have the first claim to it.

Within Value Chain projects, the basic principle is that the knowledge created during the course of the project (foreground knowledge) is the property of the inventing partner, and any background knowledge contributed to the project remains the property of the partner that provided it. Other partners have free access to the knowledge contributed to and/or generated during the project, but only to the extent necessary for developments in the project. Specific agreements are made to enable access to another partner's IP for commercial application of the knowledge outside the project.

Statistics per TA 2012	PO	PP	FPS	CT	HTE	BIP	LATFE	EOR	EMT	Corp	Total
■ Reported inventions	3	7	1	1	5			1		4	22
■ Priority filings	2	3	1	1	2					1	10
■ Foreign filings	1	3	1				1		1	1	8

# Innovation inspired by DPI



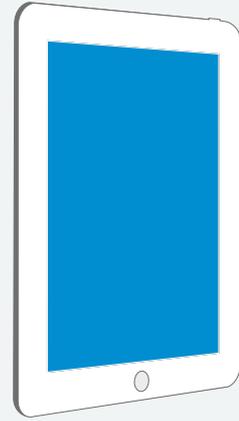
POLYCARBONATE USING CO<sub>2</sub> AS MONOMER

## Transparent roof

Polycarbonate is a robust, hard and transparent material that can handle high temperatures. It is easy to use and consequently has many applications. For example, it is used in CDs, DVDs, safety glasses, police shields, mobile telephones, drinking bottles, food packaging and many other products. The global market for polycarbonate was estimated at 3.5 million tons in 2012, which, at an average price of USD 4 per kg, represents around USD 14 billion.

Polycarbonate is made up of a repeating unit called carbonate (...-O-CO-O-...), which is formed through the polymerisation reaction of a monomer with at least a diol functionality (HO-R-OH) and another monomer possessing a carbonyl group (CO). This carbonyl group normally originates from phosgene (Cl-CO-Cl), a very dangerous monomer for which alternatives are being developed.

Researchers at DPI have found a green alternative, namely carbon dioxide (CO<sub>2</sub>). By using CO<sub>2</sub> as a monomer, the polycarbonate developed by DPI essentially absorbs CO<sub>2</sub>, the greenhouse gas. Together with elegant polymerisation chemistry, this polycarbonate is produced in a single step. All in all, the newly developed polycarbonate is one of the greenest yet available.

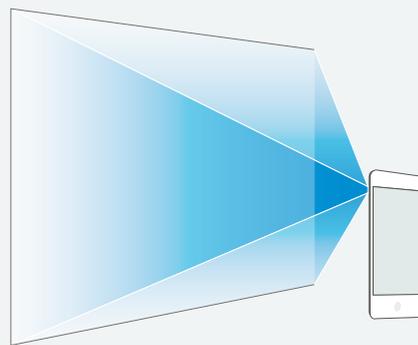
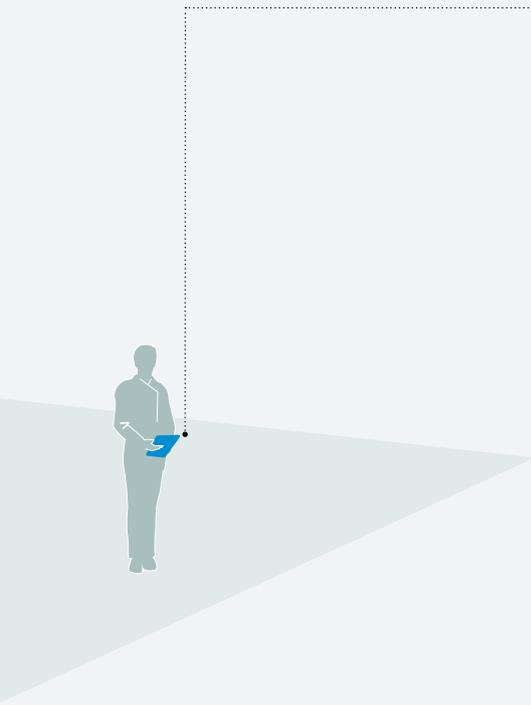


## ITO REPLACEMENT

### Touchscreens

The use of plastic electronics is rapidly increasing due to the technological advances with the material. Today, our lives are dominated by electronic devices, such as mobile phones, tablets, MP3 players. Many of these devices have touch screens with a conductive and transparent layer made from IndiumTinOxide (ITO). ITO is a scarce material, which will become more expensive as supplies of it run out. Researchers are therefore looking for substitutes for it. In 2011, DPI researchers found a replacement in a film composed of carbon nanotubes and latex particles and developed a working proof of principle.

The following year, DPI Value Centre took the technology a stage further by presenting a working proof of concept. The next step is anticipated in 2013, when the technology is positioned against the existing alternatives under commercial conditions.



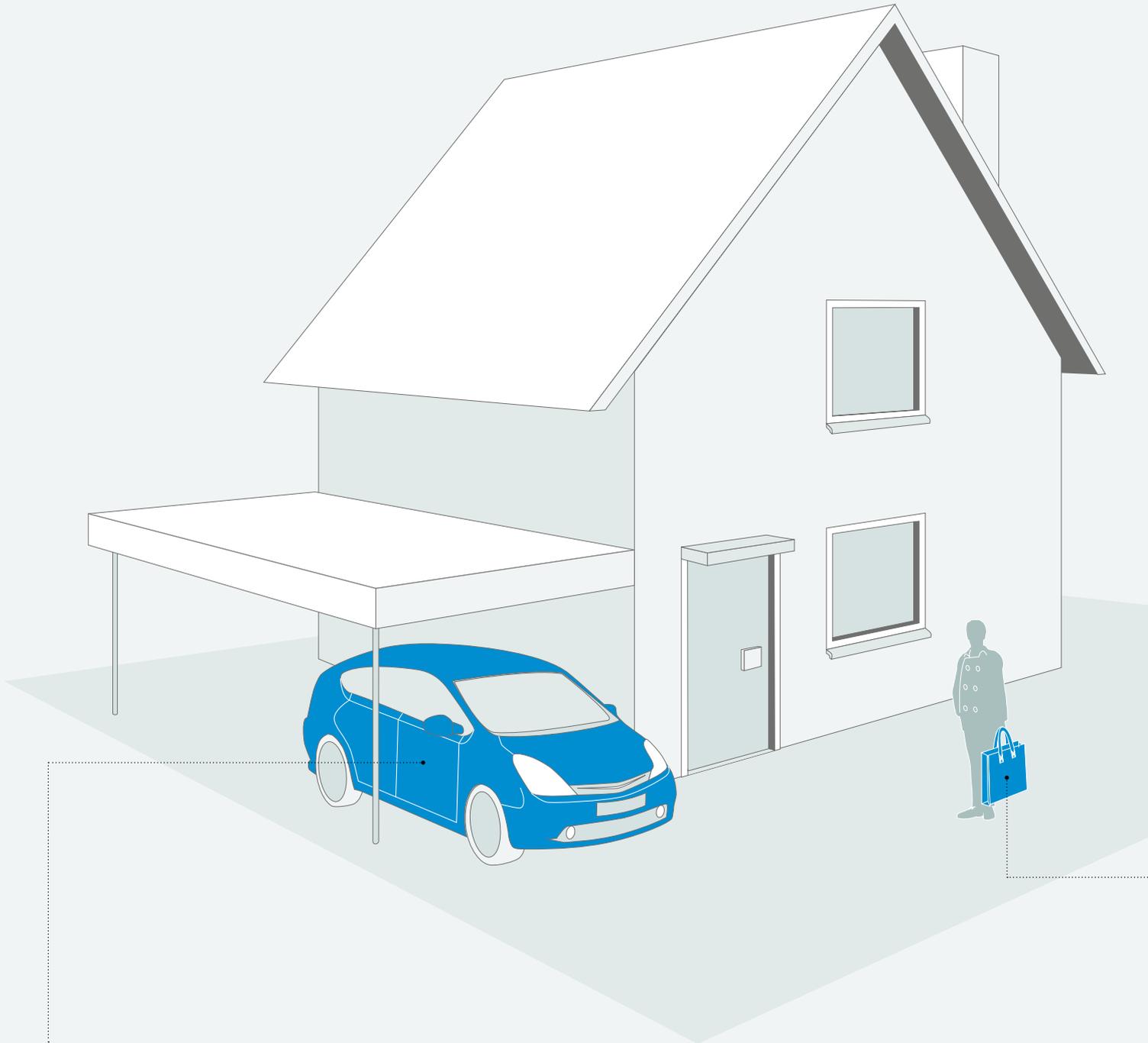
## POLYMERISATION GRATING

### Projector in mobile devices

These days almost everyone owns a mobile phone, which they often use to show pictures, movies or documents to other people. Although the screens are becoming larger, they can still only be shown to one or two people at a time. ImagineOptix has developed a technology that eliminates the restrictions imposed by the size of the screen of your mobile device in the form of a tiny beamer with the ability to project images of up to 60”.

The technology is based on a diffractive polarisation grating (PG), a polymer layer in which liquid crystals are positioned in a unique way. The resulting projection is of a superior quality with low energy consumption. This combination of functionalities makes the PG technology best suited for mobile devices.

# Innovation inspired by DPI



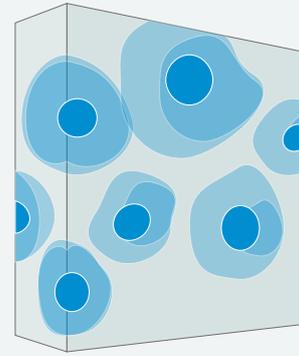
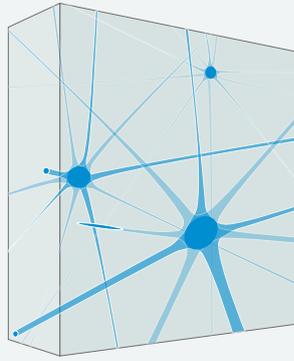
## SELF-HEALING COATING

### Paints for cars

Damage to your car's paint cannot always be prevented. Over time, it suffers from a lot of tiny scratches, which dull the high-gloss finish. You can restore the brand-new look by repainting or polishing your car, but that is expensive and the tiny scratches will eventually occur again. Researchers are working on affordable paints for cars, but also on other applications with self-healing abilities. For example, a coating that allows small

shallow scratches to heal themselves when they are exposed to sunlight.

The technology is based on adding hollow fibres with multiple cavities filled with self-healing components to the coating composition. When scratches or micro fractures appear in the coating, the hollow fibres will also break, releasing the self-healing components so that the scratches or micro fractures heal again.



## HYDROGEL FOR CELL GROWTH Growing human cells

Imagine how wonderful it would be if we could grow all kinds of human cells in one hydrogel matrix. We would be able to grow new skin for burn victims, a new kidney for transplant patients, or perhaps even a whole new ear. Such a process would improve the quality of life for a lot of people and would eventually reduce medical costs. It sounds like a pipe dream for the distant future, but it might already be possible within ten to fifteen years. It is already possible to grow human cells on a small scale, but DPI researchers have now developed a matrix material that enables cells to grow in a specific shape.

Cells need a specific template or matrix in order to grow. Nature has very specific matrices for different types of cells which are hard to mimic synthetically. Many attempts have been made to do so with synthetic polymers, and to some extent they have been successful. The matrices developed by DPI were built with amino acids, nature's own building blocks, which are able to form very specific and tailored matrices, which have initially shown a huge potential to accommodate different types of cells.

## BIO-COMPATIBLE POLYMERS

### Polymers restore damaged nerves

Over 2% of all trauma victims in hospitals suffer from damaged peripheral nerves, which results in the loss of functionality of a hand or a foot, for example. Damaged nerves normally have the ability to grow again, but as they do they tend to fan out and knot together, which causes pain. To prevent this, surgeons try to reconnect the nerve ends or replace the nerves during surgery. Unfortunately, this is not always successful.

DPI researchers have developed a new kind of biodegradable polymer to repair damaged peripheral nerves. The polymer is a porous material with a honeycomb structure to force nerve ends in the right direction. To improve the healing process, the nerve ends are placed in a tube with biodegradable polymer material that attracts growth-supporting cells to accelerate the process.

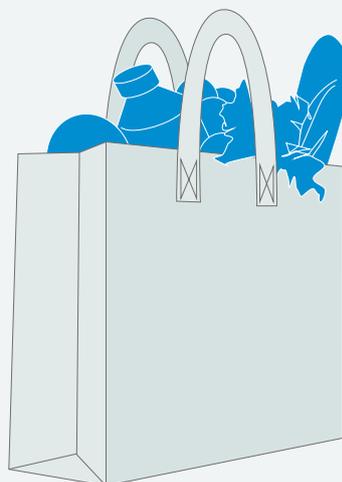


## SENSOR FOR FOOD SAFETY

### Reduction of food waste

Every year we throw away lots of food because it has reached the expiration date. The food is often still good, however. DPI researchers are currently working on a sensor that would be able to tell us whether food is still safe for consumption or not. This sensor would work throughout the value chain.

The same sensor could be used for vulnerable ICT components, particularly components that are sensitive to temperature and even more sensitive to water. The principle behind the sensor is that an ordered molecular structure is broken down into a disordered molecular structure. The change also alters the colour of the sensor, making the sensor also easy to use.



# Value Chain Projects

## The added value of cooperation in the chain

Value Chain Projects are designed to promote cooperation between companies at different stages of the chain from raw material to final product, with each of the partners providing input in its own area of expertise.

DPI and DPI Value Centre played an active role in getting the projects off the ground, for example by helping companies to find suitable partners and refine the actual project proposals. External experts were hired to assess the quality of the proposals on the basis of criteria such as technical feasibility, degree of innovation, their economic potential in relation to the costs of the project, sustainability and the project's impact on quality of life.

The proposals that have been submitted for Value Chain Projects encompass a wide variety of developments in the polymer chain, ranging from a project to produce a food grade valve for dispensers to the development of a biobased asphalt for road construction.

Thirteen Value Chain Projects involving 56 partners, including eight research institutes, commenced in 2012. The total budget for the innovation projects is over € 6.5 million.

The project leaders were all invited to pitch their projects at a Value Chain Meeting, where it became clear that all of the projects would be carried out by innovative and enthusiastic businesses working in close cooperation with each other. The aims of the projects vary from developing a new product or technology to introducing an alternative material in a process. It was apparent that cooperation has a positive impact on the pace and quality of a project and that the final outcome is a better product that can be launched in the market sooner and more successfully.



Source: KeyKegs, Lightweight Containers bv

## Pallets from recycled materials, C2CP

Plastic pallets are currently still produced from expensive monostreams or regranulates. Pallet manufacturer C2CP, waste collection company Sica Recycling, pallet pool PRS and DSM Engineering Plastics have formed a consortium for a joint project to develop pallets containing plastic waste that would normally be incinerated.

This will be accomplished by using a unique method to clean, crush and upgrade the collected waste and convert it into pallets of the necessary standard using injection moulding. By using these raw materials and creating pallet pooling facilities, they will generate a substantial reduction of CO<sub>2</sub> emissions.



## PLA carpets, Synbra Technology

A consortium consisting of Synbra Technology, Desso, Peter Holland, Bonar and Purac is currently engaged in the development of PLA yarns suitable for use in carpets.

Natural yarns are potentially interesting materials for the carpet industry provided they absorb very little moisture.

PLA yarns are a good example of this, but had not been considered up to now because PLA was not wear-proof and already became brittle at a temperature of 60 degrees Celsius. Yarns based on PLA homopolymers that overcome the boiling-water barrier have recently been developed. This new type of yarn comes in different colours and can be embedded as a top layer in the carpet and used as a non-woven carpet backing.

After use, PLA yarns, backing and underlay can now be recovered in their pure form. The treated PLA can then be depolymerised to a monomer, which can then be used again to produce PLA. The innovative aspects of this project can be summed up as follows:



- development and application of mechanical wear-resistant PLA yarns
- development and application of mechanical wear-resistant carpet backing
- use of PLA and colouring agents in yarns according to the Cradle to Cradle principle (C2C)
- increased knowledge of the processes of compounding, spinning, twining, cabling and carpet production
- testing of mechanical separation of non-woven and woven for recycling of PLA.

Features of the new type of carpet are the use of clean and healthy materials and the limited burden on the environment since renewable materials can be recycled. There is expected to be a large market for the new product because of the size of the carpet manufacturing industry in the Netherlands and abroad.

## KeyKeg: Beer in PET

The KeyKeg is a technological innovation that provides an alternative to the existing stainless steel beer barrels and also bottles and cans. Essentially, the plan is to replace them with a spherical PET container containing a sealed and laminated bag with the product (beer, but also wine). The PET container should preferably be pressurised with a propellant to squeeze the liquid from the container into the glass. The KeyKeg provides both economic and ecological benefits, since it is lighter (1.4 kilograms compared with 9 kilograms for a beer barrel, so that more product can be carried in each consignment), it is non-returnable (but can be recycled), the quality of the product is better because no propellant gas comes into contact with the product, and there is no need for CO<sub>2</sub> containers. Finally, the

innovation provide unprecedented marketing possibilities through branding of the kegs.

A new development is the KeyKeg Slimline, which contains fewer different materials and parts. The mechanical properties of the KeyKeg Slimline will be roughly 50% better than the original version, so that the KeyKeg Slimline will also be able to handle the high pressure of soft drinks and can be used in extreme tropical conditions, where the existing KeyKeg Baseline falls short. The KeyKeg Slimline will be lighter than the KeyKeg and its shape will be different to allow it to fit more snugly beneath the bar. All of these improvements will make the new product even more sustainable:

- even more product with each consignment and therefore fewer CO<sub>2</sub> emissions
- improved separation of waste because the product is made almost entirely from PET and/or the materials are easy to separate
- no pollution from the cleaning of stainless steel containers
- CO<sub>2</sub> bottles are not needed, also reducing CO<sub>2</sub> emissions
- positive LCA compared with stainless steel barrel, bottles and cans
- the KeyKeg Slimline can be used in more markets (soft drinks) and regions (tropics).

Eurokeg, the main developer of the KeyKeg Slimline, is collaborating with Alligator Plastics, Wittenburg BV, Aeson and Total Productivity.

## Anti-fogging polyolefin films, AkzoNobel

AkzoNobel, Addcomp, Oerlemans Plastics and Ouden Haveling market gardener are developing a new anti-fogging concept for greenhouse and packaging films, in cooperation with market gardeners, and packaging firms. The most important market need that has to be fulfilled for these types of films is to increase the durability of polyolefin anti-fogging films while maintaining properties such as transparency, phytotoxicity, food approval (for packaging) and recyclability. Also important in production is an easy to use, free flowing master batch.

In this project, anti-fogging agents based on existing chemistries will be evaluated and tested to establish references and standards. At the same time, new anti-fogging agents will be designed and promising molecules will be processed in master batches, films which will be produced and tested in field studies under standard greenhouse conditions.

## High-grade moulded PMMA sheets, Delta Glass

The consortium in this project is developing two new types of moulded PMMA sheet, a transparent sheet with a scratch-proof and UV-resistant coating, and a composite sheet with fiber reinforcement with PMMA as matrix.

Besides developing the new types of plate, the project includes the finishing of the sheets, which will be machined and glued and the possibilities of 2D and 3D thermoforming will be explored. The results will be used to improve the prototype sheet materials.

## Powder coatings on wood, DSM Resins

Powder coating systems are now only used on a metal substrates because processing occurs at a temperature of 180-200°C. The aim of this project is to develop a coating system that can be processed at a lower temperature, so that powder coating can also be used on plastic and wood and can compete with wet coating techniques in terms of price and performance.

The chain partners in this project each have a specific role. DSM is developing the resins and Van Wijhe is devising the formulas and coating applications, while IMS-Werkendam and Span Finishing will apply the developed coatings and contribute their knowledge of the demands of the market. The tests are being carried out at the pilot facility at Polymer Science Park and Hogeschool Windesheim is the knowledge carrier.

**SHINE project group**  
February 2013



## COMPANOCOMP

The European COMPANOCOMP project started in October 2011. The aim of the project is to develop multiscale simulation methodology and software for predicting the morphology (spatial distribution and state of aggregation of nanoparticles), thermal (glass temperature), mechanical (viscoelastic storage and loss moduli, plasticity, fracture toughness and compression strength), electrical and optical properties of soft and hard polymer matrix nanocomposites from the atomic-level characteristics of their constituent nanoparticles and macromolecules and from the processing conditions used in their preparation.

The novel ground-breaking modelling methodology should significantly improve the reliable design and processability

of nanocomposites contributing to the EU Grand Challenges for reduction of CO<sub>2</sub> emission, energy savings by light-weight high-strength nanocomposites, mobility and improved living environment. The successful outcome of the project will constitute an important advance in the state of the art and will have immediate industrial, economic and environmental impact.

The COMPANOCOMP initiative consists of two collaborative projects being executed by an EU consortium (8 partners) under the Seventh Framework Programme and a Russian consortium (4 partners) under the auspices of the Federal Russian government. DPI is acting as the coordinator of this project and Denka Hristova-Bogaerds is the Project Leader.

The project is now at its half-stage and is progressing very successfully. The results generated within the cooperative project are already included in joint publications between European and Russian partners:

P.G. Khalatur, A.R. Khokhlov, A. Gavrilov. *Unusual forms of self-assembly in the polymer world*. Book chapter 'Supercomputer Technologies in Science and Educations, Moscow: MSU, 2012, p. 184-195

A. A. Gavrilov, A. V. Chertovich, P. G. Khalatur and A. R. Khokhlov. *Effect of nanotube size on mechanical properties of elastomeric composites*. *Soft Matter* (2013), 9, 4067-4072

More information about this project: [www.companocomp.eu](http://www.companocomp.eu)

## SHINE

DPI coordinates a number of EU projects designed to create added value for its existing or prospective industrial partners, who always define the technological scope of a project. The proposal for one such project, the self-healing innovative elastomers (SHINE) project has been approved and the European Commission has awarded funding for it. The project was submitted under the call for proposals on the theme of Nanosciences, Nanotechnologies, Materials and New Production Technologies in the EU's Seventh Framework Programme (FP7).

In the SHINE project, which started in February 2013, DPI is acting as the independent coordinator of efforts to explore various self-healing material technologies in a single project.

The aim of the SHINE project is to develop self-healing elastomers for dynamic seals and vibration and noise abatement

systems. It will approach the issue from the perspective of covalent and non-covalent bonding, which can provide a repeatable healing response as a result of reversible reactivity. SHINE will investigate both the healing mechanisms of pure elastomers and composites produced with elastomers. The methods of designing these types of elastomer, tailor-made fillers and self-healing composites will be followed in a systematic manner. The SHINE project is intended to develop elastomers with mechanical properties comparable to conventional elastomers (with 60% recovery of the initial properties after healing), repeatable self-healing (preventive versus curative healing), operable at room temperature and without human intervention. A cost-benefit analysis has shown that, if successful, the SHINE project will reduce transportation costs by reducing the maintenance burden due to the degradation of infrastructure.

The overall impact of the project could be enormous because of the anticipated effects in three domains:

- economic impact: long-lasting and cost-saving seals for vehicles, heavy-duty seals for wind turbines, vibration abatement systems for roads and bridges, noise abatement systems, asphalt mixtures;
- social impact: increased reliability, enhanced safety, fewer accidents;
- environmental impact: reduction of maintenance costs, energy savings, cuts in pollutants.

The consortium carrying out the project consists of two universities, four research centres, five large companies and one SME. The total budget is € 6.4 million, including an EU subsidy of € 4.0 million.

More information about this project: [www.selfhealingelastomers.eu](http://www.selfhealingelastomers.eu)

# DPI Annual Meeting 2012

The theme of DPI's Annual Meeting on 13 and 14 November 2012 was **Polymers D Light: shedding our light on polymers**. More than 130 members attended the event.

During the first day of the meeting, several junior and senior researchers presented their vision of the latest trends in the use of polymer materials in their own disciplines.

The junior researchers were:

- **Nicole Franssen** - PostDoc at the University of Amsterdam
- **Ronald Otten** - Design Engineer at ASML
- **Alexander Kühne** - Group leader at DWI, RWTH Aachen University

Senior researchers were:

- **Christoph Weder** - Chair of Polymer Chemistry and Materials at the University of Fribourg
- **Thijs Michels** - Emeritus Professor at TU Eindhoven
- **Sir Richard Friend** - Cavendish Professor at the University of Cambridge

## GOLDEN THESIS AWARD 2012

Ronald Otten, the winner of the Golden Thesis Award 2012, Martien Cohen Stuart, Mark-Jan Spijkman and Marc Lemmers.

In the afternoon, the three nominees for the Golden Thesis Award 2012, Marc Lemmers, Ronald Otten and Mark-Jan Spijkman, gave short presentations about their completed PhD research. The jury had a hard time deciding who should win the award, but ultimately awarded the prize to Ronald Otten for his presentation and the research described in his thesis 'Self-organisation of anisometric particles: statistical theory of shape, confinement and external-field effects'.

During the breaks in the programme on 13 November, DPI researchers had an opportunity to present their research in the form of a scientific poster. Prizes were awarded for the three best posters during the conference dinner. The first prize went to Anke Teichler, the second prize to Diego Wever and the third prize to Wenshan Zhang.

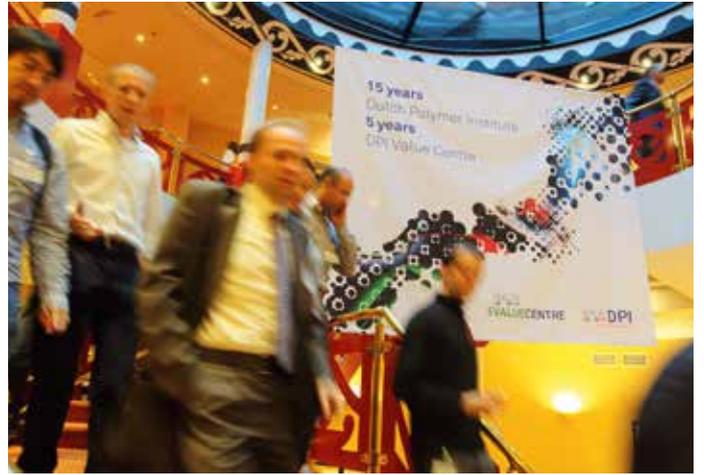
During the conference dinner, DPI Certificates of Invention were also presented to twenty researchers who had filed patent applications in the 2011-2012 academic year.

The second day of the DPI Annual Meeting was hosted by our partner organisation DPI Value Centre, and was structured around the theme, The art of connecting. There were 130 participants on the second day, including DPI researchers, partners of DPI Value Centre and others interested in innovation in polymers.

The Annual Meeting was preceded by the Young DPI day, an event organised for researchers who had recently started on a DPI project. They were given practical information about DPI and had an opportunity to connect with each other during a creative session on 'Building Bridges'.



YOUNG DPI 2012



CERTIFICATES OF INVENTION 2012  
Ulrich Mansfeld



POSTER PRIZE 2012  
Poster prize winner Anke Teichler



---

# Workshop on Polymer Synthesis

## For the purpose of function

---

The great thing about polymers is that they are so versatile: you can change the function of a polymer by adding a side chain with a specific property. In practice, however, the relationship between the molecular composition and structure of a polymer and its function is not so straightforward. Moreover, synthesising a polymer with the desired properties is not easy and can take a long time.

---

On 26 January 2012, DPI organised a workshop on current activities in the area of polymer synthesis, making full use of the available research capacity by inviting participants from all the technology areas. After a few introductory lectures, the participants from each technology area gathered to make an inventory of their wishes and ideas for functionalising polymers.

Interaction between polymer scientists at universities and in industry is essential for making any headway in polymer synthesis. This was demonstrated by the first speaker, Ruud Rulkens of DSM, who used the example of polyamide synthesis to illustrate how academic knowledge can lead to commercially interesting and successful materials. Stanyl®, a highly crystalline polyamide that is stable at high temperatures, and its successor, Stanyl®ForTii™, are synthetic polyamides with applications in the automotive and electronics industries. DSM produces them and they originated from research that Professor Reinoud Gaymans started at the University of Twente forty years ago. Building on that knowledge, DSM has developed and commercialised a partly bio-based polyamide, EcoPaXX™, a product that has the highest melting point of any aliphatic bio-based polyamide currently available on the market.

One of the reasons for synthesising polymers is to replace fossil-based polymers with more sustainable ones. In his presentation, Carsten Sinkel from BASF predicted a great future for bio-based and biodegradable polymers in applications for which fossil-based, non-degradable polymers are currently used. Most bio-based polymers (polymers synthesised from monomers originating from biomass) are developed as substitutes for their fossil-based counterparts and, hence, their functional properties are identical, but they are not, by definition, biodegradable. To make these polymers biodegradable, predetermined breaking points can be included in the polymer chain. An example of a biodegradable polymer produced by BASF is Ecoflex®, which is intended to replace polyethylene for packaging purposes. BASF is able to sell all of the Ecoflex® it produces, even though it is more expensive than polyethylene made from fossil sources. The substitution of other biodegradable applications, such as paper coated with a biopolymer, could be helped by legislation – Italy, for instance, has prohibited the use of polyethylene. Of course, customers have to be convinced of the added value of these products.

### Catalyst

Edmund Carnahan of DOW was the third industry representative to deliver a lecture. He explained how the kinetics of catalysts can result in novel microstructures, even in a mature field such as that of polyolefins. Small changes in the structure of the catalysts can have significant consequences for the properties of the resulting polymers. Building more of a co-monomer into a polymer chain, for instance, can change the rheology of a material enormously. By altering the relationship between melting point and crystallisation, injection moulding of otherwise intractable polymers would be feasible. Carnahan also showed that, in some cases, you can calculate the influence of the structure of the catalyst.

In addition to the presentations by the three speakers from industry, there were also three academic speakers.

Stephan Mecking of the University of Konstanz stressed the importance of understanding the role of the catalyst in a polymerisation process, because the properties of the resulting polymer can be influenced by the design of the catalyst. For example, polymerisation in aqueous systems with specifically designed catalysts results in the dispersion of micro- and nano-scale structures of polymer particles that can be used as a basis for coatings and films. Mecking also noted that we need a better understanding of the role of the catalyst in relation to the processing conditions for the production of polyethylene from renewable sources.

According to Klaus Müllen of the Max Planck Institute for Polymer Research, rather than striving to synthesise the polymer, we should focus on the function of the polymer. Functional nanoparticles, with shells and internal components of different compositions, can be synthesised by controlling the polymerisation reaction, by using localised catalysts, for instance. Polymers with specific electronic properties, such as the blue emitters in organic LEDs, may have other properties – such as insolubility – that preclude the most obvious processing method of spin coating. Finding solutions to these kinds of problems should not be left entirely to engineers and physicists. Organic chemists play a crucial role in synthesising polymers exhibiting specific functionalities.

How can we use monomers from biomass instead of conventional monomers to synthesise high-performance polymers, especially those with a high molecular weight? Bart Noordover of Eindhoven University of Technology listed the challenges: the reduced reactivity, limited thermal stability and differences in polarity of biomass-based monomers compared to conventional ones call for new routes to synthesis, such as the use

of low-temperature catalysts, water-borne or solvent-free systems, enzymatic reactions and replacing toxic chemicals.

### Function

After these introductory lectures, the participants broke up into four groups, one for each of the technology areas (Polyolefins, Performance Polymers, Functional Polymer Systems and Coating Technology) to discuss the challenges DPI faces in relation to the issue of synthesis. The most striking aspect of the discussions was that they focused on physics and function. The consensus seems to be that chemistry for the sake of chemistry has no role to play. What counts is the function of a polymer, not in its own right but in a specific application. The participants from all of the technology areas identified the study and understanding of interfacial phenomena and properties as an overarching topic.

A warning was not to try to tackle the whole chain of knowledge at once, but to address just one well-defined issue in each project. A fundamental approach rather than a process of trial and error will ultimately have the greatest effect. The syntheses that are currently used must be studied in depth and completely understood before new syntheses are investigated.

Another more general conclusion was that it would be very useful to hold more workshops like this one, where academic and industrial researchers meet to discuss a topic, before a call for proposals is launched, since they provide a platform for achieving a better match between industrial needs and academic curiosity.

What is badly needed is a method to characterise the small samples of newly synthesised polymers made in the high-throughput-experimentation approach, as well as a method to quickly determine aging and long-term stability. In some cases, blends and composites should be investigated to see if they give better results (PO); in others, what is being sought is extreme purity (FPS).

As might be expected, a number of participants remarked on the need to create the desired three-dimensional structures, or the architecture, required in certain applications directly in the synthesis process: the sharp interfaces between layers in organic light-emitting diodes and transistors, the gradients and cross-linked networks in coatings, membranes for filters, and nanofibres and their distribution in a polymer matrix. Although the role of catalysts in the process of creating the desired structures is not properly understood yet, an understanding of how three-dimensional structures could have an influence of the process is essential and that influence must be exploited. The same applies for surface modifications and solvents that influence the growth of subsequent layers of polymers in electronic devices.

It would be nice to get rid of unpleasant solvents, toxic components, energy-inefficient and expensive processes – why not use bio-based polymers directly for synthesising new materials instead of first breaking them up into monomers?

In all four discussion groups, the participants concluded that forming teams made up of people involved in the synthesis of the polymers and those working on their application in a device, coating or material – chemists and physicists, if you like – was essential for the success of a project. Even in a purely chemical field like polymer synthesis.

# Plastic Marine Litter

The pollution of our oceans, especially with Plastic Marine Litter (PML), has received growing public attention in the last few years. The existence and growth of extensive plastic gyres (plastic islands) in the oceans and the rising quantities of small plastic debris are increasingly being seen as threat to marine wildlife and potentially also to human health. Hence, there is an urgent need to minimise littering and other activities that cause leakages and, ultimately lead to PML. Against this background a team including DPI, DPI Value Centre, Stichting De Noordzee, IMSA Amsterdam, Utrecht University, SABIC, Van Gansewinkel and Kruidenier Foodservices launched a joint research project with a focus on PML. The objectives of the project are (1) to gain a better understanding of the sources and the pathways (leaks) leading to PML in the North Sea and (2) to identify future research strategies for gaining a deeper insight into how to prevent PML by closing the leaks of plastics into the environment.

It is important to note that due to the complexity and scale of the problem and the lack of data, it is difficult to make reliable estimates of the amount of PML in the world's oceans. Hence, the original focus of the project – an analysis of the presence of 0.5-liter plastic beverage bottles – was not feasible at this stage.

The release of plastics into the environment is mainly the result of inappropriate waste management and improper human behaviour (e.g., littering), as well as incidental and intentional spills and pollution (Barnes et al. 2009). Plastic can be found on the seabed, as floating debris in the water or on beaches (Mehlhart &

Blepp 2012). The evaluation of data from various studies indicates that, while the composition of marine litter is similar regardless independent of sampling method or location, plastic products are always the dominant category among the items found, be it at the surface, on the seabed or on the beach (Hammer et al. 2012; Barnes et al. 2009).

As figure 1 shows, plastic materials represent approximately 85% of the total marine litter found on Dutch beaches. Therefore a first hypothesis is that the composition of litter is independent of prevailing physical conditions in the North Sea, such as winds and currents. By categorising the items found, it was possible to differentiate between land-based and ocean-based sources. For the Dutch beaches that were investigated, this indicated that around 45% of all marine litter is sea-based (fisheries and shipping), 30% is land-based (sanitation and tourism for example) and another 25% is categorised as 'other' (e.g., unidentifiable materials) as depicted in figure 2.

Land-based sources are usually dominant in such research, but the fairly remote locations of the beaches in the Dutch survey and intensive fishing activities in the North Sea, could explain the relatively high proportion of ocean-based sources. First studies identified several areas of accumulation of PML on the seabed indicating so-called 'hot spots' of marine litter accumulation (Barnes et al. 2009; Maes et al. 2011).

These initial insights will be used for the next phase of the project, which is to steer and extend monitoring and to suggest

further investigation and research with the ultimate goal of identifying leaks and possible counter measures for land- and ocean-based sources of litter. However, the current gaps in our knowledge are extensive and include the total amount of litter currently in the North Sea, including a breakdown by size; annual inputs (such as micro-plastics originating from sewage-treatment plants discharged through rivers) as well as removals through different outputs/sources, a clear scientific understanding of the behaviour and pathways of marine litter, explaining the varying amounts of litter found e.g. on beaches.

## REFERENCES

- Barnes, KA, Galgani F, Thompson RC and Barlaz, M. (2009) Accumulation and fragmentation of plastic debris in global environments; *Phil. Trans. R. Soc. B* 364, 1985–1998
- Cefas contract report (2011) Authors: Thomas Maes, Manuel Nicolaus, David Stephens, Johan Van Der Molen and Allan Reese: *Marine Litter Monitoring*
- Hammer, J., Kraak, M., H.S., and Parsons, J.R. (2012) *Plastics in the Marine Environment: The Dark Side of a Modern Gift; Reviews of Environmental Contamination and Toxicology* 220
- Mehlhart, G., Blepp, M. (2012) *Study on Land-Sourced Litter in the Marine Environment - In the Context of the Initiative of the Declaration of the Global Plastics Associations for Solutions on Marine Litter Review of sources and literature; Darmstadt / Freiburg*
- OSPAR (2007) *OSPAR Pilot Project on Monitoring Marine Beach Litter - Monitoring of marine litter in the OSPAR region*

FIGURE 1 Composition of the litter found on Dutch beaches.

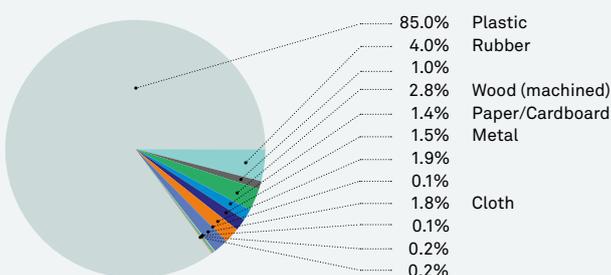
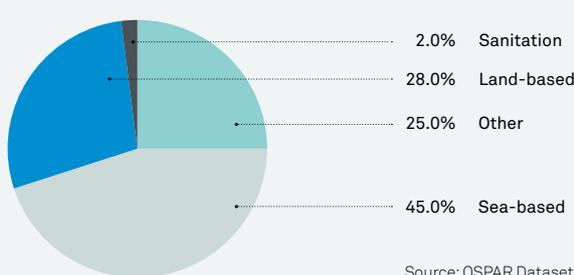


FIGURE 2 Sources in % of found litter.

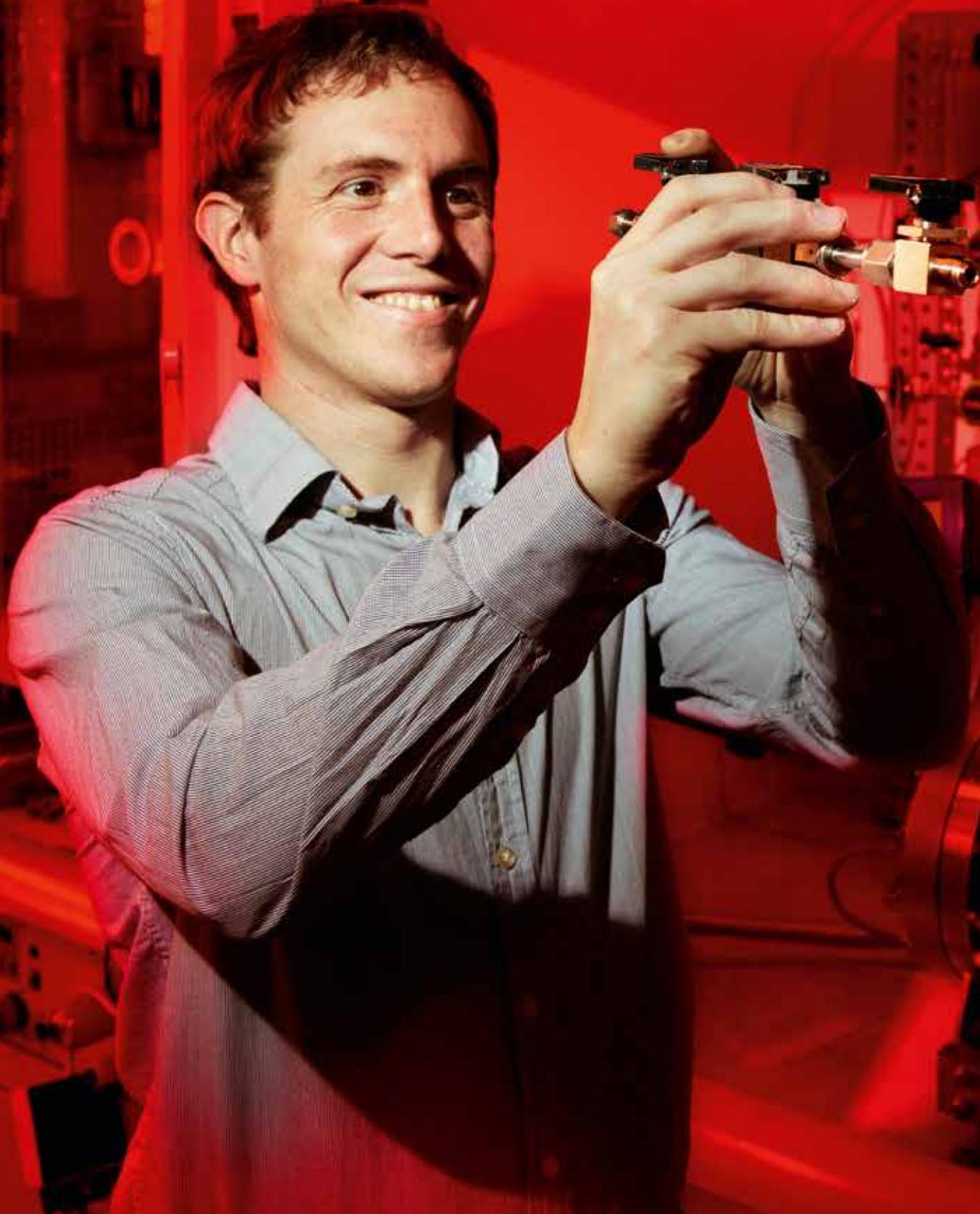


Source: OSPAR Dataset (2002-2011)

# Technology Areas



“In presenting your work, you have to be as precise as possible to get input from all technology areas.”



---

# Thomas Kröner

## The balance of mass-transfer and reaction rates

---

### POLYOLEFINS

Polyolefins (PO) are the only class of synthetic macromolecules that can be produced catalytically with precise control of stereochemistry and, to a large extent, of (co)monomer sequence distribution. Therefore, as with the letters of the alphabet, the number of constituent elements which can be assembled into meaningfully organised structures is practically infinite and, accordingly, scope of application of polyolefins is continually growing.

---

**The yield of a catalytic reaction is not only determined by the rate of the chemical reaction. In order to be able to take part in the reaction, the monomers have to reach the catalyst sites through the layers of polymers that are produced.**

“At school I liked mathematics a lot, but when I had to choose the discipline in which I would continue my studies, I chose chemical and environmental engineering because I particularly valued its possible practical applications,” says Thomas Kröner.

From 2003 to 2009, he studied at the Martin Luther University in Halle, Germany. His original plan was to go to another city for a PhD project, but when the supervisor of his Master’s thesis offered him a really interesting PhD topic (which differed from that of his Master’s thesis), he decided to stay.

Briefly, the main topic of Kröner’s project is the balance between mass-transfer and reaction rates in the production of polyolefins with Ziegler-Natta catalysts. Even though this process is widely used

in plants all over the world, the chemical aspects - the reaction mechanisms - are still not fully understood. The distributions of the molecular weight and of the chemical composition of the polymers produced in this process are very broad. Although the multi-site nature of the catalysts is believed to be the main reason for the broad distributions that are observed, concentration gradients that are attributable to diffusion resistances might also be a contributing factor. If you can decouple the two processes, you might be able to quantify the two influences.

#### Phenomenological

Kröner’s project follows an engineering approach: “We try to measure macroscopic reaction rates. We have looked at the polymerisation of high-impact polypropylene, a two-step process. In the first step, propylene is polymerised to polypropylene, and in the second step, ethylene and propylene are polymerised to a rubber-phase polymer that does not mix with the homo-propylene. The polymers grow around the catalyst particles, and before the monomers can participate in this reaction, they have to diffuse through the layer of polymers to reach the catalyst particle. A high-pressure sorption balance in which we can introduce polymer powders in a non-reacting environment allows us to measure only the rate of mass transfer. In a reactive environment, we measure a combination of the mass-transfer and the reaction rates. Based on our experiments, we have derived two models, one for the mass transfer on its own and one for the chemical reaction plus the mass transfer,” Kröner explains.

His project will end in July 2013, and he is, as we speak, transcribing the results in his dissertation: that the mass transfer does not limit the chemical reaction rate for the polypropylene reaction, and that the combined mass-transfer and reaction model has revealed pronounced limitations on diffusion for the ethylene reaction.



Apart from himself and his supervisor, the group at Martin-Luther University consisted of only two other researchers, one of whom worked alongside Kröner during the first two years and one during the last year of his project. His professor in Halle is also responsible for the Fraunhofer Polymer Pilot Plant Center (Schkopau, Germany) and can therefore only spend a limited amount of time at the university's laboratory. Consequently, the input he received at DPI project meetings was particularly beneficial for Kröner. "In their projects, my two colleagues were in direct contact with only one company, and in that situation, of course, the input you get often has a rather narrow perspective. In DPI, it is completely different. When you present the progress of your work, there are always many specialists with different technological backgrounds in the audience, so you have to be ready for questions about materials, chemical aspects, etc. You have to be as precise as possible in every respect in order to get as much useful input as possible from the various experts. And then there is also the difference between the comments from industry and academia. I must say it helps me a great deal in my work. Of course, in the beginning we had a detailed plan of what I was supposed to do, but due to the valuable input from DPI researchers, from both industry and academia, we

broadened our angle of approach, and this clearly improved the scientific quality of the project."

#### **Comparable**

Asked for an example of DPI's influence, Kröner explains: "At one of the project meetings, materials specialists said they were not sure that our approach to measuring diffusion rates on nascent powder and already molten material, pressed as films, would work. The basic question was whether, in these circumstances, the distributions of the materials and polymer properties (like crystallinity) were directly comparable. That is not a question we would have asked ourselves, but after a very thorough investigation, it turned out that our approach worked with only a very small correction to account for the differences. It really added value to our research."

Another way in which DPI helped was that experts and the expensive equipment to do the chemical analysis of the polymers were available when needed. Kröner visited Naples, where the group of Professor Busico, the scientific chairman of the Polyolefins technology area, performed these chemical characterisations for him.

There are definitely advantages for a researcher in carrying out a DPI project

compared with a contract project in which there is input from only one company. Apart from the more varied input, it is also nice to be able to visit different cities and countries for the project meetings, which are held four times a year. And you get an idea what it might be like to work in a company. "Although I don't get to know what it is like to work there on a daily basis, via all the meetings and telephone conferences we have I learn about the scientific questions they are working on. After ten years at a university, I want to work in a company and will shortly start looking for a job. Of course, I will send the polyolefin companies that were involved in my project an open application. I am sure being part of DPI will help me to find a job. We will see," concludes Kröner.

---

## FACTS AND FIGURES

### Partners from industry

- Borealis
- Braskem
- Celanese
- Dow Benelux
- DSM
- ExxonMobil
- Freeslate
- Industrial Technology Research Institute
- Lanxess Elastomers
- LyondellBasell
- Petrobras
- Sabic
- Sinopec
- Symyx
- Teijin Aramid

### Partners from the research world

- Eindhoven University of Technology
- ESCPE-Lyon
- Fraunhofer Institute for Structural Durability and System Reliability LBF
- Japan Advanced Institute of Science and Technology
- Loughborough University
- Martin-Luther University of Halle-Wittenberg
- Polymer Technology Group Eindhoven
- Queens University
- Radboud University Nijmegen
- University of Antwerp
- University of Amsterdam
- University of Groningen
- University of Manitoba
- University of Naples Federico II
- University of Ottawa
- University of Perugia
- University of Salerno
- University of Udine

### Budget and organisation

Expenditure in 2012 totalled € 2.69 million (budget: € 3.02 million). A total of k€ 51 was spent on equipment. The total number of FTEs allocated at year-end 2012 was 28.8 (46 researchers). Prof.dr. Vincenzo Busico acted as Scientific Chairman and Dr. Jan Stamhuis as Programme Area Coordinator of the Polyolefins programme.

### Publications and inventions

This technology area generated a total of 21 reviewed papers and four theses; three inventions were reported and two patent applications were filed.

For details, see page 77.

---

## OBJECTIVES

Polyolefin-based materials can be customised for a wide range of applications: from ultra-rigid thermoplastics to high-performance elastomers. This vast spectrum of performance is achieved by a variety of polyolefin molecular structures, whose common features are full atom economy in their synthesis, low cost, excellent properties, a long life cycle and ease of recycling. The research programme of the Polyolefins technology area encompasses the entire spectrum of the knowledge chain, the aim being to increase proficiency in the ever-expanding applications. Although polyolefins represent one of the oldest (if not the oldest) thermoplastic polymer families, they are still very much characterised by continuous innovation. Both gradual and step change technology renewal yield new applications and reduce the manufacturing- and user eco-footprint. The recent discovery of chain shuttling catalyst systems that enable the industrial production of polyolefin block (co)polymers with unprecedented structures, usable for a wide range of applications (from thermoplastic elastomers to optically active materials) is yet another illustration of this innovative capacity.

---

## SUB-PROGRAMMES

### Catalysis

Investigating, screening and developing (novel) homogeneous and heterogeneous catalyst systems, as well as new approaches for the immobilisation of molecular catalysts, new co-catalysts and activators.

### Polymer structure, properties and processing

Understanding, modelling and predicting structure-processing property relationships in polyolefin-based polymer systems.

### Polymer reactor engineering

Studying various reactor and technology unit operations to develop a quantitative description and acquire a thorough understanding of the crucial aspects of olefin polymerisation processes.

### New methods and exploratory research

New polymerisation and polymer characterisation methods, high-throughput screening and experimentation, embryonic research and concept development.

“You need guidelines from industry to know what is important when you want to apply your knowledge in a product.”



---

# Laurens Polgar

## Modifying rubber

---

### PERFORMANCE POLYMERS

Performance Polymers (PP) have considerable potential to contribute to reducing energy use, environmental impact and the effects of climate change through component consolidation, weight reduction, lifetime extension, recyclability and utilisation of renewable feedstock and create new opportunities for the construction, transport, appliances and electronics industries.

---

**Research should result in the practical use of the findings, according to Laurens Polgar. In his PhD project, he is investigating how rubber can be reversibly cross-linked in order to be able to recycle it.**

Laurens Polgar, in a white lab coat, safety glasses on his head and a sample in his hands, hurries down the corridor to this interview. The sample consists of several strips of synthetic rubber (EPDM), some of them specially modified and processed. Specific end groups are added with the property that they cross-link if you elicit the reaction but come loose again if you heat them. Cutting up strips of cross-linked and non-cross-linked ones, heating them and comparing the force it takes to rip them apart will tell him whether he has indeed found a reversible cross-linking mechanism for rubber.

#### Hotel

“After graduating from school in 2006, I needed time to decide what I wanted to study, so I went abroad for a year. I did not have enough money to travel around much, so for a time I worked in a hotel in London and, in no time, became the supervisor of a small international group of people that organised events such as weddings,” Polgar begins his narrative of how he

ended up at DPI. After a year, he had made up his mind about the direction he wanted to take in his studies, which was to be science. He started in Groningen with the broad Bachelor’s programme, which allows students to postpone the choice of their Bachelor’s specialisation: the lectures and exams in a number of disciplines are the same in the first year. “I could not choose between a number of science courses because I was interested in every discipline, and this allowed me to become acquainted with them all. I passed at the top of my class and received the Spinoza award from the Koninklijke Hollandse Maatschappij der Wetenschappen. At the end of the year, I opted for chemistry but still did not know whether it should be chemistry or chemical engineering. So I did both exams and passed both *cum laude*. That and the Spinoza award, as well as the fact that my former schoolmates were one year ahead of me, motivated me enormously to continue swiftly with my studies,” Polgar continues.

His Bachelor’s project was related to the chemistry of solar cells. He enjoyed it very much, but nevertheless ultimately chose chemical engineering for his Master’s, the main reason being that the useful application of all the science that he would learn was a bit closer. “I like it when I can use the knowledge I have acquired immediately, in an application or by passing it on to others. I have always helped a great many other students and pupils with their studies, given seminars, helped in practicals as a teaching assistant and participated in education and evaluation committees here at the university. Last year, one of the university professors and I launched a new series of lectures in Industrial Engineering & Management Science, and not so long ago, I took over a lecture from my professor, Francesco Picchioni. That was quite an experience: 150 people in the lecture hall and at the end they applauded,” Polgar adds. One can almost see him as a professor already.

As a Master’s student, Polgar participated in Diego Wever’s DPI project in Picchioni’s



Chemical Technology group. The project was concerned with enhanced oil recovery: by injecting a solution of polymers and water into an oil well, the oil that does not come out by itself can be forced out. "In my project, I tried to assess the relationship between the structure of the polymers – how many side chains they had and how long they were – and the viscosity of the solution," says Polgar. "The polymers were designed in a controlled way for this specific purpose and not much was known about them. I measured the viscosity of both a melt and a solution of these polymers and tried to find a relationship between the two with the ultimate goal of designing new and better polymer structures. Three articles resulted from that work."

### Rubbers

Although he was asked to continue in the same field, Polgar preferred to choose a completely new subject for his PhD project, which he started at the end of 2012. "I already knew a great deal about the polymers for enhanced oil recovery and I wanted to broaden my view. So when the opportunity was offered to work on the modification of rubbers, I chose that. Rubbers, when they are cross-linked, normally become a thermoset material that cannot be processed any more. It is a finished product that can only be burned

at the end of its life. Naturally, that is not a desirable method of disposing of it. If the cross-linking could be reversed, perhaps it would be possible to reuse the rubbers, or at least parts of them. So what I have done up to now is to review all the possible modification methods for rubbers: which functional groups can be incorporated and what that implies for the properties of these rubbers. For a few of them, I have already investigated – using the strips mentioned before – which ones could result in reversible cross-links," says Polgar to explain the present status of his project. Reversible cross-linking is not unknown in polymers such as ketones and others, but it is new for commercial rubbers.

The fact that his project is a DPI project is certainly valuable to Polgar. Doing research just to satisfy his curiosity is not enough for him. "As a scientist, of course you are interested in knowing why something works, but you need guidelines from industry to know what is important when you want to apply your knowledge in a product. For example, I might intend to use a system that breaks its cross-links at a temperature of 150°C, but if someone from industry told me that the product would then lose its strength, I could decide to try something else. That is the kind of information you get from DPI's industrial

partners," says Polgar. During his internship with Nyrstar, a zinc smelter in the Netherlands, he also gained some hands-on experience of working in industry. He found analysing every aspect of a problem, not only the technical but also the organisational and managerial aspects (the cadmium mass balance in a specific reactor, in his case) very interesting.

When his PhD project is finished, he would either like to go into industry or secure a post-doc position abroad, but with both routes preferably ending in a professorship at a university. That is where his ambition lies. With his drive (he reinstated the weekly progress meetings in Picchioni's group and revitalised the safety procedures in the department, which he thought had become a bit too slack compared with what he saw in Nyrstar) that is probably where he will end up.

---

## OBJECTIVES

The Performance Polymers (PP) technology area combines Engineering Polymers and Rubber Technologies and is positioned between bulk plastics and specialty polymers such as functional polymer systems. Performance polymers possess improved chemical, mechanical and physical properties, especially beyond ambient conditions. They are applied as material systems under (cyclic or continuous) load-bearing conditions and frequently consist of multi-component mixtures with various polymers, reinforcements and additives.

The performance requirements of complex parts and assemblies in polymer materials necessitate close technological cooperation between polymer supplier, converter and end user. That in turn calls for a thorough understanding of polymerisation and polymer modification, as well as the processing, properties and design of polymer systems. Moreover, the wide variety of base polymers in this technology area demands a special effort to identify commonality in those themes along the value chain. This is reflected in the strategy and objectives of the Performance Polymers technology area, which include investigation of fundamental issues in the value chain using a 'chain of knowledge' approach in terms of energy saving, durability, ultimate performance and sustainability.

---

## FACTS AND FIGURES

### Partners from industry

- AkzoNobel
- BASF
- Bayer
- Bekaert
- DSM
- Lanxess Elastomers
- Sabic
- SKF
- Teijin Aramid

### Partners from the research world

- Delft University of Technology
- DWI an der RWTH Aachen
- Eindhoven University of Technology
- Fraunhofer Institute for Structural Durability and System Reliability LBF
- Leibniz-Institut für Polymerforschung, Dresden
- National Technical University of Athens
- Queen Mary & Westfield College, University of London
- University of Amsterdam
- University of Groningen
- University of Twente
- Wageningen University

### Budget and organisation

Expenditure in 2012 totalled € 1.44 million (budget: € 1.89 million). A total of k€ 126 was spent on equipment. The total number of FTEs allocated at year-end 2012 was 14 (26 researchers). Prof.dr. Costantino Creton acted as Scientific Chairman. Dr. Jan Stamhuis acted as Programme Area Coordinator of the Performance Polymers programme.

### Publications and inventions

This technology area generated a total of 26 reviewed papers and ten theses; seven inventions were reported and three patent application were filed.

For details, see page 78.

---

## SUB-PROGRAMMES

### Polymer and network chemistry and modification

Studies aimed at expanding the use of bio-based materials, by identifying their unique properties and reducing their eco-footprint. Further studies are designed to reduce the costs and energy use in polymerisation. Other objectives are network formation and the development of new concepts for monomer polymer molecular structure to achieve gradual changes in the balance of flow properties, static and dynamic mechanical behaviour and other functional properties.

### Processing for properties, polymer physics and modelling

Understanding the relationship between the molecular structure, processing and properties of polymers. Studies of the processing effects of intermolecular interactions, e.g. hydrogen bonding. Processing, modification and vulcanisation studies of elastomer blends. Studies of complex flow behaviour, e.g. in particle reinforced visco-elastic materials.

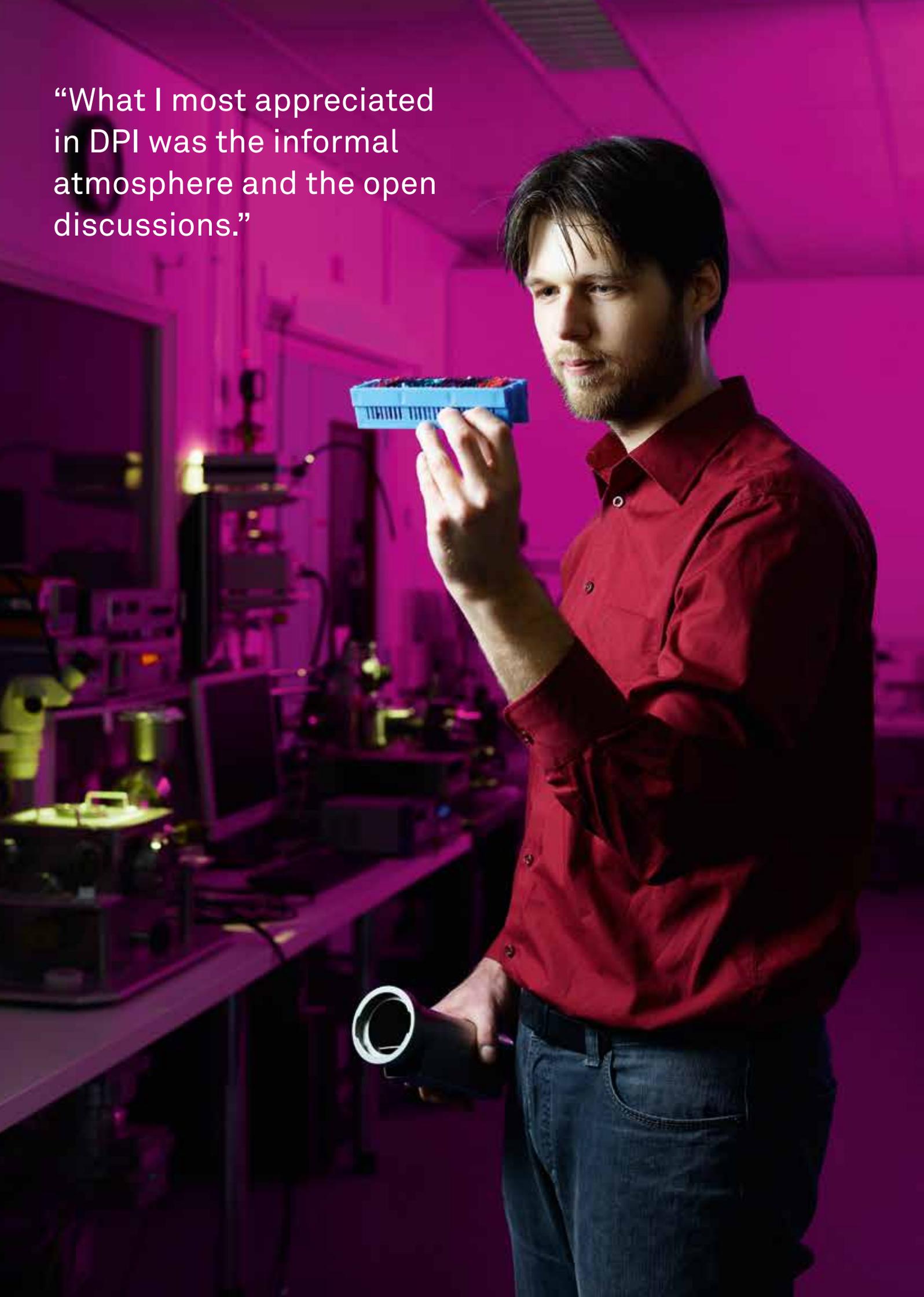
### Advanced reinforced thermoplastics and synthetic fibres

Studies of the interface effects in fibre-reinforced composite systems, the effects of nano-reinforcement on polymer material properties on macroscopic and microscopic scale with a focus on the effects at the matrix-filler interface, friction and wear studies of fibre-reinforced thermoplastics and elastomers.

### Long term stability and performance

Investigation of the chemical and physical ageing mechanisms and their interaction, with the ultimate objective of predicting lifetime and attaining a fit-for-purpose design over the entire lifecycle. Studies of self-healing in polymeric materials as paradigm shift to realise improved fit-for purpose lifetimes.

“What I most appreciated in DPI was the informal atmosphere and the open discussions.”



---

# Paul de Bruyn

## About tandem and hybrid solar cells

---

### FUNCTIONAL POLYMER SYSTEMS

The Functional Polymer Systems (FPS) technology area performs research on polymers, small organic molecules and their prototype devices that are capable of an electrical, optical, magnetic, ionic or photo-responsive function and that offer potential for industrial application.

---

**There are obvious directions you can take to improve solar cells: place two with different spectral properties on top of each other; or combine the best of the organic and inorganic materials. But it is easier said than done.**

“Half way through my course in applied physics at the University of Groningen, I began to develop a lively interest in one particular subject: organic electronics. I was highly motivated to continue studying in that field and therefore decided to do my Master’s project in the Physics of Organic Semiconductors group, which at that time was still headed by Professor Paul Blom,” says Paul de Bruyn, as he explains how he became involved in polymer research and in DPI. “Solar energy was another subject that appealed to me, so when I was offered a PhD project in which I could combine both interests, the choice was easy.”

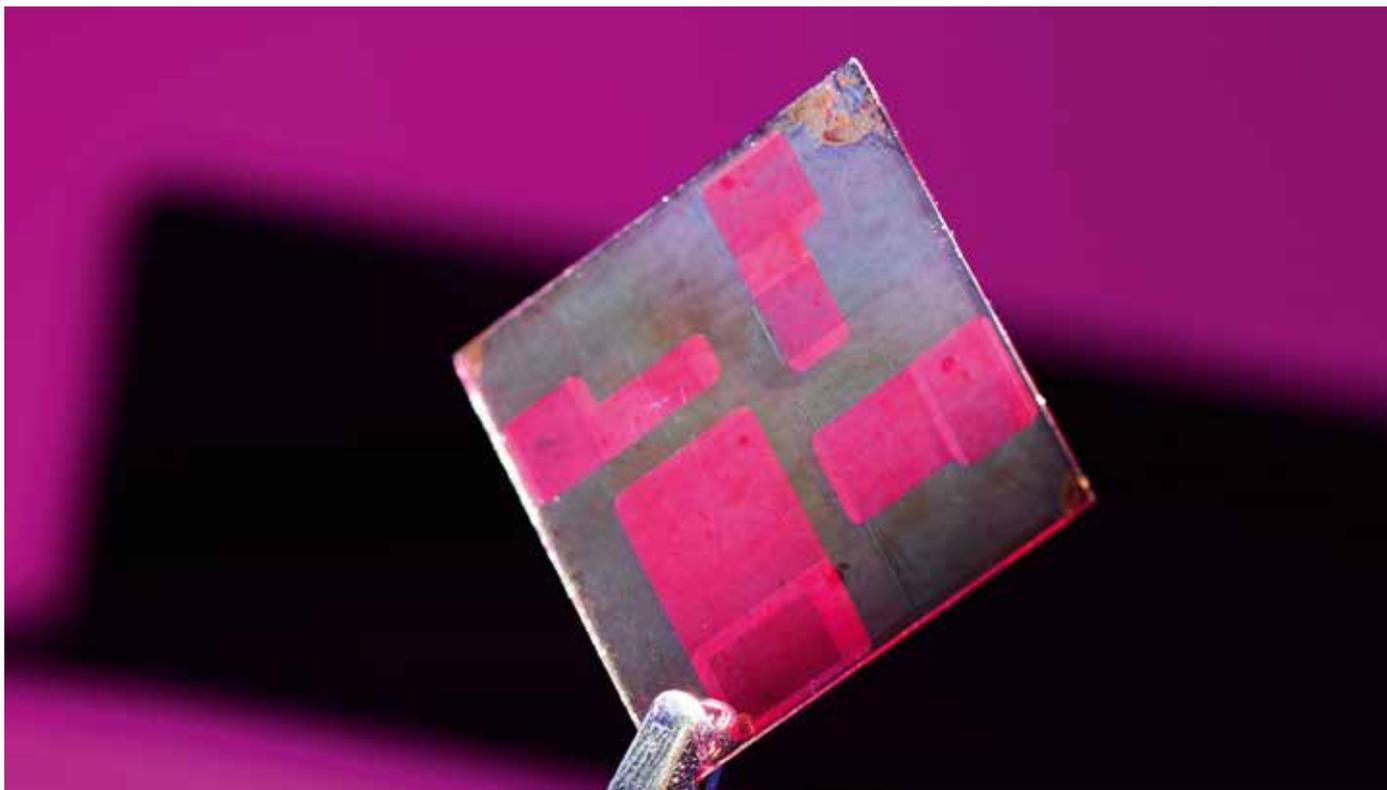
#### Orthogonal

During his Master’s project, De Bruyn investigated how to combine two organic solar cells that absorbed sunlight in different regions of the spectrum. Placed on top of each other, the efficiency of the combination would be greater than that of two separate solar cells. The idea was to make this tandem solar cell in single

process. Organic solar cells are produced using a process called spin coating: a polymer is deposited from a solution on a spinning disc, the polymer covers the surface uniformly and the solvent evaporates. When several layers are placed on top of each other, the solvents used have to be ‘orthogonal’, which means that the previous layer should not dissolve in the solvent used to deposit the following layers. This is difficult enough with the layers of one solar cell, but the constraints are even greater when another set of layers for the second solar cell has to be deposited on top of that. “For my Master’s project, I conducted the experiments to find out which combinations of polymers and solvents worked,” De Bruyn explains.

“My supervisor at the time investigated how the charge transport was affected in such a combination. In the end, we found a nice combination of polymers and accompanying solvents that gave satisfying results,” he says.

In the course of his Master’s project De Bruyn was already asked whether he would be interested in doing a PhD project in the same field. Since he liked Groningen and enjoyed the subject, he accepted the offer. Once again, the subject was solar cells, but this time the project involved hybrid solar cells. De Bruyn: “I was asked to look at the combination of an organic donor polymer and an inorganic acceptor, in particular zinc oxide. Mixing the organic semiconductor donor material with nanoparticles of zinc oxide had already produced working solar cells. In the next step, the particles would not be mixed in the donor material, but the zinc oxide would be produced in situ in a chemical reaction (hydrolysis) that occurred when the layer was formed. To create that effect, a precursor material containing zinc is mixed with the donor material. Some work had already been done with diethylzinc as precursor material, but that material was so reactive that it immediately reacted with the atmospheric water. The properties of resulting layers were completely



unpredictable.” So De Bruyn tried other precursor materials in the hope of finding one with which the process could be controlled.

### **Cathode**

That hope proved in vain, at least for the active layers in solar cells. The problem is that precursor materials with longer side chains are not easily removed from the layer after the zinc oxide is produced. They subsequently start to act as charge traps and detrimentally disturb the charge transport. However, one of the materials De Bruyn experimented with appeared to result in zinc oxide layers that could be used for the cathodes of the solar cells, for which barium or calcium, very reactive materials demanding very good encapsulation, are normally used. Zinc oxide is already an oxide and is therefore not so reactive. Although some encapsulation is still required, it is less demanding. “So, via a side path, my project produced a useful result after all,” says de Bruyn. “Researchers at the Holst Centre are now investigating how to incorporate zinc oxide cathodes in the production process of organic solar cells and LEDs.” The fact that the reaction is rapid and that the temperatures involved are not extremely high, which would damage the polymers, will ultimately allow the cathodes to be used in a roll-to-roll production process

for organic semiconductor devices on plastic foils.

De Bruyn completed the experimental work for his thesis several months ago and is busy writing the last two articles for the thesis. He has already started a new job that is, ironically, related to fossil energy resources. At GasTerra, a Dutch company engaged in the worldwide trade and supply of natural gas, he has been employed as a business analyst and is currently developing models on price appreciation. He enjoys his work very much. “It is completely different to what I did before, but also very interesting,” says De Bruyn, who was seeking to broaden his perspective and wanted to find a job that would allow him to stay in Groningen. “I am enjoying it immensely for now, but I do not rule out the possibility that I may return to the organic semiconductor world in the future. In that case, DPI and the contacts I have made there could be helpful. What I appreciated most in DPI was the informal atmosphere in which all of the activities took place. Discussions were always very open. Companies are more inclined to exchange information when they see their peers in other industries doing the same thing. That is something you miss in projects in which only one industry is involved. The international aspect also appealed to me. Project meetings must

be of great value for people if they are prepared to come from as far away as London and the south of Germany to attend them. DPI is an institution with a good reputation and even when you look for work beyond its scope, as I did, having done a DPI project looks good on your curriculum vitae.”

For his project work and the contacts with the Holst Centre, the direct lines he had via his supervisor Paul Blom, who moved from Groningen to the Holst Centre, and former colleagues who followed in Blom’s footsteps, were more important than the DPI meetings. But De Bruyn believes that, even if this had not been the case, DPI could certainly have been instrumental in ensuring the continuation and application of his project. And the excellent analytical facilities available to the Holst Centre at the Eindhoven University of Technology certainly brought added value to his research project.

---

## OBJECTIVES

The FPS research programme is structured along application lines in the following sub-programmes: polymer lighting and field-effect transistors; polymers for information and communication technology; solar cells (photovoltaics); and responsive materials, (bio)sensors and actuators.

---

## FACTS AND FIGURES

### Partners from industry

- BASF
- DSM
- ECN
- Industrial Technology Research Institute
- Philips
- Rolic Technologies
- Sabic
- Solvay
- TNO

### Partners from the research world

- Delft University of Technology
- ECN
- Eindhoven University of Technology
- Imperial College London
- Nanoforce Technology
- University of Cologne
- University of Groningen
- University of Wuppertal

### Budget and organisation

Expenditure in 2012 totalled € 1.65 million (budget: € 1.51 million). A total of k€ 15 was spent on equipment. The total number of FTEs allocated at year-end 2012 was 16.4 (31 researchers). Prof.dr. Frans de Schryver acted as Scientific Chairman and Dr. John van Haare as Programme Area Coordinator.

### Publications and inventions

The research programme in this technology area generated a total of 21 reviewed papers and eleven theses. One invention was reported and one patent application was filed.

For details, see page 80.

---

## SUB-PROGRAMMES

### Polymer lighting and field-effect transistors

Research in this field is designed to generate a thorough fundamental understanding of the behaviour of materials under operational conditions and create breakthroughs in device performance and related architectures. New materials and innovative approaches are explored in the search for a significant improvement in the efficacy (lm/W) of polymer lighting applications and improved mobility/stability for field-effect transistors. The research focuses on understanding materials and device performance, photo-physics and charge transport of emitting materials, mobility improvements and stability under ambient conditions (air, water).

### Polymers for information and communication technology

The objective of this sub-programme is to develop scalable techniques for structuring polymers on a nano- and micro-scale by combining 'top-down' approaches with 'bottom-up' techniques based on self-assembly or supramolecular chemistry in order to produce new or greatly enhanced properties for optical, electrical, biomedical and sensor applications.

### Photovoltaics (PV)

This area is dedicated to exploring new materials and gaining a fundamental understanding of all (photo-) physical processes occurring in polymer and small organic molecule bulk heterojunction PV. Organic PV is one of many promising PV technologies offering the prospect of large area cost-effective PV for sustainable energy production in the long term. The research focuses on novel low-bandgap materials, hybrid (inorganic-organic) blends, stable materials under ambient conditions, non-radiative decay processes, efficient charge separation, morphology control, tandem solar cells and a thorough understanding of materials behaviour under operational device conditions.

### Responsive materials, (bio)sensors and actuators

The purpose of the research is to develop new materials and processes that result in a change of shape and/or large displacement upon an external electrical, magnetic, optical and/or chemical trigger.



“DPI also serves as a bridge, connecting industry and the academic field, that facilitates a very open debate.”

# Yingyuan Li

## Environment-friendly coatings

### COATINGS TECHNOLOGY

Within the Coatings Technology (CT) area frontier research in the general field of organic coatings is performed. The aim is to develop fundamental insights that will lead to innovative coatings technologies, The research is pre-competitive and is focussed at achieving sustainability, quality of life improvements, economic growth and preparing the coatings industry for future challenges.

**The challenge facing Yingyuan Li is to produce waterborne polyurethane coatings based entirely on renewable resources, not only with controlled pre-polymer composition and chain end groups, but also well-controlled dispersion stability and degree of chain extension.**

“My supervisor in the polymer chemistry group at Eindhoven University of Technology, Professor Cor Koning, described my project as the most challenging of all his group’s projects,” says Yingyuan Li, when asked about her project in the DPI Coatings Technology area. She is researching whether, and if so how, waterborne coatings can be made entirely from renewable resources. “When I started the project, nobody in our group had any experience in making polyurethane dispersions. Fortunately, the industrial partners involved in this project were extremely helpful. Nevertheless, the dispersion process, and especially the chain-extension step, has turned out to be far more complicated than we originally thought.”

#### Challenge

Li uses the word ‘challenge’ more than once during the interview. In 2003, after

earning her Bachelor’s degree in Polymer Material Science and Engineering at SiChuan University in the south of China, Li returned to Beijing, where she was born. She started to work as a commercial assistant for Charna, a Chinese-Japanese chemical company. After a while, she moved to DSM Beijing, where she found a more challenging and more interesting job. After three years working in commercial and marketing-related affairs, she realised that she wanted to be more closely involved with science and technology and moved to another Dutch company, Hofung Technology, an agency for Western companies seeking to introduce their products and technology in China. Here, Li often attended the technical meetings between the foreign companies and the Chinese customers and learned about specific technologies and products in detail. This experience inspired her next decision. “In 2007, I came to the conclusion that I wanted to know more about the technology, to gain more in-depth knowledge. Through my contacts at DSM, I knew that Eindhoven University of Technology has a strong programme in polymers, and I started my Master’s study there,” explains Li. By then she had already set her heart on the next challenge, a PhD project, which she embarked on soon after earning her Master’s degree in 2008.

Waterborne PU coatings as such are not new. They have been developed since the 1960s. But renewable raw materials normally have a different molecular structure than petrochemical raw materials, thus their reactivity, and especially their regioselectivity, had to be investigated. It turned out that isosorbide and lysine-based diisocyanate are indeed suitable to make waterborne PU dispersions. The next step was to prepare stable dispersions of high molecular weight with a tunable glass transition temperature, i.e. tunable coating properties such as hardness and flexibility. “For that I had to combine the soft and the rigid PU building blocks at different ratios. Currently, we can



formulate coatings with a renewable content of between 92% and 98% by weight. The non-renewable content is the petrochemical-based stabilising agent, for which there is not yet a renewable-based alternative. The resulting coatings are glossy and transparent, and some of them display good mechanical properties. I am now comparing the properties of these renewable-based coatings with the commercially available ones,” explains Li.

### **Purity**

The obvious goal of research into waterborne coatings based on renewable resources is to develop a coating system, that is less toxic, non-flammable and contains a much smaller amount of volatile organic solvent. The availability of renewable-based PU building blocks makes it possible to prepare fully renewable-based coatings. “But there is still a price gap between renewable-based and petrochemical-based materials,” says Li. “That can be due to many factors, including differences in the scale of production, the purification steps and the product yield, etc. For example, one of the renewable-based functional groups involved in this project requires multi-step purification and has a relatively low yield. There is a significant amount of research being conducted worldwide nowadays, in companies and in universities, so I expect that the

price disadvantage of renewable-based materials could gradually be reduced. But, besides the price, legislation also plays an important role.”

“The system I investigated still needs improvement. For instance, the molecular weight is not yet comparable to the coatings that are currently commercially available. That might be due to the relatively low purity of renewable-based compounds and the low compatibility between the reaction partners. Many things can be done to improve the current system, such as improving the purity of the renewable-based materials and replacing the toxic isocyanates compounds. A lot of practical work is still required before this system can be applied. The companies that have been involved in my project, DSM, AkzoNobel and Evonik, are conducting similar research of their own. Combining their experience and results with the university’s contribution will certainly accelerate the progress.”

### **Home**

Input from and direct contact with other researchers doing similar work is particularly important for PhD projects in a field that is completely new to a university research group. In that sense, DPI has played an important role in Li’s project, as she explains: “I feel kind of at home in DPI.

DPI provides a platform for information transfer between industrial partners and universities. For instance, I was given the opportunity to learn how to make polyurethane dispersions at DSM (Waalwijk), a skill that would have taken me far longer to learn if I had had to do it on my own. I like the cluster meetings and the Annual Meeting, where you get to know people from all of the technology areas and learn about their research. DPI also serves as a bridge connecting industry and the academic field, but not a static bridge. It is a bridge that facilitates a very open debate between the partners.”

When her contract ends in May, Li would like to spend some time finalising a number of publications and her thesis. “I have been working on this project for more than four years and I want my thesis to demonstrate the value of all that work. After my doctorate, I would like to continue working in research. I have devoted a lot of time to renewable waterborne coatings and my interest still lies in that area, but I can also work on other research topics in order to broaden my experience in new fields,” she says. Her great ambition is to continue conducting research into polymers, regardless of whether it is at a university or in industry.

---

## OBJECTIVES

The research programme for Coatings Technology (CT) concentrates on exploring novel coating materials and technologies and acquiring fundamental insights into the structure-properties relationships of coatings to enable the coatings industry to meet future challenges. The research programme is based on three pillars: renewable raw materials and novel, environmentally friendly coating technologies; functional (smart) coatings; durability and testing of coatings.

---

## FACTS AND FIGURES

### Partners from industry

- AkzoNobel
- Altana
- DSM
- Lawter
- Saint Gobain

### Partners from the research world

- Eindhoven University of Technology
- University of Groningen
- University of Haute-Alsace
- Wageningen University

### Budget and organisation

Expenditure in 2012 totalled € 0.86 million (budget: € 0.95 million). A total of € 29k was spent on equipment. The total number of FTEs allocated at year-end 2012 was 8.5 (12 researchers). Prof. Claus Eisenbach acted as Scientific Chairman and Dr. Harold Gankema as Programme Area Coordinator of the Coatings Technology programme.

### Publications and inventions

The research programme in this technology area generated a total of thirteen reviewed papers, three theses. One invention was reported and one patent application was filed.

For details, see page 81.

---

## SUB-PROGRAMMES

### Renewable raw materials, formulation and powder coatings

There are currently three projects underway to study the feasibility of applying sustainable, renewable resources in coatings technology without compromising the properties of the final coating (film). The programme focuses on bio-based building blocks and raw materials as substitutes for materials derived from petrochemistry and their use in novel coating technologies. Systems being studied include polycarbonate powder coatings or waterborne polyurethane dispersions, as well as starch-based performance coating materials. The results are promising in that coatings have already been obtained which match and/or improve on the properties of purely synthetic coatings.

### Functional (smart) coatings

'Smart coatings' are capable of responding to an external stimulus, such as light, temperature, pressure, pH, odours or gas. The stimulus causes a change in the coating's properties which may be permanent or reversible. Coatings with self-healing properties in response to mechanical damage or with light- or moisture-induced self-cleaning properties are of particular interest and have already been studied. Research on protective coatings that can adapt to their environment and/or conditions under which they are used is at the embryonic stage, but such systems, as well as tailored coatings for medical diagnostics (e.g. test strips) and implants, seem feasible in the future. The same applies for coatings with special optoelectronic and electronic properties that could be used in electronic devices and information technology.

### Durability and testing of coatings

The aim is to gain a fundamental understanding of the degradation mechanisms of coatings used in outdoor exposure to enhance durability. Another objective of this sub-programme is to develop new testing methods for coatings, e.g. methods for testing adhesion, gloss or scratch resistance, which correlate to meaningful physical parameters. Last but not least, DPI collaborates intensively with the Materials Innovation Institute's 'Materials to Innovate' (M2i) programme in the study of anti-corrosion coatings.



“At the interface between chemistry and biology, you gain a fundamental understanding and are close to an application.”

---

# Marco Emanuele Favretto

## Fundamental understanding and specific applications

---

### HIGH-THROUGHPUT EXPERIMENTATION

High-Throughput Experimentation (HTE) and combinatorial materials research open the way to the rapid construction of libraries of polymers, blends and materials through systematic variation of composition. Detailed characterisation of such libraries will help to develop an in-depth understanding of structure property relationships.

---

**In the synthesis of polymers for drug or gene delivery, chemical properties are the main point of attention. Naturally, biological safety is equally important and should be considered from an early stage according to Marco Emanuele Favretto.**

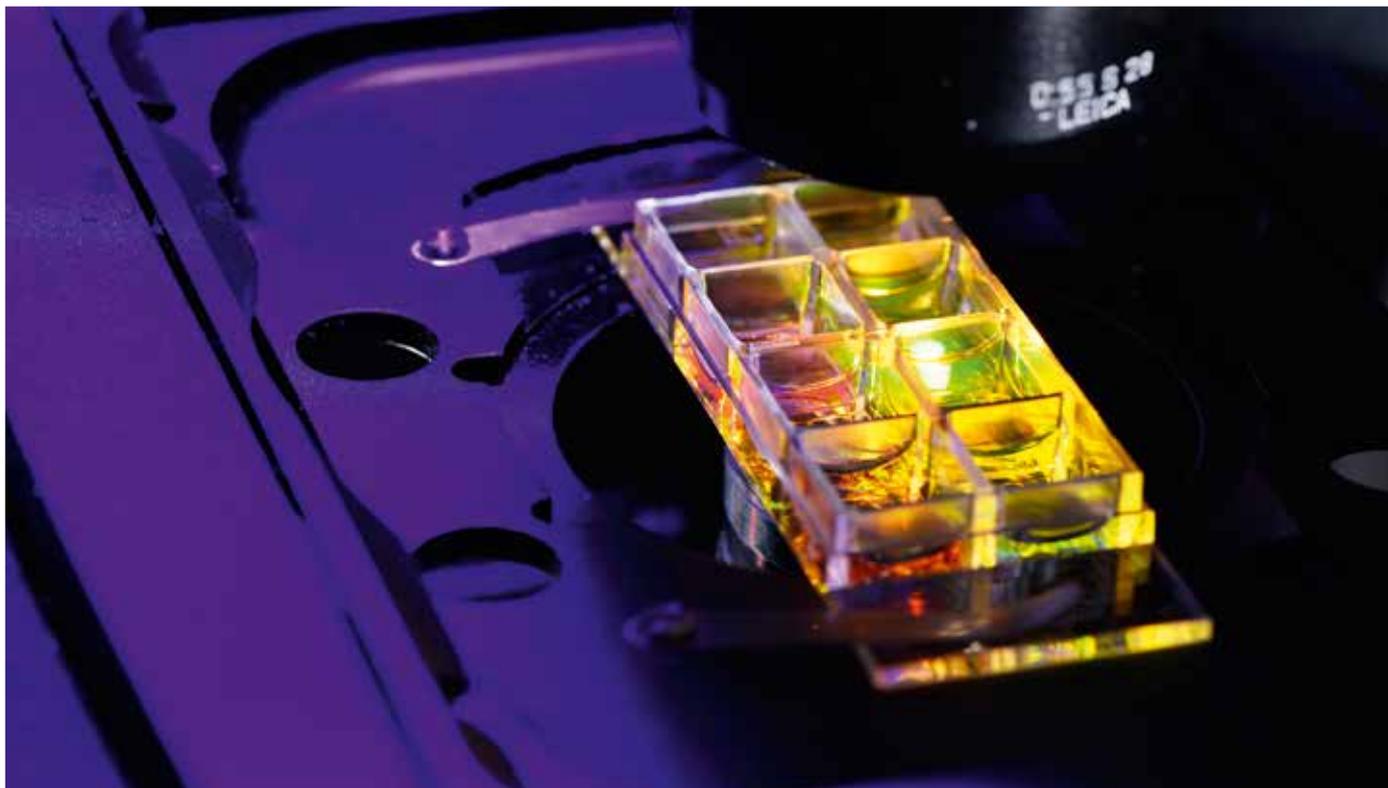
“I was kind of in shock when I started my PhD project in 2007, because I had never seen a cell in my life,” says Marco Emanuele Favretto, who studied pharmaceutical chemistry in Trieste in Italy before he went to the University of Kent in the United Kingdom for his doctorate. “By the time I had completed my Master’s thesis in Trieste, I realised that pure chemistry was not exactly the right choice for me, since I wanted to see how molecules are applied in biology. In my opinion, the really interesting things are happening at the interface between chemistry and biology. You obtain a fundamental understanding of how the molecules that you have just synthesised work, but you are also quite close to a very specific application. I started as a chemist who thinks like a biologist, and now I am becoming more like a biologist who thinks like a chemist. And that suits me fine.”

#### Circle

During his Master’s internship, Favretto worked on the synthesis of highly branched

polymers for drug delivery, with the aim of improving the solubility of extremely hydrophobic drugs and increasing their circulation time in the bloodstream. He had the good fortune that the Medway School of Pharmacy at the University of Kent was looking for a PhD candidate with a strong background in chemistry and an open mind towards biological applications. During his PhD project, Favretto was able to successfully formulate liposomes that are able to accumulate in brain tumours, while developing complex cellular models of the blood-brain barrier. The experience with biological applications Favretto had acquired in the United Kingdom induced Professor Roland Brock to ask him to come to the Radboud University in Nijmegen, the Netherlands, in 2011. The Biochemistry department was looking for someone with a biological mindset and a strong background in chemistry. The circle was complete.

In his present project, which is about gene delivery to cells with the help of polymers, Favretto collaborates with Professor Ulrich Schubert’s group in Jena, Germany. Favretto explains how this fits in with his specific background: “It used to be that chemists would synthesise polymers solely with the aim of improving the internalisation and release of nucleic acids in the cells. Such polymers were tested and, in the end, the most promising ones were optimised and selected for (expensive) preclinical and clinical trials. However, during these trials, it was often found that these polymers were not compatible with blood or produced severe side-effects. A great deal of money had been spent and there were no useful results. If you search for information about blood compatibility in the literature, you will find it only for a very small number of polymers. We tried to reverse this paradigm. We asked the chemists to synthesise a library of polymers with specific functionalities, inspired by nature, that might possibly improve their ability to deliver genes to the target and limit the side-effects. What I now do



is test the polymers for their biological safety in an earlier phase and I do that also in a high-throughput way. Are the promising polymers compatible with blood and not toxic, do they not cause inflammations and are they stable enough for their intended use? The number of possible polymers you end up with is smaller, some two or three instead of the former thirty, but the chance of success in preclinical and clinical trials is higher. It is more than simply testing, however. In the process we try to understand what happens inside the cell, and this fundamental understanding will help us and the group in Jena in selecting the building blocks for the synthesis of new polymers for specific purposes.”

#### **Expertise**

What Favretto noticed was that biologists and chemists, even though their goal is the same and they are thinking along the same lines, frequently do not know how to communicate with each other, not only because of the language but also because of the way they are used to think. “Therefore, it is easier to get useful results if you can assemble the biological and chemical expertise to work on the same topic at least in the same laboratory, but preferably in the same person, than when you have to look for that expertise outside your team. Of course, you still have to

talk to people outside your group - useful information often comes from outside - but the input from both these backgrounds on a daily basis really accelerates a project.” Favretto has developed a workflow to biologically test polymers that he and Schubert’s group consider promising candidates for delivery of a specific gene and that can be produced in large enough quantities.

The biological aspects of polymers have been playing a role for quite some time in other technology areas of DPI, but this is the first time that they have done so in the High-Throughput Experimentation technology area. And it has already had a positive effect on other technology areas, as Favretto explains: “At one of the DPI Annual Meetings, I met Martien Cohen Stuart, who offered me access to their facilities in Wageningen, the Netherlands, if I wanted to take the characterisation of our polymers a step further. It actually happened the other way round: they came to us to test some of their polymers for biological compatibility. So we have now set up a collaboration in which the biologically-oriented work flow we developed here is instrumental.”

#### **Teaching**

Favretto’s present project in Nijmegen was due to end in June, but an extension has

been granted until the end of 2013. He will then start looking for a position at a university. “My idea is to remain in academia, but in what role is still a big question. I love to teach; I love students. I really think that giving everyone, especially young students, the possibility to be part of the world of science and to understand something of science is absolutely essential. Unfortunately, there are not many positions available where you can teach as well as doing research, at least not here in the Netherlands, so I may be forced to go back to the United Kingdom. It will be impossible in Italy, given the present situation, and by that, I do not mean only the financial situation. There they tend to draw from the same pool of scientists when there is a vacancy, kind of recycle them.” Favretto believes his DPI network will definitely help him find a job.

---

## OBJECTIVES

In the long term, it is envisioned that 'materials informatics' will facilitate the design and preparation of customised materials and devices with predetermined properties based on previously established structure-property relationships. DPI's unique combination of leading industrial and academic partners provides an excellent basis for successful output. It also guarantees early pre-competitive evaluation of the new (platform) technologies and their rapid transfer into the commercial R&D programmes of the industrial partners.

---

## FACTS AND FIGURES

### Partners from industry

- Chemspeed Technologies
- Evonik
- Forschungsgesellschaft Kunststoffe
- Michelin
- Microdrop Technologies

### Partners from the research world

- Fraunhofer Institute for Structural Durability and System Reliability LBF
- Eindhoven University of Technology
- Friedrich-Schiller University, Jena
- Radboud University Nijmegen

### Budget and organisation

Expenditure in 2012 totalled €1.15 million (budget: € 0.66 million). A total of € 31k was spent on equipment. The total number of FTEs allocated at year-end 2012 was 11.4 (21 researchers). Prof.dr. Ulrich Schubert acted as Scientific Chairman and Dr. Harold Gankema as Programme Area Coordinator.

### Publications and inventions

This technology area generated a total of 57 reviewed papers and one thesis. Five inventions were reported and two patent applications were filed.

For details, see page 82.

---

## SUB-PROGRAMMES

### Synthesis, catalysis & formulation

Besides fundamental research on the use of microwave irradiation, studies are conducted into the feasibility of scaling up microwave assisted polymerisation procedures. The synthesis efforts have been intensified in the direction of water-soluble polymers. In addition to fast synthesis and formulation platforms, other subjects being investigated include the incorporation of high-throughput screening techniques for molar mass, polymerisation kinetics and thermal and surface properties.

### Thin-film library preparation & screening

This sub-programme focuses on gaining a detailed understanding of thin-film preparation technologies, the application of these technologies and the screening of thin-film material properties with automated atomic force microscopy and nano indentation technologies. Areas of application include the processing of light emitting materials, surface patterning, cell screening and the preparation of conductive tracks on polymeric substrates.

### Combinatorial compounding

The objective is to develop a process to accelerate the preparation, characterisation and optimisation of plastic formulations. The combinatorial extrusion line used for this purpose has been equipped with in-line and on-line screening techniques (e.g. IR, UV/Vis, rheometry, ultrasonic spectroscopy) as well as systems for data acquisition, analysis and visualisation.

### Materials informatics & modelling

This programme concerns data handling, database construction and the build-up of integrated knowledge capture systems for combinatorial materials and polymer research as well as experimental design, hard and soft modelling tools and tools for deriving quantitative structure-property relationships. A model is being developed for the screening of MALDI matrices to facilitate faster screening of molar mass.

### Characterisation techniques

This sub-cluster is engaged in the development of detailed characterisation methods. An important aspect of the research is the combination of different measurement techniques to characterise multiphase or multi-component materials at macro, micro and nano scale. Another focal point is the analysis of branched polymers by means of two-dimensional liquid chromatography. Tools and models for nano scale characterisation of interfaces using AFM technology are also being developed.

“We replace its building blocks with bio-based monomers and try to determine the effect on the final properties.”



# Karel Wilsens

## Towards bio-based high-performance fibres

### BIO-INSPIRED POLYMERS

Within the Bio-Inspired Polymers (BIP) programme, the main driver for the development of future materials is sustainability, with nature being regarded as an important source of inspiration for finding new leads and possibilities.

**Designing high-performance fibres based on renewable resources by polymerising bio-based monomers is a leap into the unknown. Replacing small amounts of monomers with their bio-based equivalents and determining the effect on the final properties is perhaps a better way to go.**

“The nice thing about my PhD project with DPI, compared with working on a project on your own at a university, is that I have access to a network of people who are doing similar projects,” says Karel Wilsens, a PhD student at Eindhoven University of Technology. He knows what he is talking about, since his project was initially sponsored by Teijin for a year before becoming a DPI project. “This is particularly true in my project, which is, in fact, one of a trio of projects that are all related to a specific bio-based monomer, furandicarboxylic acid. Two of the projects are based in Wageningen: one is related to optimising monomer and polymer synthesis, and in the other, the researchers are investigating how the monomer can be polymerised with enzymes. My task is to determine the possibilities of using bio-based monomers and to develop new high-performance bio-based polyesters.”

#### Internship

As with many other students, Wilsens’ choice of what to study after leaving

school was related to the subjects he was good in. In his case, it was chemistry. The chemistry programme at Eindhoven University of Technology had a good reputation and it was close to his home town, Tilburg, so he started his Bachelor’s course in chemical engineering in 2005 and continued with his Master’s in the polymer chemistry group of Cor Koning. He has never regretted these choices. “In my Master’s project I investigated whether it would be possible, and if so how, to make polymer gels, originally intended for drug-delivery purposes and for regenerative medicine for healing wounds,” says Wilsens. This project focused mainly on chemical synthesis and that is still what I enjoy most. Part of my Master’s programme was a three-month internship with Teijin Aramid. I ended up spending five months there, since I did not think I could get a good idea of what working in a company was like in just three months.” Nevertheless, he was not interested in working in a company immediately after graduating. “I first wanted to do a PhD project. I like doing chemistry, working in the laboratory, researching things. Fortunately, during my internship with Teijin Aramid, my supervisor there, Professor Sanjay Rastogi, asked me whether I would be interested in doing a PhD project with Teijin. Of course I was, and that’s how I have ended up here at Eindhoven University of Technology in a project sponsored by Teijin.” Teijin Aramid is engaged in producing high-performance fibres - aramids - and during his five-month internship, Wilsens worked with those materials. Strong fibres are stiff and therefore inherently difficult to process into the desired form. His work during the internship involved investigating and possibly adapting the synthesis of the aramids in such a way that they could be more easily processed. Five months was not long enough to achieve that goal. “But we certainly gained more insight into the process,” says Wilsens, whose current project is also related to strong fibres, but, in this case, polyester fibres rather than aramids.



The idea is to design new liquid-crystalline polyester fibres by incorporating bio-based monomers. More and more bio-based monomers are appearing on the market today, and although they are still expensive, research is underway to find applications for them. Apart from the obvious purpose of replacing fossil-based monomers with bio-based monomers – in view of the predictable and inevitable depletion of fossil resources – the hope is also that these new bio-based polymers will exhibit interesting properties. “Of course, you hope that strong fibres can eventually be made completely from bio-based materials, but it is better to start with a process that is understood and does not present problems chemically. Vectran, a commercially available polyester with liquid-crystalline properties, is our starting point. We replace its building blocks with bio-based monomers and try to determine the effect on the final properties. I am now half-way through my project and we now understand the chemistry of such processes: we know which building blocks we can successfully incorporate and understand the effect they have on the end result. In the coming period, we will focus on the fibre-spinning process, test the properties of the fibres and assess whether the bio-based polymers might indeed possess the desired properties,”

Wilsens says of the present phase of his project.

Small quantities are usually sufficient to show that it is chemically possible to substitute monomers, but when fibres have to be spun, more material is required. Two new reactors have been purchased to cope with the demanding reaction conditions, which require reaction temperatures of between 250°C and 350°C and the distillation of corrosive acetic acid. Wilsens is glad that all these costs (including a trip to Grenoble for special synchrotron XRD analyses, a visit he will probably repeat) can be covered in a DPI project.

In Rastogi, he has a supervisor who specialises in the physics involved in the project, while he can turn to Bart Noordover, his supervisor at the university, for expertise in chemical synthesis. Wilsens really appreciates the combination of expertise that DPI projects offer.

#### **Finished product**

The three related projects are discussed once a year at a special meeting in addition to the regular cluster meetings for the Bio-Inspired Polymers technology area. According to Wilsens, discussing your results with people who are more or less at the same stage of their research

projects provides extra motivation and inspiration. In that sense, he also regards the Young DPI meeting for researchers who have recently started their projects as a valuable complement to the regular DPI meetings, not only now but also in the longer term. “Through DPI, I have met new people and interesting companies, and once I finish my PhD project, I hope that these connections will help me to find a job at one of those companies. The experience and the knowledge I have gained will hopefully prove useful in finding a job in an industrial environment. For now, I find it very interesting to study the fundamental aspects in depth, but eventually I want to go all the way from the chemistry and physics right up to the development of a final product.” Wilsens concludes the interview on a less optimistic note, however: “The future will probably not be as bright as it was sketched when we started our studies in 2005, when we were told that we would all find a job within three months after graduating.”

---

## OBJECTIVES

The aim of the Bio-Inspired Polymers (BIP) programme is to develop advanced polymeric materials and methodologies for new and existing applications. The development of these materials is inspired by natural polymeric structures and principles of natural systems such as self-assembly and bio-catalysis.

---

## FACTS AND FIGURES

### Partners from industry

- Food and Biobased Research, Wageningen UR
- FrieslandCampina
- Petrobras
- Sabic
- Teijin Aramid

### Partners from the research world

- Eindhoven University of Technology
- Food and Biobased Research, Wageningen UR
- Friedrich-Schiller-University, Jena

### Budget and organisation

Expenditure in 2012 totalled € 1.22 million (budget: € 0.76 million). A total of € 96k was spent on equipment. The total number of FTEs allocated at year-end 2012 was 9.8 (19 researchers). Prof.dr. Gerrit Eggink acted as Scientific Chairman and Dr. Peter Nossin as Programme Area Coordinator of the Bio-Inspired Polymers technology area.

### Publications and inventions

The research programme in this technology area generated a total of seven reviewed papers and three theses.

For details, see page 85.

Bio-Inspired Polymers can be produced from renewable or fossil resources through either chemocatalysis or enzymatic/microbial catalysis. The structure-property relationships of the novel materials are studied to elucidate why they exhibit unique properties. One important line of research is intended to develop a generic toolbox for new bio-based polymers with a view to creating new business opportunities. Aspects addressed by a bio-based polymer programme include the identification of new or improved (multi-)functionalities of bio-based building blocks and polymers and the assessment of relevant technologies in the bio-based value chain.



“The project worked out more than great and I hope it can be continued. The collaboration was excellent.”

---

# Qian Chen, Paulo Rocha and Benjamin Bory

## The relationship between resistive switching and OLED reliability

---

### LARGE-AREA THIN-FILM ELECTRONICS

Large-Area Thin-Film Electronics (LATFE) is the step in the value chain devoted to studying fundamental issues related to processing for large-area deposition and disruptive architectures for large-area organic electronic devices. Large-Area Thin-Film Electronics is an excellent example of a highly interdisciplinary research area, extending from chemistry and physics to engineering.

---

**Organic Light Emitting Diodes (OLEDs) suffer from early failure. As this extensive project shows, that phenomenon could be related to the formation of native oxides that cause OLEDs to function as an organic non-volatile memory.**

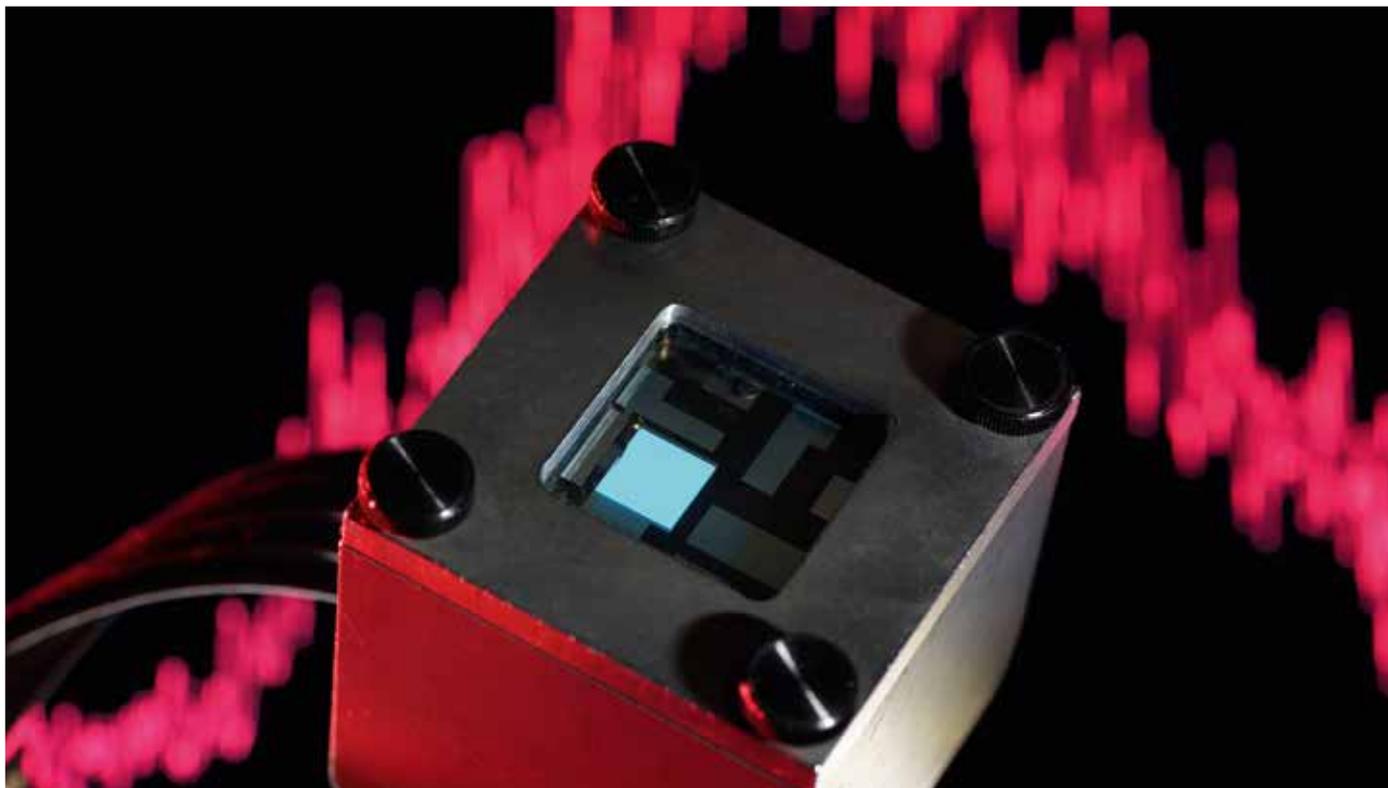
It is a morning in April 2013 and the BISTABLE project team is assembled around a few telephones in Eindhoven in the Netherlands, Faro in Portugal, Mainz in Germany and Haikou in China. Given the routine nature of the conversation, this has apparently happened more often during this large-scale project. There are no fewer than three PhD students and their supervisors participating in the conference call. They are joined by Professor Dago de Leeuw of the University of Groningen, who is currently working in Mainz, who initiated the project and recalls how the idea occurred to him. “I collected a batch of faulty OLEDs from the Philips OLED factory and they turned out to be beautiful non-volatile memories.”

It was thought at the time that short-circuits due to polluting particles or degradation of the luminescent materials were the cause of the early and unpredictable failure of the OLEDs. The faulty OLEDs displayed a phenomenon called ‘resistive switching’: a polymer layer between electrodes can be made conductive by applying a high voltage that causes a conduction path, which can then be switched on and off by applying an appropriate voltage. De Leeuw recognised the parallel between the faulty OLEDs and non-volatile memory, and wrote a project proposal to investigate the matter further. His long-standing relationship with Henrique Gomes’ group in Faro and with Stefan Meskers in René Janssen’s group in Eindhoven resulted in a joint project by three PhD students, Qian Chen and Paulo Rocha, who were working in Faro, and Benjamin Bory, who worked in Eindhoven.

### Background

“OLEDs are expected to be important products in the building industry by 2018 and therefore attract a lot of interest,” says Rocha, explaining how he became involved in the project. “The OLED industry will grow and I felt it was an interesting field with tremendous possibilities and wanted to be part of it.” With his background in electrical engineering, Rocha’s role involved trying to unravel the effects related to the resistive switching phenomenon.

For Chen, it was not the first time she had come to Europe. She had studied chemistry in Denmark for three years, before returning to China and working for two years in the clean-energy industry. “In Shanghai, where I worked, there was a firm of head hunters active on the campus,” she recalls. “They found me and introduced me to this project. I was very



interested and the idea of returning to Europe appealed to me. I thought it might be an opportunity to gather knowledge about OLEDs and about organic memories, and later bring that knowledge back home to China again. So I went to Portugal, and have enjoyed my time there very much.” Chen’s work permit expired and she is now back in China, where she is currently writing her thesis.

Bory, a materials scientist who studied in Grenoble and Lyon, also hopes to bring the knowledge he acquires in the project back to his home town of Grenoble, where organic electronics is, in his words, ‘quite present’. His task is to try to understand resistive switching, to make devices with known and controlled amounts of nano particles so that they can later be related to the electrical properties found by his two colleagues in Faro. From the start, the three PhD students, and their supervisors, hoped to benefit from the cooperation, and they were not disappointed. As Janssen puts it, “We definitely learned from each other, which helped us to make progress that would have been impossible for each of the groups to make alone.”

#### **Glue**

The three PhD students are now nearing the end of their projects. The short-circuiting was originally thought to be

induced by defects such as the presence of particles. However, a decade of research had neither confirmed nor refuted this. The present project has shown that it is not electrical short-circuits that cause the problem: the ‘dead OLED’ is a non-volatile organic memory. The common source of both the problems with reliability and the switching in non-volatile organic memories is the formation of oxide on the aluminium electrode. But the three have also shown that when other metal oxides or halides are involved – such as spin-coated layers of nanoparticles of aluminium oxide, cerium oxide, titanium oxide, lithium fluoride or indium tin oxide in diodes – this resistive switching also occurs. There are also metal oxide layers in other organic electronic devices, so the results are also significant for fields other than OLEDs. De Leeuw, who initiated the project and provided the ‘glue’ that kept everyone motivated with his enthusiasm, was more than satisfied with the results. “The project worked out more than great and I hope it can be continued. The collaboration was excellent.”

The interest of industrial partners can change during the course of a project. When truly fundamental and longer-term issues are being tackled, the applications are not immediately around the corner. Ultimately, however, because the results

have implications for all sorts of applications of organic electronics, they will find their way into better-performing devices or diagnostic tools for OLED reliability. It is of course difficult to pinpoint when and where this will happen. For the three PhD students, the interaction with the industrial partners was not limited to the DPI meetings. Chen: “We talked to both academic and industrial partners and received suggestions for further research at those meetings, but not only there. External conferences were also important for us.”

All three PhD students praise the open-minded working atmosphere during the meetings. Meetings in Eindhoven and in Faro and working together were fun and, although communicating via e-mail was not always easy, they would all do it again. “When I arrived there, it took me some time to get used to the late start in the morning that appeared to be normal in Faro,” Chen recalls. “But once I stopped fighting against it, it was fine.” Rocha corroborates this view. “It took us some time to get used to our respective working methods, but after a year we had learned how to communicate clearly with each other.” Bory remembers that it took him some time to find out what everyone was supposed to do, but “in the end we were not doing the same things, what we were doing was complementary.”

---

## OBJECTIVES

Whereas Functional Polymer Systems (FPS) focuses on materials development and initial device performance, Large-Area Thin-Film Electronics (LATFE) is the obvious next step in the value chain. The fundamental knowledge generated should facilitate the reliable production and operation of organic electronic devices.

---

## FACTS AND FIGURES

### Partners from industry

- BASF
- DSM
- Philips
- Solvay
- TNO

### Partners from the research world

- Eindhoven University of Technology
- Imperial College London
- Max Planck Institute für Polymerforschung
- University of Algarve
- University of Cologne
- University of Groningen
- University of Twente
- University of Wuppertal

### Budget and organisation

Expenditure in 2012 totalled € 1.09 million (budget: € 1.32 million). A total of € 80k was spent on equipment. The total number of FTEs allocated at year-end 2012 was 11.7 (21 researchers). The position of Scientific Chairman of the Large-Area Thin-Film Electronics programme is still vacant; Dr. John van Haare acted as Programme Area Coordinator.

### Publications and inventions

This technology area generated a total of two reviewed papers and three theses.

For details, see page 85.

---

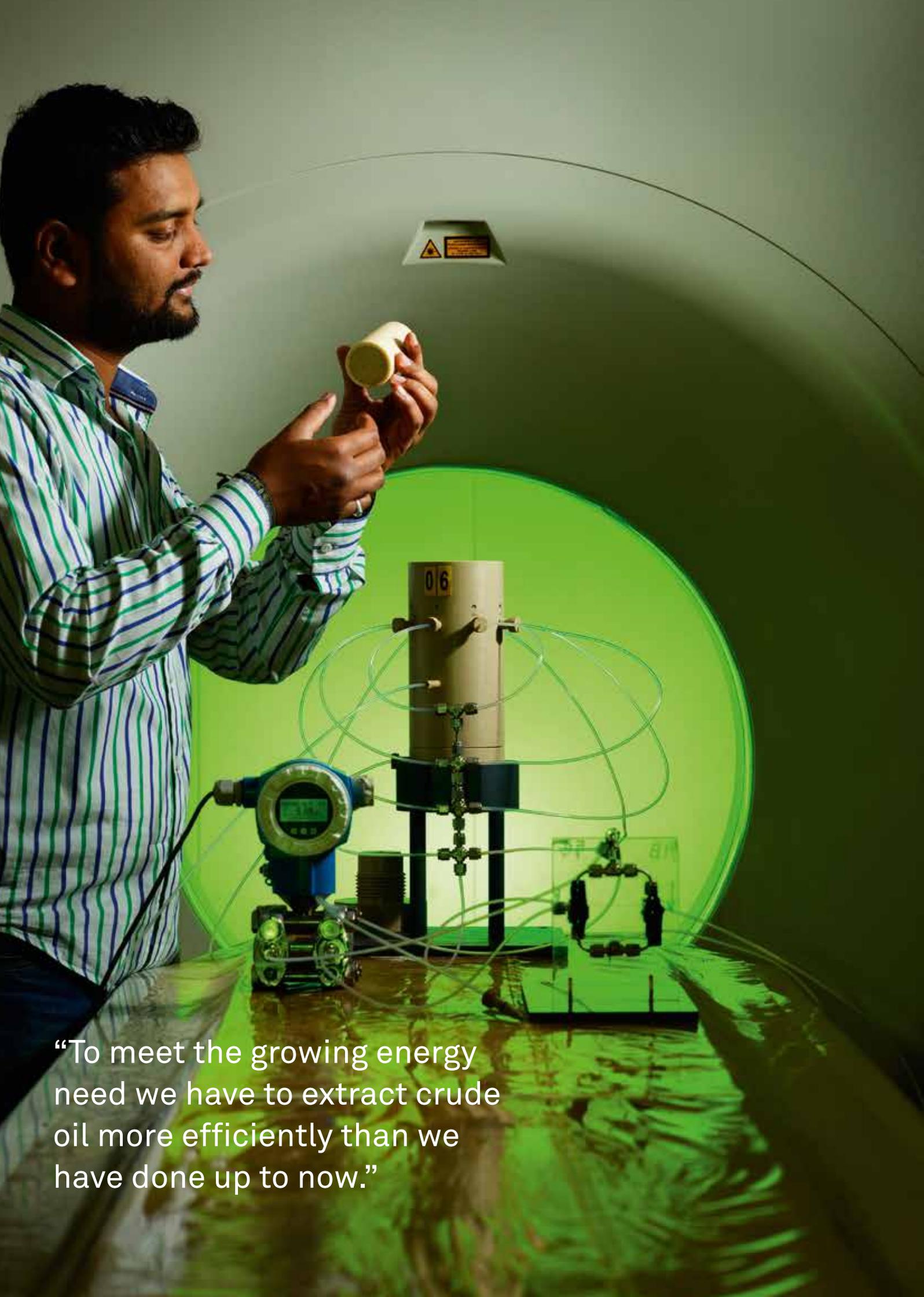
## SUB-PROGRAMMES

### Large-area material deposition using solution processing

The objective is to study fundamental issues of large-area polymer and small-molecule material deposition using roll-to-roll solution processing (gravure, flexo, screen, slot-die) to make the transition from lab scale to industrial scale for reliably processed devices. For patterning of structures inkjet printing is explored. Although lab-scale devices have superb performance, we lack the industrial processes and the fundamental knowledge about large-area material deposition from solution and patterning needed to choose the right deposition method per layer for mass production.

### Disruptive device architectures

The purpose of this research is to develop disruptive device architectures for more reliable and easier production and to understand the failure mechanisms occurring in industrially produced devices. Current device architectures require very thin films (~ 100 nm) with less than 2% thickness deviation, which imposes very strict demands on the processing and production of devices. At the moment, this results in poor yields, high costs and many uncomprehended failures. There is an urgent need for new device architectures that allow more robust processing and production and improve yield without affecting device performance (efficacy, homogeneity of light output).



“To meet the growing energy need we have to extract crude oil more efficiently than we have done up to now.”

---

# Durgesh Kawale

## Rheology in oil reservoirs

---

---

### POLYMERS FOR ENHANCED OIL RECOVERY

---

Polymers for Enhanced Oil Recovery represent an important application of water-soluble polymers. With the increasing complexity of oil recovery from existing and new reservoirs, this technology could contribute significantly to more efficient recovery of the world's energy resources. Originally a sub-programme in the Emerging Technologies (EMT) technology area, DPI has now created a new, separate technology area for polymers for enhanced oil recovery.

---

**A thorough understanding of the flow of polymer solutions in porous media, which differs from that outside these porous media, is needed if these solutions are to be used effectively to produce more oil from deep geological formations.**

Enhanced Oil Recovery is a new technology area for DPI and, consequently, Durgesh Kawale is also a newcomer to the institute. He started his PhD project in the Petroleum Engineering group at Delft University of Technology six months ago. The project is concerned with the extraction of crude oil from maturing oil-bearing deep geological formations. Kawale is eager to explain why his subject is so important. "Recovering even only a small fraction of the oil left in the existing oil reservoirs worldwide would represent several billion barrels of additional oil."

#### Infrastructure

In many oil fields about 15% to 20% of the oil flows out because of the inherent energy in the reservoir, while another 20% to 30% can be pushed out by injecting water and steam. That leaves around 50% to 65% of the oil trapped in the reservoir,

and if methods can be found to force that oil out, it could serve us well in helping to meet the growing energy demand. Kawale: "We have to extract crude oil more efficiently than we have done up to now. Injecting polymers into a reservoir has been shown to improve oil recovery." The flow of polymer solutions through the (porous) reservoir rock is related to the individual pore-scale flow phenomena. But what is the relationship between this pore-scale polymer rheology and the polymer rheology in a reservoir and, more specifically, how does it improve oil recovery? That is what Kawale's project is all about. Since the results of injecting the polymer solutions into the reservoir only materialise over a period of time, it is particularly important to make reliable predictions of the effect of the injection process at the start.

The central problem in his project is to discover the relationship between the 'apparent viscosity' of the polymer solution in a porous medium and the viscosity measured in simple flow geometries, such as in commercial rheometers. The term 'apparent viscosity' is used because the viscosity of a polymer solution in a porous medium, such as the sandstone of an oil reservoir, is a function of the permeability. With a series of hand gestures, Kawale tries to explain why the viscosity is such an important parameter. "This is my reservoir saturated with oil, and here is the oil layer. If we pump in water, channels will form in this direction, due to the large difference in viscosity. The water follows the path of least resistance. It will come out through these channels, and thus not mobilise the oil in the surrounding region. If we use a polymer solution, the difference between the viscosities of the solution and the oil is smaller and fewer, if any, channels will be formed. Consequently, more oil will be mobilised." To find this relationship, the polymer solutions will be studied in the laboratory in small microfluidic channels with well-defined flow geometries (sinusoidal tubes, for instance). From there, the behaviour will be related to that in typical porous media



like sandstone rock or packed beds. Apart from studying the existing literature to familiarise himself with the subject, Kawale is busy with the experimental set-up. Naturally, it is still too early for a resumé of the results of the project.

Six months after starting his project, Kawale is pleased with how things are organised in DPI. SNF, the French polymer producer, oil company Shell and the University of Groningen are also involved in his project. "There are now about 15 people working in this technology area. That makes it easy to maintain close contact with the other participants. I have already received some useful resources from one of them. When I applied for the job, I had to deal primarily with the university, so my impression of DPI dates from the cluster meetings."

### **Multiphase flows**

After his Bachelor's course in chemical engineering at the University of Mumbai, like so many of his compatriots, Kawale started his professional career at a Norwegian company with an office in India. The company performed dynamic process simulations of the upstream oil stabilisation/sweetening process, the first process that the crude oil is subjected to on board the oil rigs or the Floating Production Storage and Offloading units

(FPSOs). "I used commercially available simulation software and my task was to find out how the whole process was affected if, for example, different controller settings and different scenarios were employed," Kawale explains. "But after a while I wanted to learn more about the multiphase flows that occur. One of the people in the company advised me to consider going to Delft where, he said, 'they are at the forefront of research and there is a well-known research group in this field'. I looked up more information and was happy with what I found, and have not been disappointed since I arrived in Delft. I really like the university and the way problems are tackled. It is quite hands-on, the approach is pragmatic and the emphasis is on the application of the acquired knowledge. In India, I learned several technical theories, but the application side was not as strong. I like that part of it in Delft."

Kawale's Master's thesis dealt with preventing liquid loading of gas wells. During gas production, a certain amount of water also flows out together with the gas. Over time, as the pressure drop over the well declines, water accumulates in the well. The additional back pressure due to that is undesirable from the perspective of steady maximum production. To prevent this, soap is usually injected into the well

where it creates foam. Foam lowers the fluid density and therefore delays the onset of liquid accumulation. Summarising his Master's project, Kawale says "The key question was which physical-chemical property of a soap solution would serve as a handle to model such phenomena. Or, more precisely, how does the dynamic surface tension relate to foam mass density. It was found that dynamic surface tension has little or no effect on the mass density. We are now writing an article on this study."

Master's students normally spend their three-month internship at a company, but since he had already worked in a company, Kawale was allowed to go to the Norwegian University of Science and Technology in Trondheim (NTNU). NTNU has extensive laboratory facilities to study liquid-fluid interfaces and it gave him an opportunity to investigate interfacial rheology and build on the results of his work in Delft.

"When I was there I told one of my supervisors that I was looking for a PhD project, and he mentioned this project. I was interviewed via Skype one morning and at about half past eight that evening they called and offered me the position."

---

## OBJECTIVES

Although the underlying mechanisms may be similar for a range of applications of water-soluble polymers, this specific application warrants the establishment of a specific programme focusing on the structure-property relationships of polymers in solutions and their behaviour in the reservoir.

---

## FACTS AND FIGURES

### Partners from industry

- Shell
- SNF

### Partners from the research world

- Delft University of Technology
- University of Groningen

### Budget and organisation

Expenditure in 2012 totalled € 0.25 million (budget: € 0.31 million). A total of k€ 15 was spent on equipment. The total number of FTEs allocated at year-end 2012 was 3.5 (4 researchers). Prof.dr. Martien Cohen Stuart acted as Scientific Chairman and Dr. Jan Stamhuis as Programme Area Coordinator of the Enhanced Oil Recovery programme

### Publications and inventions

One reviewed paper was published and one invention was reported.

For details, see page 86.

---

## SUB-PROGRAMMES

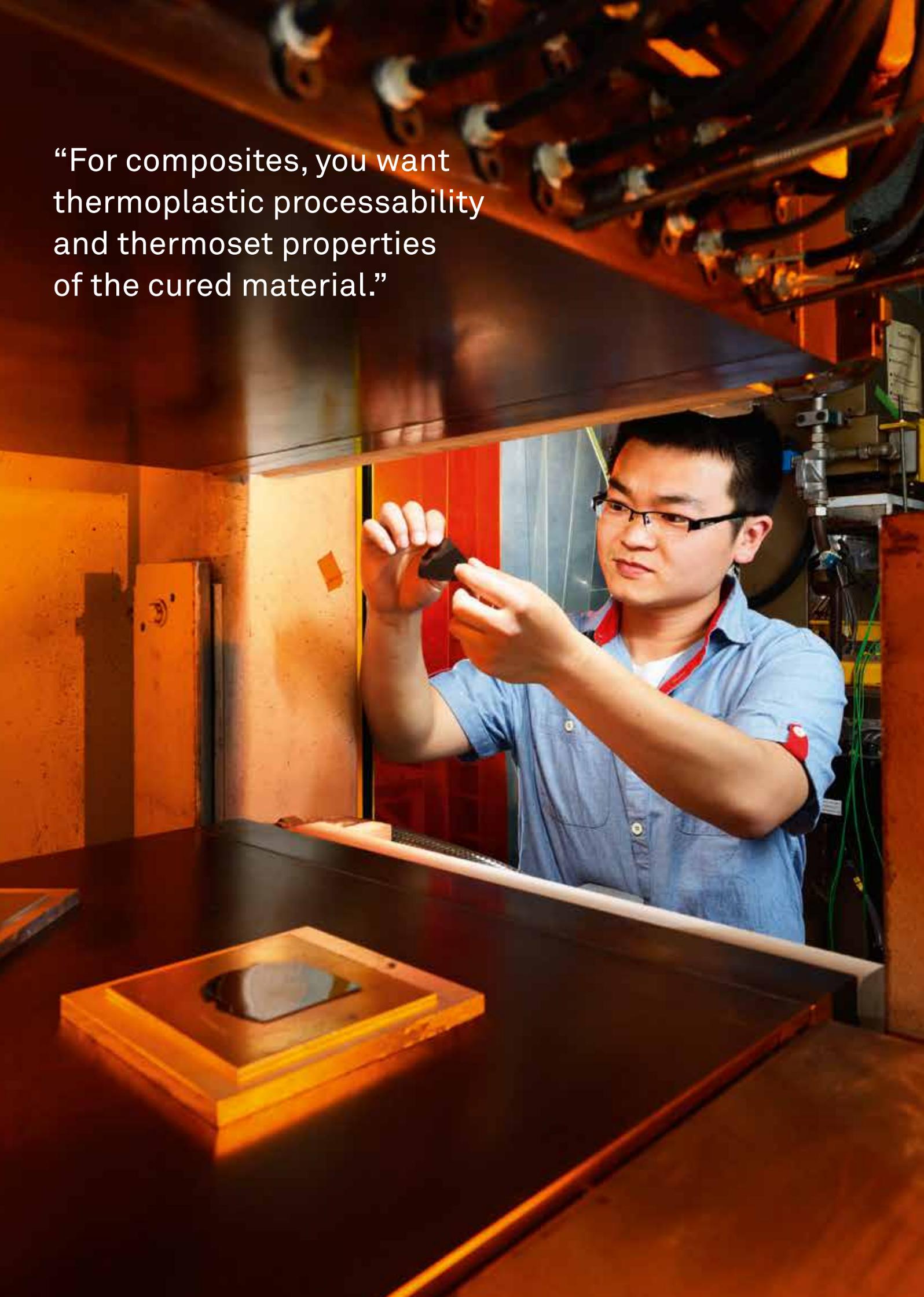
### Structure–property relationships and the design of new model macromolecules

Controlled radical polymerisation techniques will be employed to investigate the effects of macromolecular topology, for example branching, on polymer solution properties and on viscosity and/or visco-elasticity. These novel structures are evaluated in core flow experiments to determine their injectivity and impact on the recovery of oil in porous media. The effects of polymeric surfactants, i.e. high molecular weight amphiphilic structures that have the potential to decrease the interfacial tension and enhance oil recovery compared with that obtained with the current polymer flooding applications, are also being investigated.

### Relating polymer rheology to apparent viscosity in porous media

The objective of this sub-programme is to develop reliable models to predict the relationship of polymer-apparent viscosity in porous media to porous-medium properties, bulk rheological parameters and superficial velocity in the medium and establish the relationship with enhanced oil recovery.

“For composites, you want thermoplastic processability and thermoset properties of the cured material.”



---

# Qingbao Guan

## A balancing act

---

---

### EMERGING TECHNOLOGIES: ADVANCED COMPOSITES

---

The aim of the Emerging Technologies (EMT) technology area is to promote the exploration investigation of new ideas from industry concerning new technologies that do not fit into any of the existing technology areas. When a company approaches DPI with a proposal for a project on a new topic, DPI will find an academic partner to carry out the research.

---

**Although they consist to a substantial extent of polymers, composites are a relatively new field of research for DPI. Qingbao Guan has taken up the challenge of producing the required properties in a workable process.**

Eighteen months ago, Qingbao Guan started his PhD project in the polymer group of Professor Theo Dingemans at Delft University of Technology. “During my Master’s, I did a project on the use of high-performance polymers in composites. The subject interested me enormously and I was looking for a university that was conducting cutting-edge research in this field, and, naturally, a ‘big name’ institution”, says Guan, to explain why he chose Delft. He received a scholarship from the Chinese Scholarship Council, a non-profit organisation that provides financial assistance to Chinese citizens wishing to study abroad and to foreign nationals wishing to study in China, in order to strengthen the educational, scientific, technological and cultural ties between China and other countries. DPI became involved in the project when it had been underway for eight months.

#### **Viscosity**

After earning his Bachelor’s degree in polymer engineering in Suzhou, a city close to

Shanghai, Guan did his Master’s project on the use of composite materials in various kinds of electronic devices. The problem is always that the viscosity of the polymer to be combined with carbon or other fibres is too high for melt processing. In a composite, you want the polymer to really penetrate the fabric structure before it cures. Guan’s task was to reduce the viscosity, and he did so by incorporating hyper-branched structures in bismaleimides. In composite materials for all kinds of applications, what you are always looking for is outstanding thermal stability, which means that they can be used at high temperatures and maintain their strength. In addition, they should be stable in the presence of all kinds of fluids and should adhere well to the fibres.

Viscosity is again the pivotal aspect of his current PhD project. “In aerospace engineering, the issue is always to reduce the weight of the material,” says Guan. “You would like to replace metal structures with the lightest possible materials, but the performance of such materials should be of a similar quality to that of metals. That is why we want to produce composites with high-quality mechanical properties, chemical resistance against all kinds of fluids and good temperature stability. But they also need to be processable; you want thermoplastic processability and, ultimately, thermoset properties. I am now investigating polyesteramides and polyesterimides, high-performance polymers with specific end groups that give them all these qualities but which, unfortunately, also have a really high melting point. To process them into useful structures or parts, you will have to lower this melting point, which means that you have to reduce its molecular weight by modifying the chemical structure, without affecting the other properties. That boils down to ‘cutting’ the backbone of the molecule into smaller pieces, in other words, preparing oligomers, without affecting the after-cure performance, and introducing reactive end-groups that can polymerise these oligomers in a second consecutive



heat treatment step.” It is obviously a balancing act.

For the polyesteramides, Guan has found an acceptable solution. He has characterised the material and tested its mechanical and thermal properties, and is satisfied with the end product. He is now trying to surpass that with the polyesterimides and has already found some interesting phenomena. The molecule can be stretched many times after cure, which raises the glass temperature. This means that the same material, with different pre-stretched molecules, can be used for different applications that require different properties in relation to the glass temperature. When it comes to a commercial product, the material can be produced in large quantities and thus at lower cost. The process he has developed has the additional advantage that it runs in a closed system. It is an environmentally benign polymerisation method with no waste products and can easily be scaled up to commercially viable quantities in the future.

#### **Instrumental**

Composites are versatile materials that combine the best of two worlds. Unfortunately, there was no clear home base for research into these materials in the Netherlands in either of these worlds. DPI recognised the seriousness of that

situation and was looking for ways of playing a relevant role in composites research. Accordingly, it became involved in Guan’s project in June 2012. DPI is now covering some of the additional costs of the project, but that is not the only benefit of DPI’s involvement in the project. “I was looking for a community where I could discuss my project and DPI has given me the opportunity to meet other researchers in the polymer world, people outside my direct sphere of interest, and they have been able to make some useful suggestions,” says Guan, who is also very positive about the meetings organised by DPI. “You learn about the properties, physics, chemistry and processing of polymers. Professors and lecturers from all the universities in the Netherlands inform us about what they are doing in these fields and that is very useful. The contacts with other PhD students who are in the same situation are also useful. This network could maybe help me later on in my career.”

“When I return to China after my PhD project, I could perhaps be instrumental for the country’s growing aircraft industry.” China’s aircraft industry needs new composite chemistry, new fibres and more knowledge about what happens at the polymer-fibre interface. Naturally, they will want to learn from mistakes that have been made elsewhere.

The grant from the Chinese Scholarship Council requires Guan to return to China to work when he completes his PhD project. So in addition to helping China’s economy, Guan could also be instrumental in promoting DPI, which is building a strong presence in the country. But that time is still two-and-a-half years away. Guan already has one suggestion for DPI: “I believe DPI could play an even greater role in facilitating research than it already does by making equipment it has paid for available to more researchers than just the person it was bought for. A database with details of all the equipment that is available and where it can be found would help in that respect.”

Coming from China to the Netherlands was, of course, a huge culture shock for Guan. It took him some time to get used to the different hierarchical structure. “It is unimaginable that you would address your professor by his first name in China. Here, I just knock on his door and say, ‘Theo, could I have a word with you?’ And I still am surprised when motorists wave me on to proceed when I am waiting to cross the street.” Other striking differences between living in China and in the Netherlands that Guan mentions are the clean air – he studied in a city close to Shanghai where pollution rules due to the heavy traffic – and the fact that you do not have to worry about the quality of the food here.

---

## OBJECTIVES

Projects in the Emerging Technologies technology area are handled like any other DPI projects. However, after two years a decision is made on whether the project will be extended for another two years, by which time at least one other industrial party, in addition to the industrial party that initiated the project, must be willing to participate. The project can then be absorbed into another technology area. As in the case of projects in the Corporate Research technology area, the intellectual property (IP) generated in the first two years is owned by all of DPI's partners. If a project is continued after two years, the IP is treated in the same way as in other technology areas. In 2012, Water-Soluble Polymers, Smart Packaging and Advanced Composites were selected as the focus areas for Emerging Technologies. Potential projects in these areas are currently being discussed with industry. However, other opportunities are emerging that would promote DPI's mission of studying and developing new sustainable polymer technologies in cooperation with industry and academia.

---

## FACTS AND FIGURES

### Partners from industry

- DPI partners
- M2i partners

### Partners from the research world

- Delft University of Technology

### Budget and organisation

Expenditure in 2012 totalled € 0.01 million (budget: € 0.07 million). The total number of FTEs allocated at year-end 2012 was 0.3 (one researcher). Prof.dr. Martien Cohen Stuart acted as Scientific Chairman and Dr. Jan Stamhuis as Programme Area Coordinator of the Emerging Technologies programme.

### Publications and inventions

This technology area has generated no output in 2012.

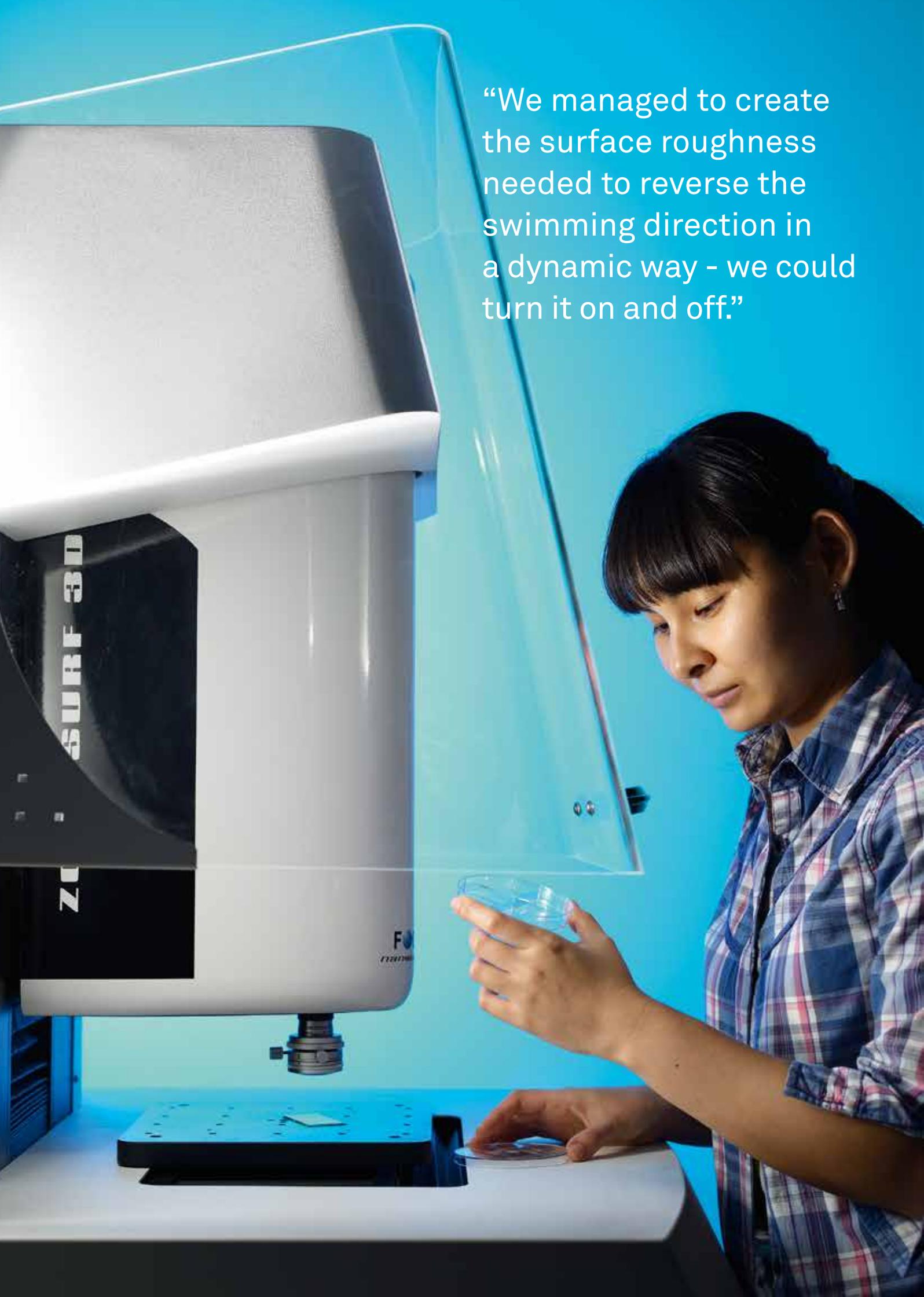
For details, see page 86.

---

## SUB-PROGRAMMES

In 2012, on-going projects involving water-soluble polymers to be used for enhanced oil recovery (EOR) were transferred to a new technology area, Polymers for EOR (page 65). A new project to investigate High Performance Matrices for Advanced Composites was launched in 2012. This project, which is being carried out in association with Delft University of Technology, is part of a new collaboration with the Dutch materials programme, M2i. In this joint programme, DPI is studying base materials, for example matrix and fibres, whilst M2i is investigating the design and properties of composites. Interface studies and processing/composite manufacturing are a joint focus area.

“We managed to create the surface roughness needed to reverse the swimming direction in a dynamic way - we could turn it on and off.”



# Sandeep Namdeo and Danqing Liu

## Micro-bots 'swim' upstream

### CORPORATE RESEARCH

The role of the Corporate Research programme is to initiate and support enabling science and conceptual new science that is of interest to all of the partners in DPI because of its long-term potential impact.

**By actuating modified polymers with external stimuli, such as magnetic fields and light, micro-robots can move with and against the stream. Simulations are used to optimise the polymers' properties for this effect.**

In no time, Sandeep Namdeo has covered the sheet of paper on the table in front of him with small sketches of bacteria and other micro-organisms with one or more tails, and with graphs showing parameters such as their speed. Terms like 'bio-inspired', 'nano-' and 'micro-scale' and 'multi-physics' whizz past. His enthusiasm about his project is evident. "If you cannot use inertial forces for propulsion, as is the case with bacteria, you have to rely on viscous forces. In my project, I am trying to find conditions and parameters similar to the properties of micro-organisms that allow active transport of micro-bots, small robots that can be used to deliver drugs in the human body or to transport something from one location to another in a lab-on-a-chip device, for example," he says. Namdeo is a mechanical engineer who specialised in structural design at IIT-Bombay, a prestigious university in India. After a few years in industry, he came to the University of Groningen for his present PhD project.

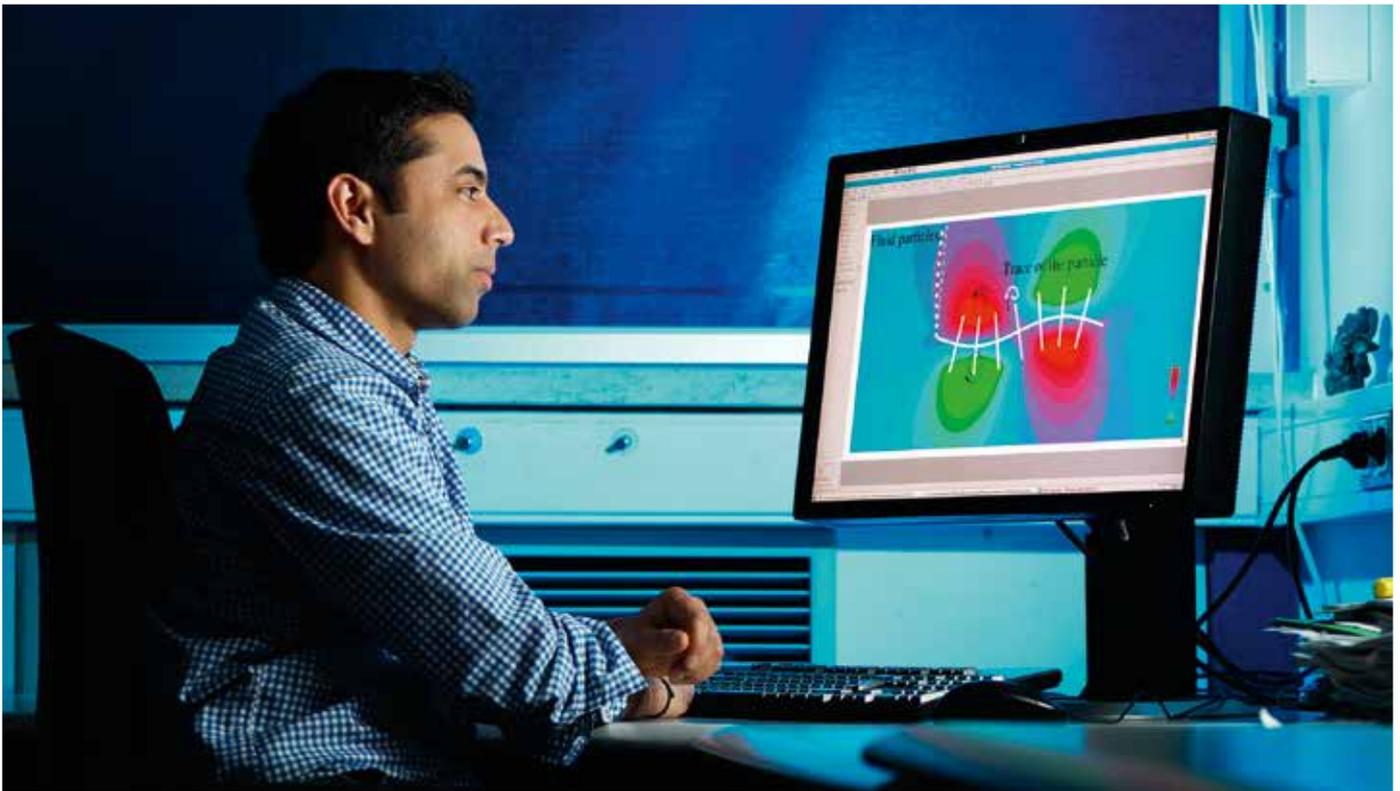
#### Tail

One of the ways in which micro-organisms move in a fluid is by generating a wave in a long tail. If this tail has a certain

roughness, the micro-organism can move in a direction opposite to the stream. The idea is to mimic this with polymers, and Namdeo is exploring the parameters of such polymers by performing simulations. The energy that is needed to generate the wave in the tail is applied externally, by a magnetic field, for example, and light can be used to induce the surface roughness. "From my simulations, it appears that two parameters are particularly important: the wavelength of the wave generated in the tail and the height of the bumps on it - the surface roughness," says Namdeo. "These are determined by a combination of the properties of the material, the fluid dynamics and the influence of the external stimuli (the magnetic field and the light)."

That is all very well, but can it work in practice? That is, of course, the main question. In a related DPI PhD project, Danqing Liu, an electrical engineer who did her Master's at Delft University of Technology, has investigated whether there are polymers that exhibit this behaviour. She actually started before Namdeo did, and it took her a year to modify a specific type of polymer so that it could be used as a long tail in which a wave can be induced by a magnetic field. "But once I had shown that it was, in principle, possible (and for some configurations varied the parameters in the way Sandeep calculated), I wanted to focus on the second part of our project. So in the remaining time, we managed to create the surface roughness needed to reverse the swimming direction in a dynamic way - we could turn it on and off - and that appealed to me much more," says Liu, who in the meantime has defended her thesis and is now involved in a post-doc DPI project to exploit this dynamic control of the polymer's roughness.

When light falls on a specific type of polymer with side chains, these side chains protrude from the surface and thus produce the desired surface roughness. When the light is switched off, the side chains lie parallel to the surface, making it flat.



“Two parameters are important: the wavelength of the wave generated in the tail and the height of the bumps on it.”

“There are more applications for this effect than changing the direction of the ‘swimmers’, as the polymer micro-bots are called,” says Liu. “You can, for instance, think of self-cleaning properties, the lotus effect: if the roughness is turned on, the surface is very hydrophobic and water flowing on the surface will be pushed away, accompanied by any dirt that has accumulated on that surface. If you do not need this effect, to prevent damage to these bumps, you turn the effect off by switching the light off. The polymers showing this effect can be made in a coating a few microns thick that can be applied to window panes or any other surface that needs to be self-cleaning.”

#### Dynamic

Neither Liu nor Namdeo are chemists with a polymer background. For Namdeo, it does not matter much what chemical structure the polymers have, as long as the relevant material parameters are available. It took him some time to get used to the formulas of chemical structures that filled the presentations at DPI meetings, and he took care not to use too

many mathematical equations in his own presentations. For Liu, the chemistry of polymers was a new subject that she had to immerse herself in deeply for her project. “For my Master’s project in Delft, I worked in lithography and, since these micro-bots will eventually have to be made with lithographic methods, Dick Broer, my supervisor in the chemical department here, thought it would be useful to hire me. Little did he know that for electrical engineers lithography is nothing more than opening the machine, putting in the wafer and taking it out again when it is ready,” she laughs. “But I learned a lot of chemistry from him. He taught me from scratch how to make the swimmers and the roughness.”

Coming to the Netherlands from countries like China and India must have been quite a change for them. But both say they have enjoyed the move very much. “The atmosphere is relaxed, and people are nice in the Netherlands, not only at the university. They greet or smile at you in the street, which would be very strange in China,” says Liu. Namdeo agrees and

mentions that “most people speak English here; however, once you have acquired some vocabulary, Dutch is easy to understand. Additionally, what I appreciate in DPI is that they are interested in you as a person; they invest in you. I was allowed to follow an international management programme at Nyenrode Business University, which helped me to adjust to the international and multicultural environment.” When his project ends, later this year, he will look for a job in an innovation-driven company, not necessarily related to polymers, and it could be anywhere in the world. After his education in India, he worked for some years in industry in India, but there he found that the atmosphere lacked encouragement for new innovations. Liu also wants to work in industry after completing her post-doc. She hasn’t done so before and intends to get an idea of what it is like by speaking to the industrial partners in her DPI project.

---

## OBJECTIVES

This programme is primarily science-driven, based on a vision of future industrial needs and opportunities. It operates at the forefront of scientific knowledge and capabilities in the field of polymer science. The programme activities are arranged in several sub-clusters.

---

## FACTS AND FIGURES

### Partners from industry

- All DPI partners take part in Corporate Research

### Partners from the research world

- Delft University of Technology
- Fraunhofer Institute for Structural Durability and System Reliability LBF
- Eindhoven University of Technology
- ESRF, Grenoble
- Foundation for fundamental research on matter (FOM)
- Radboud University
- TI Food and Nutrition (TIFN)
- University of Groningen
- University of Twente
- Wageningen University

### Budget and organisation

Expenditure in 2012 totalled € 1.86 million (budget: € 1.55 million). A total of € 9k was spent on equipment. The total number of FTEs allocated at year-end 2012 was 15.9 (21 researchers). Prof.dr. Martien Cohen Stuart is the Scientific Chairman and Dr. Monique Bruining is the Programme Area Coordinator of the Corporate Research programme.

### Publications and inventions

This research programme generated a total of 23 reviewed papers and two theses. Four inventions were reported and one patent application was filed.

For details, see page 86.

---

## SUB-PROGRAMMES

### Enabling science

- Polymer characterisation (surfaces and interfaces (applying mainly microscopic techniques), molecular characterisation (SEC techniques on cross-linked architectures and networks, for example, and analysis of molar mass distribution)).
- Structure vs. performance: multiscale modelling, fluid dynamics (rheology) and solid-state properties (bulk materials and surface properties).

### New science

Development of new concepts in polymer chemistry and polymer physics with a view to meeting long-term requirements in terms of sustainability, durability and bio-related polymer systems.

### Infrastructure

Corporate Research also strengthens the research infrastructure by investing in equipment for the benefit of the entire DPI community.

### DPI fellowship programme

Under this programme, talented young researchers with a tenured or tenure-track position at a Dutch university can be appointed as a 'DPI fellow'. The aim of the programme is to secure their commitment to the Dutch polymer science community and give them the opportunity to attain scientific leadership qualities in an area matching DPI's current or future strategy.

### Bio-Related Materials (BRM) programme

In association with FOM and TIFN, DPI has established an Industrial Partnership Programme on biomaterials and bio-related materials. The aim of the programme is to understand how to move from the scale of complexes and aggregates to the mesoscopic scale, taking account of both the time dependent interactions and structures in their chemical detail and the resulting dynamic and spatially varying mesoscale physical properties.

### Understanding the visco-elasticity of elastomer-based nanocomposites (VEC) programme

Filled rubbers are widely used in industry. Adding silica particles to a polymer matrix increases the mechanical properties of the material but causes various non-linear effects, notably a dramatic decline in elasticity under high strain (the Payne effect). This effect is still not understood very well. During this project systematic experiments will be conducted with rubbers of varying compositions. On the macroscopic scale, we are performing rheological measurements and combining them with microscopic characterisations in order to link behaviour on a macroscopic scale with the micro-structure of the sample.

# Output



## POLYOLEFINS

### Projects

**#632:** Experimental and computational study of dense gas-fluidised beds with liquid injection

**#633:** Understanding structure/performance relationships for non-metallocene olefin polymerization catalysts

**#635:** Measuring active site concentration of olefin polymerization catalysts

**#638:** Thermally stable olefin polymerization catalysts by reversible intramolecular alkyl shuttling

**#641:** High-Throughput Computational Pre-Screening of Catalysts

**#642:** Development of High-Temperature 2-Dimensional Liquid Chromatography for the Characterization of Polyolefins

**#646:** New Functionalized Materials by Rh and Pd Mediated Carbene Homo-Polymerization and Olefin/Carbene Co-Polymerization

**#674:** Rheology Control by Branching Modeling

**#706:** Intrinsic effect of catalyst immobilization techniques on catalyst activity and selectivity

**#707:** Advanced Static and Dynamics Modeling of Heterogeneous Ziegler-Natta Catalytic Systems

**#708:** Structure-property relations of olefinic block copolymers

**#709:** Integrated Models for PolyOlefin Reactors

**#710:** Linking chemically specific structure information to physical properties of polyolefins

**#711:** Mass transfer & kinetics in heterophasic copolymerization of propylene

**#712:** Elucidation and control of the active surface structure and chemistry in MgCl<sub>2</sub>-supported Ziegler-Natta catalysis: an integrated experimental and computational approach

**#714:** Putting values to a model for Flow Induced Crystallization

**#728:** Structural investigations on MAO and design of alternative well-defined cocatalysts and single-component catalysts

**#731:** Main group metal-alkyl cocatalysts and scavengers in molecular olefin polymerization catalysis: a mechanistic investigation

**#732:** Strategies for stabilizing trivalent vanadium and chromium propylene polymerization catalysts

**#750:** Optimisation and Calibration of High-Temperature Liquid Chromatographic Separation of Polypropylene and Propylene based Copolymers

**#751:** Predictive Modelling of Polyolefin Reactors

**#753:** Impact of the geometric parameters of catalyst supports on the kinetics and morphology of polyolefins

**#754:** Direct insight into elusive active Ti species of high-yield Ziegler-Natta Catalysts

**#757:** Influence of entanglement on rheological response of Ultra High Molecular Weight Polyethylene from linear to nonlinear viscoelastic behaviour

### Theses

Maria Ranieri  
Measuring of main kinetic parameters of molecular catalyst for olefin polymerization using high-pressure-type quenched flow technique

Shaneeh Vadake Kulangara  
Novel catalysts for ethylene polymerisation and oligomerisation

Anton Ginzburg  
Development of High Temperature Two Dimensional Liquid Chromatography of Polyolefins

Nicole Franssen  
Functional (co) Polymers From Carbenes

### Scientific publications

A. J. C. Walters, E. Jellema, M. Finger, P. Aarnoutse, J. M. M. Smits, J. N. H. Reek and B. de Bruin  
*Rh-mediated carbene polymerization: From multistep catalyst activation to alcohol-mediated chain-transfer*  
Acs Catalysis 2(2) 246-260

E. Tioni, R. Spitz, J. P. Broyer, V. Monteil and T. McKenna

*Packed-bed reactor for short time gas phase olefin polymerization: Heat transfer study and reactor optimization*  
Aiche Journal 58(1) 256-267

Y. Shaikh, K. Albahily, M. Sutcliffe, V. Fomitcheva, S. Gambarotta, I. Korobkov and R. Duchateau  
*A highly selective ethylene tetramerization catalyst*  
Angewandte Chemie-International Edition 51(6) 1366-1369

M. Finger, M. Lutz, J. N. H. Reek and B. de Bruin  
*Synthesis and reactivity of ester-functionalized 5-membered rhi-kappa 2-c,o-chelates and their relevance in rh(cod)-mediated carbene polymerization*  
European Journal of Inorganic Chemistry 9) 1437-1444

W. Godlieb, S. Gorter, N. G. Deen and J. A. M. Kuipers  
*Experimental study of large scale fluidized beds at elevated pressure*  
Industrial & Engineering Chemistry Research 51(4) 1962-1969

E. Tioni, J. P. Broyer, V. Monteil and T. McKenna  
*Influence of reaction conditions on catalyst behavior during the early stages of gas phase ethylene homo- and copolymerization*  
Industrial & Engineering Chemistry Research 51(45) 14673-14684

Z. Bartczak, P. F. M. Beris, K. Wasilewski, A. Galeski and P. J. Lemstra  
*Deformation of the ultra-high molecular weight polyethylene melt in the plane-strain compression*  
Journal of Applied Polymer Science 125(6) 4155-4168

R. Barenwald, Y. Champouret, K. Saalwachter and K. Schaler  
*Determination of chain flip rates in poly(ethylene) crystallites by solid-state low-field h-1 nmr for two different sample morphologies*  
Journal of Physical Chemistry B 116(43) 13089-13097

T. B. van Erp, D. Cavallo, G. W. M. Peters and L. E. Govaert  
*Rate-, temperature-, and structure-dependent yield kinetics of isotactic polypropylene*  
Journal of Polymer Science Part B-Polymer Physics 50(20) 1438-1451

A. V. Cheruvathur, E. H. G. Langner, J. W. Niemantsverdriet and P. C. Thune  
*In situ atr-ftir studies on mgcl2-diisobutyl ziegler-natta catalysts*  
Langmuir 28(5) 2643-2651

G. Ciancaleoni, N. Fraldi, R. Cipullo, V. Busico, A. Macchioni and P. H. M. Budzelaar  
*Structure/properties relationship for bis(phenoxyamine)zr(IV)-based olefin polymerization catalysts: A simple dft model to predict catalytic activity*  
Macromolecules 45(10) 4046-4053

Z. Ma, L. Balzano and G. W. M. Peters  
*Pressure quench of flow-induced crystallization precursors*  
Macromolecules 45(10) 4216-4224

A. Correa, R. Credendino, J. T. M. Pater, G. Morini and L. Cavallo  
*Theoretical investigation of active sites at the corners of mgcl2 crystallites in supported ziegler-natta catalysts*  
Macromolecules 45(9) 3695-3701

N. M. G. Franssen, K. Rernerie, T. Macko, J. N. H. Reek and B. de Bruin  
*Controlled synthesis of functional copolymers with blocky architectures via carbene polymerization*  
Macromolecules 45(9) 3711-3721

S. V. Kulangara, A. Jabri, Y. Yang, I. Korobkov, S. Gambarotta and R. Duchateau  
*Synthesis, x-ray structural analysis, and ethylene polymerization studies of group IV metal heterobimetallic aluminum-pyrrolyl complexes*  
Organometallics 31(17) 6085-6094

S. V. Kulangara, C. Mason, M. Juba, Y. Yang, I. Thapa, S. Gambarotta, I. Korobkov and R. Duchateau  
*Synthesis and catalytic oligomerization activity of chromium catalysts of ligand systems with switchable connectivity*  
Organometallics 31(17) 6438-6449

Y. Shaikh, J. Gurnham, K. Albahily, S. Gambarotta and I. Korobkov  
*Aminophosphine-based chromium catalysts for selective ethylene tetramerization*  
Organometallics 31(21) 7427-7433

C. Descour, T. Meijer-Vissers, T. Macko, M. Parkinson, D. Cavallo, M. van Drongelen, G. Hubner, H. Goossens and R. Duchateau  
*Random and block copolymers based on 4-methyl-1-pentene and 1-pentene*  
Polymer 53(15) 3096-3106

C. Descour, T. Meijer-Vissers, T. Macko, M. Parkinson, D. Cavallo, M. van Drongelen, G. Hubner, H. Goossens and R. Duchateau  
*Random and block copolymers based on 4-methyl-1-pentene and 1-pentene (vol 53, pg 3096, 2012)*  
Polymer 53(18) 4018-4018

J. Mazzolini, O. Boyron, V. Monteil, F. D'Agosto, C. Boisson, G. C. Sanders, J. P. A. Heuts, R. Duchateau, D. Gigmes and D. Bertin

*Polyethylene end functionalization using thia-michael addition chemistry*  
Polymer Chemistry 3(9) 2383-2392

J. A. Laverman, X. Fan, A. Ingram, M. V. Annaland, D. J. Parker, J. P. K. Seville and J. A. M. Kuipers  
*Experimental study on the influence of bed material on the scaling of solids circulation patterns in 3d bubbling gas-solid fluidized beds of glass and polyethylene using positron emission particle tracking*  
Powder Technology 224(297-305)

### Filed patent applications

**#638:** S. Kulangara, Y. Yang, R. Duchateau and S. Gambarotta  
Process for producing an oligo(alpha-olefin) and the use of a particular form of methylaluminoxane in such process

**#732:** S. Licciulli, S. Gambarotta, R. Duchateau  
Process for producing an oligo(alpha-olefin) and the use of a particular form of methylaluminoxane in such process

### Reported inventions

**#646/647:** N.M.G. Franssen and B. de Bruin  
Carpool II

**#638:** S. Kulangara, Y. Yang, R. Duchateau and S. Gambarotta  
I-hexene Philips+

**#732:** S. Licciulli, S. Gambarotta and R. Duchateau  
Pure 1-Hexene

### PERFORMANCE POLYMERS

### Projects

**#623:** Fundamental aspects of Nanocomposites

**#647:** New Functionalized Materials by Rh and Pd Mediated Carbene Homo-Polymerization and Olefin/Carbene Co-Polymerization

**#648:** Graphene-based nanocomposites- A study on the potential of graphene nano-sheets as an alternative low-cost filler for multi-functional polymeric materials

**#649:** Thermoplastic elastomers via living radical graft polymerization from functional elastomers

**#650:** Molecular Modelling of Cavitation in Polymer Melts and Rubbers

**#651:** Smart Surface Modifiers for Engineering Plastics

**#652:** Rubber/silica nano-composites via reactive extrusion

**#653:** Biodegradable Thermoplastic Polyurethanes from Renewable Resources

**#654:** Effects of the nano-scale structure of polymer surfaces on their adhesion and friction

**#656:** Green Rigid blocks for Engineering plastics with ENhanced pERformance

**#664:** Sustainable elastomers and Thermoplastics by short fibre reinforcement

**#671:** Optimized plastication in extruders for better economy and product properties

**#697:** Creating multiple distributed healing in fibre composites using compartmented fibres liquid filled fibres

**#742:** Membranes with Adjustable Interior in their Nanopores

**#743:** Curable Semi-aromatic or aliphatic Semicrystalline Thermoplastics

**#744:** Molecular Simulations of Polymer Networks: Stress-Strain Relations, Cavitation, and Dynamics in Confinement

**#745:** Microstructure-based Modeling of the Intrinsic Kinetics of Aging and Deformation of Polymer Glasses

**#746:** Particles at Fluid-Fluid Interfaces

**#747:** Polyamide/silica nanocomposites: a systematic investigation

**#749:** The chemistry of rubber modification and crosslinking: New approaches towards an old problem

**#755:** MONodisperse OLIGOamide building blocks for thermoplastic elastomers (TPEs) revisited

**#756:** Do contacts in electrically conductive particulate composites really exist?

### Theses

Nicole Franssen  
Functional (co) Polymers From Carbenes

Dmytro Hudzinsky  
Atomistic Modeling of Structure and Dynamics of Sheared Atactic Polystyrene Films

- Jing Wu  
Carbohydrate-based Building Blocks and Step-growth Polymers
- Morteza Shirazi  
Aromatic polyamide short fibres-reinforced elastomers: Adhesion mechanisms and the composites performance properties
- Natlia Rodriguez Pareja  
Contact and Friction in Systems with Fibre reinforced Elastomers
- Gözde Tuzcu  
Thermoplastic Elastomers via Controlled Radical Polymerization
- Evgeniy Tkalya  
Graphene based Polymer Nanocomposites
- Marcos Gomes Ghislandi  
Nano-Scaled Carbon Fillers and their Functional Polymer Nanocomposites
- Christian Hinze  
Influence of processing induced morphology on mechanical properties short aramid fibre filled elastomer composites.
- Gemma Sanders  
Exploring the Frontiers of Macromonomer Chemistry
- Scientific publications**
- A. J. C. Walters, E. Jellema, M. Finger, P. Aarnoutse, J. M. M. Smits, J. N. H. Reek and B. de Bruin  
*Rh-mediated carbene polymerization: From multistep catalyst activation to alcohol-mediated chain-transfer*  
Acs Catalysis 2(2) 246-260
- A. Alekseev, D. L. Chen, E. E. Tkalya, M. G. Ghislandi, Y. Syurik, O. Ageev, J. Loos and G. de With  
*Local organization of graphene network inside graphene/polymer composites*  
Advanced Functional Materials 22(6) 1311-1318
- M. Ghislandi, G. G. Hoffmann, E. Tkalya, L. J. Xue and G. De With  
*Tip-enhanced raman spectroscopy and mapping of graphene sheets*  
Applied Spectroscopy Reviews 47(5) 371-381
- S. D. Mookhoek, H. R. Fischer and S. van der Zwaag  
*Alginate fibres containing discrete liquid filled vacuoles for controlled delivery of healing agents in fibre reinforced composites*  
Composites Part A-Applied Science and Manufacturing 43(12) 2176-2182
- Y. J. Choi, M. A. Hulsen and H. E. H. Meijer  
*Simulation of the flow of a viscoelastic fluid around a stationary cylinder using an extended finite element method*  
Computers & Fluids 57(183-194)
- E. E. Tkalya, M. Ghislandi, G. de With and C. E. Koning  
*The use of surfactants for dispersing carbon nanotubes and graphene to make conductive nanocomposites*  
Current Opinion in Colloid & Interface Science 17(4) 225-231
- M. Finger, M. Lutz, J. N. H. Reek and B. de Bruin  
*Synthesis and reactivity of ester-functionalized 5-membered rhi-kappa 2-c,o-chelates and their relevance in rh(cod)-mediated carbene polymerization*  
European Journal of Inorganic Chemistry 9) 1437-1444
- G. J. E. Biemond, K. Brasspenning and R. J. Gaymans  
*Synthesis and selected properties of polyurethanes with monodisperse hard segments based on hexane diisocyanate and three types of chain extenders*  
Journal of Applied Polymer Science 124(2) 1302-1315
- D. Hudzinsky, M. A. J. Michels and A. V. Lyulin  
*Mechanical properties and local mobility of atactic-polystyrene films under constant-shear deformation*  
Journal of Chemical Physics 137(12)
- R. H. J. Otten and P. van der Schoot  
*Deformable homeotropic nematic droplets in a magnetic field*  
Journal of Chemical Physics 137(15)
- D. J. A. Senden, T. A. P. Engels, S. H. M. Sontjens and L. E. Govaert  
*The effect of physical aging on the embrittlement of steam-sterilized polycarbonate*  
Journal of Materials Science 47(16) 6043-6046
- Y. J. Choi and M. A. Hulsen  
*Alignment of particles in a confined shear flow of a viscoelastic fluid*  
Journal of Non-Newtonian Fluid Mechanics 175(89-103)
- S. H. Chikkali, R. Bellini, B. de Bruin, J. I. van der Vlugt and J. N. H. Reek  
*Highly selective asymmetric rh-catalyzed hydroformylation of heterocyclic olefins*  
Journal of the American Chemical Society 134(15) 6607-6616
- D. L. Tang, B. A. J. Noordover, R. J. Sablong and C. E. Koning  
*Thermoplastic poly(urethane urea)s from novel, bio-based amorphous polyester diols*  
Macromolecular Chemistry and Physics 213(23) 2541-2549
- J. Wu, P. Eduard, S. Thiyagarajan, L. Jasinska-Walc, A. Rozanski, C. F. Guerra, B. A. J. Noordover, J. van Haveren, D. S. van Es and C. E. Koning  
*Semicrystalline polyesters based on a novel renewable building block*  
Macromolecules 45(12) 5069-5080
- L. Jasinska-Walc, D. Dudenko, A. Rozanski, S. Thiyagarajan, P. Sowinski, D. van Es, J. Shu, M. R. Hansen and C. E. Koning  
*Structure and molecular dynamics in renewable polyamides from dideoxy-diamino isohexide*  
Macromolecules 45(14) 5653-5666
- G. C. Sanders, R. Duchateau, C. Y. Lin, M. L. Coote and J. P. A. Heuts  
*End-functional styrene-maleic anhydride copolymers via catalytic chain transfer polymerization*  
Macromolecules 45(15) 5923-5933
- J. Wu, L. Jasinska-Walc, D. Dudenko, A. Rozanski, M. R. Hansen, D. van Es and C. E. Koning  
*An investigation of polyamides based on isoidide-2,5-dimethylethylamine as a green rigid building block with enhanced reactivity*  
Macromolecules 45(23) 9333-9346
- L. Jasinska-Walc, M. Villani, D. Dudenko, O. van Asselen, E. Klop, S. Rastogi, M. R. Hansen and C. E. Koning  
*Local conformation and cocrystallization phenomena in renewable diaminoisoidide-based polyamides studied by ft-ir, solid state nmr, and waxd*  
Macromolecules 45(6) 2796-2808
- N. M. G. Franssen, K. Rernerie, T. Macko, J. N. H. Reek and B. de Bruin  
*Controlled synthesis of functional copolymers with blocky architectures via carbene polymerization*  
Macromolecules 45(9) 3711-3721
- R. M. W. van Bijnen, R. H. J. Otten and P. van der Schoot  
*Texture and shape of two-dimensional domains of nematic liquid crystals*  
Physical Review E 86(5)
- R. H. J. Otten and P. van der Schoot  
*Connectedness percolation of elongated hard particles in an external field*  
Physical Review Letters 108(8)
- K. B. Lu, M. van Duin, J. Loos and G. de With  
*On the volume organisation of thermoplastic vulcanisates (tpvs) as revealed by scanning transmission electron microscopy (stem) tomography*  
Polymer 53(19) 4171-4177

G. C. Sanders, B. G. P. van Ravensteijn, R. Duchateau and J. P. A. Heuts  
*The unexpected behaviour of epoxidised macromonomers derived from catalytic chain transfer during ring opening copolymerisation*  
Polymer Chemistry 3(8) 2200-2208

B. Marinho, M. Ghislandi, E. Tkalya, C. E. Koning and G. de With  
*Electrical conductivity of compacts of graphene, multi-wall carbon nanotubes, carbon black, and graphite powder*  
Powder Technology 221(351-358)

L. C. A. van Breemen, L. E. Govaert and H. E. H. Meijer  
*Scratching polycarbonate: A quantitative model*  
Wear 274(238-247)

### Filed patent applications

**#656:** J. Wu, P. Eduard and D.S. van Es  
Polymer, process for producing such polymer and composition comprising such polymer

**#651:** R. Duchateau, J.P.A. Heuts, T. Hoeks and G.C. Sanders  
Graft copolymer, process for producing such graft copolymer and composition comprising such graft copolymer

**#664:** M. Shirazi, E. van de Ven, P. J. de Lange, L. Vertommen and A.G. Talma  
Coated reinforcement fiber, process for the manufacturing of such fiber and polymer composite comprising such fiber

### Reported inventions

**#656:** J. Wu, P. Eduard and D. van Es  
Greener 1C-DIOL

**#656:** J. Wu, P. Eduard and D. van Es  
Greener 1C-DIACID

**#651:** R. Duchateau, J.P.A. Heuts, T. Hoeks and G.C. Sanders  
Smurf

**#664:** M. Shirazi, E. van de Ven, P.J. de Lange, L. Vertommen and A.G. Talma  
Sustfiber II

**#656:** J. Wu, L. Jasinska-Walc, D. van Es, B.A.J. Noordover and C.E. Koning  
Greener 1C-diamine

**#656:** J.W. ten Brinke and T.J. Dingemans  
Greener III

**#656:** S. Thuyagarajan and D. van Es  
Greener IV

## FUNCTIONAL POLYMER SYSTEMS

### Projects

**#518:** Singlet to triplet exciton formation in polymeric light-emitting diodes (LED/FET)

**#624:** Electronic noses for high-volume system in foil applications.

**#625:** Polymeric Sensors in Smart Packaging

**#626:** Hardening of elastomers (and gels) in response to magnetic fields

**#627:** Air-stable n-type field-effect transistors

**#628:** Tuning the (electro)luminescent properties of a polymeric film by controlling inter- and /or intramolecular interactions.

**#629:** Polymer lighting with new triplet emitters and multi-layer structural design.

**#630:** Functional polymer based nano- and micro-optics for solid state lighting management

**#631:** Triplet recombination in polymer solar cells

**#660:** Bulk heterojunction polymer:zinc oxide solar cells from novel organozinc precursors

**#661:** Structurally defined conjugated dendrimers and hyperbranched polymers in solar cells

**#677:** Understanding interactions between polymer surfaces and proteins: towards an ideal polymer biosensor substrate material

**#678:** Air stable organic photovoltaics

**#679:** Smart textiles

**#680:** Charge carrier transport and recombination in advanced OLEDs

**#681:** Hybrid solar cells based on Si nanoparticles and conjugated polymers

**#682:** Creation of functional nanostructures in solution/dispersion

**#683:** Photoembossed gratings for efficient light harvesting in organic solar cells

### Theses

Fatemeh Gholamrezaie  
Self-assembled monolayers in organic electronics

Nan Tian  
Phosphorescent copolymers and their applications

Ties de Jong  
Diffractive nonimaging optics

Daniele Di Nuzzo  
Optoelectronic Processes at Polymer - Fullerene Heterojunctions

Jeroen Cottaar  
Modeling of charge-transport processes for predictive simulation of OLEDs

Rein de Vries  
Development of a charge transport model for white OLEDs

Marco Carvelli  
Study of photophysical processes in organic light-emitting diodes based on light-emission profile reconstruction

Ricardo Bouwer  
Fullerene Bisadducts for Organic Photovoltaics

Ilona Stengel  
Transition Metal Complexes and Ligand Design for Organic Optoelectronics

Oleksandr Mikhnenko  
Dynamics of singlet and triplet excitations in organic semiconductors

Haining An  
Rheological properties of magneto-responsive copolymer gels

### Scientific publications

G. J. A. H. Wetzelaer, M. Kuik and P. W. M. Blom  
*Identifying the nature of charge recombination in organic solar cells from charge-transfer state electroluminescence*  
Advanced Energy Materials 2(10) 1232-1237

V. S. Gevaerts, A. Furlan, M. M. Wienk, M. Turbiez and R. A. J. Janssen  
*Solution processed polymer tandem solar cell using efficient small and wide bandgap polymer: Fullerene blends*  
Advanced Materials 24(16) 2130-2134

N. F. Hughes-Brittain, O. T. Picot, M. Dai, T. Peijs and C. W. M. Bastiaansen  
*Effect of polymer binder on surface texturing by photoembossing*  
Applied Surface Science 258(22) 8609-8612

O. V. Mikhnenko, H. Azimi, M. Scharber, M. Morana, P. W. M. Blom and M. A. Loi  
*Exciton diffusion length in narrow bandgap polymers*  
Energy & Environmental Science 5(5) 6960-6965

## Projects

- #606:** Real-time 3D imaging of microscopic dynamics during film formation.
- #617:** Mobility of water and charge carriers in polymer/oxide/aluminium alloys
- #657:** Dyktiogenic Polymer Ions
- #658:** Waterborne polyurethane dispersions based on renewable resources
- #672:** Dopamine modification of interfaces between polymers and metals
- #673:** Starch based performance coating materials
- #675:** Drying of a waterborne coating: spontaneous phase inversion in jammed systems
- #676:** UV to daylight curing of organic coatings
- #713:** Physical aspects and modeling of weathering of polyester-urethane coatings
- #758:** Self-replenishing hydrophobic coatings with intrinsic hardness cured by LED's
- #759:** Novel Isocyanate-free, Chain-Extended Polyurethane Dispersions Containing Alternative Internal Dispersing Agents

## Theses

- Dina Ribena  
Dopamine Modification of Interfaces between Polymers and Metals
- Marc Lemmers  
Physical Gels based on Charge-Driven Co-Assembly
- Mustafa Yagci  
Self-Stratifying Antimicrobial Coatings

## Scientific publications

- T. Dikic, W. Ming, R. A. T. M. van Benthem, A. C. C. Esteves and G. de With  
*Self-replenishing surfaces*  
Advanced Materials 24(27) 3701-3704

I. Stengel, C. A. Strassert, E. A. Plummer, C. H. Chien, L. De Cola and P. Bauerle  
*Postfunctionalization of luminescent bipyridine ptii bisacetylides by click chemistry*  
European Journal of Inorganic Chemistry (11) 1795-1809

R. K. M. Bouwer, G. J. A. H. Wetzelaer, P. W. M. Blom and J. C. Hummelen  
*Influence of the isomeric composition of the acceptor on the performance of organic bulk heterojunction p3ht:Bis-pcbm solar cells*  
Journal of Materials Chemistry 22(30) 15412-15417

H. N. An, B. Sun, S. J. Picken and E. Mendes  
*Long time response of soft magnetorheological gels*  
Journal of Physical Chemistry B 116(15) 4702-4711

D. H. K. Murthy, M. Gao, M. J. W. Vermeulen, L. D. A. Siebbeles and T. J. Savenije  
*Mechanism of mobile charge carrier generation in blends of conjugated polymers and fullerenes: Significance of charge de localization and excess free energy*  
Journal of Physical Chemistry C 116(16) 9214-9220

S. A. Muntean, H. M. J. M. Wedershoven, R. A. Gerasimov and A. V. Lyulin  
*Representation of hydrogen atoms in molecular dynamics simulations: The influence on the computed properties of thin polystyrene films*  
Macromolecular Theory and Simulations 21(2) 90-97

S. A. Muntean, R. A. Gerasimov and A. V. Lyulin  
*Dynamics of water near oxidized polystyrene films*  
Macromolecular Theory and Simulations 21(8) 544-552

C. K. Chang, C. W. M. Bastiaansen, D. J. Broer and H. L. Kuo  
*Discrimination of alcohol molecules using hydrogen-bridged cholesteric polymer networks*  
Macromolecules 45(11) 4550-4555

O. T. Picot, M. Dai, T. Peijs and C. W. M. Bastiaansen  
*Manufacturing of fibres with new reflective properties and their application in textiles*  
Multifunctional Polymer-Based Materials 1403(113-118)

M. Carvelli, A. van Reenen, R. A. J. Janssen, H. P. Loebl and R. Coehoorn  
*Exciton formation and light emission near the organic-organic interface in small-molecule based double-layer oleds*  
Organic Electronics 13(11) 2605-2614

P. de Bruyn, D. J. D. Moet and P. W. M. Blom  
*All-solution processed polymer light-emitting diodes with air stable metal-oxide electrodes*  
Organic Electronics 13(6) 1023-1030

S. Bubel, A. Ringk, P. Strohrriegel and R. Schmechel  
*N-type perylene to fill voids in solution processed nanoparticulate zinc oxide thin films*  
Physica E-Low-Dimensional Systems & Nanostructures 44(10) 2124-2127

O. V. Mikhnenko, J. Lin, Y. Shu, J. E. Anthony, P. W. M. Blom, T. Q. Nguyen and M. A. Loi  
*Effect of thermal annealing on exciton diffusion in a diketopyrrolopyrrole derivative*  
Physical Chemistry Chemical Physics 14(41) 14196-14201

G. J. A. H. Wetzelaer, M. Kuik, Y. Olivier, V. Lemaure, J. Cornil, S. Fabiano, M. A. Loi and P. W. M. Blom  
*Asymmetric electron and hole transport in a high-mobility n-type conjugated polymer*  
Physical Review B 86(16) 165203

O. V. Mikhnenko, R. Ruiter, P. W. M. Blom and M. A. Loi  
*Direct measurement of the triplet exciton diffusion length in organic semiconductors*  
Physical Review Letters 108(13) 137401

H. N. An, S. J. Picken and E. Mendes  
*Nonlinear rheological study of magneto responsive soft gels*  
Polymer 53(19) 4164-4170

M. Dai, T. M. de Jong, C. Sanchez, O. T. Picot, D. J. Broer, T. Peijs and C. W. M. Bastiaansen  
*Surface structuring of bi-component fibres with photoembossing*  
Rsc Advances 2(26) 9964-9968

H. N. An, S. J. Picken and E. Mendes  
*Direct observation of particle rearrangement during cyclic stress hardening of magnetorheological gels*  
Soft Matter 8(48) 11995-12001

## Filed patent application

**#679:** O.T. Picot, C.W.M. Bastiaansen, E. Bilotti and A.A. Peijs  
Optical Strain Sensor

## Reported invention

**#630:** T.M. de Jong, D.K.G. de Boer and C.W.M. Bastiaansen  
Funoptics II

I. D. Gunbas, M. E. L. Wouters, M. M. R. M. Hendrix, R. A. T. M. van Benthem, C. E. Koning and B. A. J. Noordover  
*Maleic anhydride based copolymer dispersions for surface modification of polar substrates*  
Journal of Applied Polymer Science 125(3) 1745-1757

C. Croutxe-Barghorn, M. De Brito, X. Allonas, C. Belon, A. Chemtob, L. Ni, N. Moreau, H. De Paz, B. El Foughaili and C. Dietlin  
*Organic and hybrid interpenetrated polymer networks for advanced materials*  
Journal of Photopolymer Science and Technology 25(2) 131-135

H. Salmi, X. Allonas, C. Ley, D. Marechal and A. Ak  
*Photopolymerization using photolabile amine catalysts*  
Journal of Photopolymer Science and Technology 25(2) 147-151

M. Lemmers, E. Spruijt, S. Akerboom, I. K. Voets, A. C. van Aelst, M. A. C. Stuart and J. van der Gucht  
*Physical gels based on charge-driven bridging of nanoparticles by triblock copolymers*  
Langmuir 28(33) 12311-12318

D. Ribena, A. Alekseev, O. van Asselen, G. J. A. Mannie, M. M. R. M. Hendrix, L. G. J. van der Ven, N. A. J. M. Sommerdijk and G. de With  
*Significance of the amide functionality on dopa-based monolayers on gold*  
Langmuir 28(49) 16900-16908

D. L. Tang, B. A. J. Noordover, R. J. Sablong and C. E. Koning  
*Thermoplastic poly(urethane urea)s from novel, bio-based amorphous polyester diols*  
Macromolecular Chemistry and Physics 213(23) 2541-2549

J. Wu, P. Eduard, S. Thiyagarajan, L. Jasinska-Walc, A. Rozanski, C. F. Guerra, B. A. J. Noordover, J. van Haveren, D. S. van Es and C. E. Koning  
*Semicrystalline polyesters based on a novel renewable building block*  
Macromolecules 45(12) 5069-5080

M. de Brito, X. Allonas, C. Croutxe-Barghorn, M. Palmieri, C. Dietlin, S. Agarwal, D. Lellinger and I. Alig  
*Kinetic study of photoinduced quasi-simultaneous interpenetrating polymer networks*  
Progress in Organic Coatings 73(2-3) 186-193

V. Maurin, C. Croutxe-Barghorn and X. Allonas  
*Photopolymerization process of uv powders. Characterization of coating properties*  
Progress in Organic Coatings 73(2-3) 250-256

G. Ye, F. Courtecuisse, X. Allonas, C. Ley, C. Croutxe-Barghorn, P. Raja, P. Taylor and G. Bescond  
*Photoassisted oxypolymerization of alkyd resins: Kinetics and mechanisms*  
Progress in Organic Coatings 73(4) 366-373

P. Malanowski, S. Huijser, F. Scaltro, R. A. T. M. van Benthem, L. G. J. van der Ven, J. Laven and G. de With  
*Photodegradation of poly(neopentyl terephthalate)*  
Progress in Organic Coatings 74(1) 165-172

M. Lemmers, E. Spruijt, L. Beun, R. Fokkink, F. Leermakers, G. Portale, M. A. C. Stuart and J. van der Gucht  
*The influence of charge ratio on transient networks of polyelectrolyte complex micelles*  
Soft Matter 8(1) 104-117

### Filed patent application

**#617:** N.N.A.H. Meis, R.A.T.H. van Benthem, L.G.J. van der Ven and G. de With  
Curable coating composition

### Reported invention

**#617:** N.N.A.H. Meis, R.A.T.H. van Benthem, L.G.J. van der Ven and G. de With  
Super Interphase

.....  
HIGH-THROUGHPUT EXPERIMENTATION

### Projects

**#502:** Combinatorial approaches to rational coating design: from polymerization kinetics via coating libraries to structure-property relationships and mathematical descriptors

**#543:** Polymer manufacturing using new approaches

**#589:** High-Throughput screening of functional materials in plastic electronics: Optimizing ink-jet printing and electro-optical property pre-screening

**#611:** From Polymer synthesis to mechanical testing by high-throughput experimentation

**#612:** High-throughput investigations on well-defined (co)polymers with lower critical solution temperature (LCST) behavior

**#620:** Rapid-prototyping and inkjet printing using polyurethane precursors

**#621:** In-Stu preparation of Polymer nanoblends

**#622:** Combinatorial screening of polymer solubility

**#666:** 3D Printing of Hydrogels Based on Liquid Free-Form Fabrication of Modified Polysaccharides

**#668:** Microwave-assisted synthesis of polyamides from amines and carboxylic acids

**#690:** Libraries of poly (ethylene oxide) via parallel living anionic polymerization

**#729:** High-throughput screening technologies applied to compatibility maps

**#730:** Cellular pharmacokinetics of polymers for drug delivery - A high-throughput approach to polymers with optimum targeting characteristics

### Thesis

Ece Koç  
Linear Low-Density Polyethylene Synthesis by High-Throughput Approach

### Scientific publications

E. F. J. Rettler, M. V. Unger, R. Hoogenboom, H. W. Siesler and U. S. Schubert  
*Water uptake of poly(2-n-alkyl-2-oxazoline)s: Temperature-dependent fourier transform infrared (ft-ir) spectroscopy and two-dimensional correlation analysis (2dcos)*  
Applied Spectroscopy 66(10) 1145-1155

C. von der Ehe, K. Kempe, M. Bauer, A. Baumgaertel, M. D. Hager, D. Fischer and U. S. Schubert  
*Star-shaped block copolymers by copper-catalyzed azide-alkyne cycloaddition for potential drug delivery applications*  
Macromolecular Chemistry and Physics 213(20) 2146-2156

A. Krieg, C. Weber, R. Hoogenboom, C. R. Becer and U. S. Schubert  
*Block copolymers of poly(2-oxazoline)s and poly(meth)acrylates: A crossover between cationic ring-opening polymerization (crop) and reversible addition-fragmentation chain transfer (raft)*  
Acs Macro Letters 1(6) 776-779

J. Perelaer, R. Abbel, S. Wunscher, R. Jani, T. van Lammeren and U. S. Schubert  
*Roll-to-roll compatible sintering of inkjet printed features by photonic and microwave exposure: From non-conductive ink to 40% bulk silver conductivity in less than 15 seconds*  
Advanced Materials 24(19) 2620-2625

- J. Perelaer, R. Jani, M. Grouchko, A. Kamyshny, S. Magdassi and U. S. Schubert  
*Plasma and microwave flash sintering of a tailored silver nanoparticle ink, yielding 60% bulk conductivity on cost-effective polymer foils*  
Advanced Materials 24(29) 3993-3998
- C. Friebe, M. D. Hager, A. Winter and U. S. Schubert  
*Metal-containing polymers via electropolymerization*  
Advanced Materials 24(3) 332-345
- T. Janoschka, M. D. Hager and U. S. Schubert  
*Powering up the future: Radical polymers for battery applications*  
Advanced Materials 24(48) 6397-6409
- A. Wild, A. Winter, M. D. Hager and U. S. Schubert  
*Fluorometric sensor based on bisterpyridine metallopolymer: Detection of cyanide and phosphates in water*  
Analyst 137(10) 2333-2337
- A. C. Crecelius, R. Steinacker, A. Meier, T. Alexandrov, J. Vitz and U. S. Schubert  
*Application of matrix-assisted laser desorption/ionization mass spectrometric imaging for photolithographic structuring*  
Analytical Chemistry 84(16) 6921-6925
- A. Wild, K. Babiuch, M. Konig, A. Winter, M. D. Hager, M. Gottschaldt, A. Prokop and U. S. Schubert  
*Synthesis of a glycopolymeric pt-ii carrier and its induction of apoptosis in resistant cancer cells*  
Chemical Communications 48(51) 6357-6359
- A. Wild, A. Winter, M. D. Hager and U. S. Schubert  
*Fluorometric, water-based sensors for the detection of nerve gas g mimics dmmp, dcp and dcnp*  
Chemical Communications 48(7) 964-966
- K. Kempe, A. Krieg, C. R. Becer and U. S. Schubert  
*Clicking on/with polymers: A rapidly expanding field for the straightforward preparation of novel macromolecular architectures*  
Chemical Society Reviews 41(1) 176-191
- M. Jager, S. Schubert, S. Ochrimenko, D. Fischer and U. S. Schubert  
*Branched and linear poly(ethylene imine)-based conjugates: Synthetic modification, characterization, and application*  
Chemical Society Reviews 41(13) 4755-4767
- B. Happ, A. Winter, M. D. Hager and U. S. Schubert  
*Photogenerated avenues in macromolecules containing re(i), ru(ii), os(ii), and ir(iii) metal complexes of pyridine-based ligands*  
Chemical Society Reviews 41(6) 2222-2255
- A. Winter, M. Gottschaldt, G. R. Newkome and U. S. Schubert  
*Terpyridines and their complexes with first row transition metal ions: Cytotoxicity, nuclease activity and self-assembly of biomacromolecules*  
Current Topics in Medicinal Chemistry 12(3) 158-175
- A. M. Breul, C. Pietsch, R. Menzel, J. Schafer, A. Teichler, M. D. Hager, J. Popp, B. Dietzek, R. Beckert and U. S. Schubert  
*Blue emitting side-chain pendant 4-hydroxy-1,3-thiazoles in polystyrenes synthesized by raft polymerization*  
European Polymer Journal 48(7) 1339-1347
- V. V. Rajan, R. Waber and J. Wieser  
*Comparative investigation of the ultraviolet stabilization of polycarbonate/poly(acrylonitrile-butadiene-styrene) with different ultraviolet absorbers*  
Journal of Applied Polymer Science 124(5) 3988-3995
- A. Baumgaertel, E. Altuntas and U. S. Schubert  
*Recent developments in the detailed characterization of polymers by multidimensional chromatography*  
Journal of Chromatography A 1240(1-20)
- E. M. Reingruber, A. Chojnacka, E. Jellema, B. de Bruin, W. Buchberger and P. J. Schoenmakers  
*Chromatographic examination of the chemical composition and sequence distribution of copolymers from ethyl and benzyl diazoacetate*  
Journal of Chromatography A 1255(259-266)
- A. Chojnacka, K. Kempe, H. C. van de Ven, C. Englert, R. Hoogenboom, U. S. Schubert, H. G. Janssen and P. Schoenmakers  
*Molar mass, chemical-composition, and functionality-type distributions of poly(2-oxazoline)s revealed by a variety of separation techniques*  
Journal of Chromatography A 1265(123-132)
- K. W. Yang, J. T. Delaney, U. S. Schubert and A. Fahr  
*Fast high-throughput screening of temoporfin-loaded liposomal formulations prepared by ethanol injection method*  
Journal of Liposome Research 22(1) 31-41
- E. Altuntas, K. Knop, L. Tauhardt, K. Kempe, A. C. Crecelius, M. Jager, M. D. Hager and U. S. Schubert  
*Tandem mass spectrometry of poly(ethylene imine)s by electrospray ionization (esi) and matrix-assisted laser desorption/ionization (maldi)*  
Journal of Mass Spectrometry 47(1) 105-114
- E. Altuntas, A. Winter, A. Baumgaertel, R. M. Paulus, C. Ulbricht, A. C. Crecelius, N. Risch and U. S. Schubert  
*Determination of the relative ligand-binding strengths in heteroleptic ir(III) complexes by esi-q-tof tandem mass spectrometry*  
Journal of Mass Spectrometry 47(1) 34-40
- R. Siebert, Y. X. Tian, R. Camacho, A. Winter, A. Wild, A. Krieg, U. S. Schubert, J. Popp, I. G. Scheblykin and B. Dietzek  
*Fluorescence quenching in zn2+-bis-terpyridine coordination polymers: A single molecule study*  
Journal of Materials Chemistry 22(31) 16041-16050
- S. Wunscher, S. Stumpf, A. Teichler, O. Pabst, J. Perelaer, E. Beckert and U. S. Schubert  
*Localized atmospheric plasma sintering of inkjet printed silver nanoparticles*  
Journal of Materials Chemistry 22(47) 24569-24576
- I. Y. Perevyazko, A. Vollrath, C. Pietsch, S. Schubert, G. M. Pavlov and U. S. Schubert  
*Nanoprecipitation of poly(methyl methacrylate)-based nanoparticles: Effect of the molar mass and polymer behavior*  
Journal of Polymer Science Part a-Polymer Chemistry 50(14) 2906-2913
- M. J. Barthel, K. Babiuch, T. Rudolph, J. Vitz, S. Hoepfener, M. Gottschaldt, M. D. Hager, F. H. Schacher and U. S. Schubert  
*Bis-hydrophilic and functional triblock terpolymers based on polyethers: Synthesis and self-assembly in solution*  
Journal of Polymer Science Part a-Polymer Chemistry 50(14) 2914-2923
- A. M. Breul, J. Schafer, G. M. Pavlov, A. Teichler, S. Hoepfener, C. Weber, J. Nowotny, L. Blankenburg, J. Popp, M. D. Hager, B. Dietzek and U. S. Schubert  
*Synthesis and characterization of polymethacrylates containing conjugated oligo(phenylene ethynylene)s as side chains*  
Journal of Polymer Science Part a-Polymer Chemistry 50(15) 3192-3205
- L. Tauhardt, K. Kempe and U. S. Schubert  
*Toward the design of lpei containing block copolymers: Improved synthesis protocol, selective hydrolysis, and detailed characterization*  
Journal of Polymer Science Part a-Polymer Chemistry 50(21) 4516-4523
- M. J. Barthel, T. Rudolph, S. Crotty, F. H. Schacher and U. S. Schubert  
*Homo- and diblock copolymers of poly(furfuryl glycidyl ether) by living anionic polymerization: Toward reversibly core-crosslinked micelles*  
Journal of Polymer Science Part a-Polymer Chemistry 50(23) 4958-4965

- T. Janoschka, A. Teichler, A. Krieg, M. D. Hager and U. S. Schubert  
*Polymerization of free secondary amine bearing monomers by raft polymerization and other controlled radical techniques*  
Journal of Polymer Science Part A-Polymer Chemistry 50(7) 1394-1407
- I. Y. Perevyazko, M. Bauer, G. M. Pavlov, S. Hoepfner, S. Schubert, D. Fischer and U. S. Schubert  
*Polyelectrolyte complexes of DNA and linear pvi: Formation, composition and properties*  
Langmuir 28(46) 16167-16176
- K. Babiuch, D. Pretzel, T. Tolstik, A. Vollrath, S. Stanca, F. Foertsch, C. R. Becer, M. Gottschaldt, C. Biskup and U. S. Schubert  
*Uptake of well-defined, highly glycosylated, pentafluorostyrene-based polymers and nanoparticles by human hepatocellular carcinoma cells*  
Macromolecular Bioscience 12(9) 1190-1199
- B. Happ, G. M. Pavlov, I. Perevyazko, M. D. Hager, A. Winter and U. S. Schubert  
*Induced charge effect by co(ii) complexation on the conformation of a copolymer containing a bidentate 2-(1,2,3-triazol-4-yl)pyridine chelating unit*  
Macromolecular Chemistry and Physics 213(13) 1339-1348
- G. M. E. Pozza, H. Harris, M. J. Barthel, J. Vitz, U. S. Schubert and P. J. Lutz  
*Macromonomers as well-defined building blocks in the synthesis of hybrid octafunctional star-shaped poly(ethylene oxide)s*  
Macromolecular Chemistry and Physics 213(20) 2181-2191
- A. M. Breul, J. Schafer, C. Friebe, F. Schlutter, R. M. Paulus, G. Festag, M. D. Hager, A. Winter, B. Dietzek, J. Popp and U. S. Schubert  
*Synthesis and characterization of poly(methyl methacrylate) backbone polymers containing side-chain pendant ruthenium(ii) bis-terpyridine complexes with an elongated conjugated system*  
Macromolecular Chemistry and Physics 213(8) 808-819
- G. M. Pavlov, A. M. Breul, M. D. Hager and U. S. Schubert  
*Hydrodynamic and molecular study of poly{4-[4-(hexyloxy)phenyl]ethynylphenyl methacrylate} in dilute solutions and conformational peculiarities of brush-like macromolecules*  
Macromolecular Chemistry and Physics 213(9) 904-916
- M. M. Bloksma, R. M. Paulus, H. P. C. van Kuringen, F. van der Woerd, H. M. L. Lambermont-Thijs, U. S. Schubert and R. Hoogenboom
- Thermoresponsive poly(2-oxazine)s*  
Macromolecular Rapid Communications 33(1) 92-96
- A. Vollrath, D. Pretzel, C. Pietsch, I. Perevyazko, S. Schubert, G. M. Pavlov and U. S. Schubert  
*Preparation, cellular internalization, and biocompatibility of highly fluorescent pmma nanoparticles*  
Macromolecular Rapid Communications 33(20) 1791-1797
- R. Siebert, A. Winter, M. Schmitt, J. Popp, U. S. Schubert and B. Dietzek  
*Light-induced dynamics in conjugated bis(terpyridine) ligands - a case study toward photoactive coordination polymers*  
Macromolecular Rapid Communications 33(6-7) 481-497
- C. Friebe, A. Wild, J. Perelaer and U. S. Schubert  
*Inkjet printing of zinc(ii) bis-2,2':6',2''-terpyridine metallopolymer: Printability and film-forming studies by a combinatorial thin-film library approach*  
Macromolecular Rapid Communications 33(6-7) 503-509
- A. Wild, A. Winter, M. D. Hager, H. Gorgs and U. S. Schubert  
*Perfluorophenyl-terpyridine ruthenium complex as monomer for fast, efficient, and mild metallopolymerizations*  
Macromolecular Rapid Communications 33(6-7) 517-521
- B. Schulze, C. Friebe, S. Hoepfner, G. M. Pavlov, A. Winter, M. D. Hager and U. S. Schubert  
*Ruthenium(ii) metallo-supramolecular polymers of click-derived tridentate ditopic ligands*  
Macromolecular Rapid Communications 33(6-7) 597-602
- C. Weber, T. Neuwirth, K. Kempe, B. Ozkahraman, E. Tamahkar, H. Mert, C. R. Becer and U. S. Schubert  
*2-isopropenyl-2-oxazoline: A versatile monomer for functionalization of polymers obtained via raft*  
Macromolecules 45(1) 20-27
- C. Weber, J. A. Czaplowska, A. Baumgaertel, E. Altuntas, M. Gottschaldt, R. Hoogenboom and U. S. Schubert  
*A sugar decorated macromolecular bottle brush by carbohydrate-initiated cationic ring-opening polymerization*  
Macromolecules 45(1) 46-55
- C. Pietsch, U. Mansfeld, C. Guerrero-Sanchez, S. Hoepfner, A. Vollrath, M. Wagner, R. Hoogenboom, S. Saubern, S. H. Thang, C. R. Becer, J. Chiefari and U. S. Schubert
- Thermo-induced self-assembly of responsive poly(dmaema-b-degma) block copolymers into multi- and unilamellar vesicles*  
Macromolecules 45(23) 9292-9302
- E. F. J. Rettler, T. Rudolph, A. Hanisch, S. Hoepfner, M. Retsch, U. S. Schubert and F. H. Schacher  
*Uv-induced crosslinking of the polybutadiene domains in lamellar polystyrene-block-polybutadiene block copolymer films - an in-depth study*  
Polymer 53(25) 5641-5648
- C. Weber, K. Babiuch, S. Rogers, I. Y. Perevyazko, R. Hoogenboom and U. S. Schubert  
*Unexpected radical polymerization behavior of oligo(2-ethyl-2-oxazoline) macromonomers*  
Polymer Chemistry 3(10) 2976-2985
- G. Vancoillie, S. Pelz, E. Holder and R. Hoogenboom  
*Direct nitroxide mediated (co)polymerization of 4-vinylphenylboronic acid as route towards sugar sensors*  
Polymer Chemistry 3(7) 1726-1729
- M. A. M. Mballa, S. I. Ali, J. P. A. Heuts and A. M. van Herk  
*Control of the anisotropic morphology of latex nanocomposites containing single montmorillonite clay particles prepared by conventional and reversible addition-fragmentation chain transfer based emulsion polymerization*  
Polymer International 61(6) 861-865
- C. Weber, R. Hoogenboom and U. S. Schubert  
*Temperature responsive bio-compatible polymers based on poly(ethylene oxide) and poly(2-oxazoline)s*  
Progress in Polymer Science 37(5) 686-714
- K. Babiuch, M. Gottschaldt, O. Werz and U. S. Schubert  
*Particulate transepithelial drug carriers: Barriers and functional polymers*  
Rsc Advances 2(28) 10427-10465
- A. R. Liberski, J. T. Delaney, A. Liberska, J. Perelaer, M. Schwarz, T. Schuler, R. Moller and U. S. Schubert  
*Printed conductive features for DNA chip applications prepared on pet without sintering*  
Rsc Advances 2(6) 2308-2313
- T. S. Druzhinina, S. Hoepfner, U. S. Schubert  
*New Design Concepts for the Fabrication of Nanometric Gap Structures: Electrochemical Oxidation of OTS Mono- and Bilayer Structures*  
Small 8(6) 852 - 857
- M. M. Bloksma, S. Hoepfner, C. D'Haese, K. Kempe, U. Mansfeld, R. M. Paulus, J. F. Gohy, U. S. Schubert and R. Hoogenboom

*Self-assembly of chiral block and gradient copolymers*  
Soft Matter 8(1) 165-172

J. C. Ribot, C. Guerrero-Sanchez, T. L. Greaves, D. F. Kennedy, R. Hoogenboom and U. S. Schubert  
*Amphiphilic oligoether-based ionic liquids as functional materials for thermoresponsive ion gels with tunable properties via aqueous gelation*  
Soft Matter 8(4) 1025-1032

B. Happ, J. Schafer, C. Friebe, H. Gorgs, A. Winter, M. D. Hager, J. Popp, B. Dietzek and U. S. Schubert  
*Chelating fluorene dyes as mono- and ditopic 2-(1*h*-1,2,3-triazol-4-yl)pyridine ligands and their corresponding ruthenium(II) complexes*  
Synthesis-Stuttgart 44(14) 2287-2294

### Filed patent applications

**#690:** U.S. Schubert, S. Hoepfner and U. Mansfeld  
Observation method by TEM or SEM and specimen for use therein

**#620:** S. Wüchner, J. Perelaer, A. Teichler and U.S. Schubert  
Atmospheric plasma sintering

### Reported inventions

**#730:** M.E. Favretto, R. Brock, A. Krieg, Schubert and U.S. Schubert  
RAFT

**#612:** A. Baumgaertel, S. Crotty, K. Scheubert, M. Engler, A.C. Crecelius, S. Böcker and U.S. Schubert  
MS<sup>3</sup> Analysis

**#620:** S. Wüchner, J. Perelaer, A. Teichler and U.S. Schubert  
Induction flash sintering

**#729:** J. Vitz, S. Uebe and U.S. Schubert  
FLEX WELL-PLATE

**#620:** S. Wüchner, J. Perelaer, A. Teichler and U.S. Schubert  
Atmospheric plasma sintering

### BIO-INSPIRED POLYMERS

#### Projects

**#587:** Keratins as cheap feedstock for novel self-organising oligomers and polymers

**#684:** Smart Materials with programmable response

**#685:** Ionic interactions in water at superheated state and its implications on the dissolution of biopolymers

**#686:** Thermal Catch and Release

**#687:** Functionality of novel amphiphilic biomaterials synthesized by enzymatic linking of food polysaccharides, food proteins and fatty acids

**#688:** Lessons from biomineralization: Self-Organizing and Mineralization-Directing Block Copolymers

**#689:** Bio-inspired hairy surfaces for actuation or sensing, produced with roll-to-roll technology

**#737:** Exploring novel biobased polymers comprising furandicarboxylic acids, 2,2,4,4-tetramethyl 1,3-cyclobutanediol (CDBO) derivatives and substituted hydroxy benzoic acids as biobased rigid monomers

**#738:** Tailored water-based materials assembled from sponge-like building blocks

**#739:** Melt processable Bio-based Aromatic Polymers

**#740:** Enzymatic catalysis for the production of biobased monomers and polymers based upon them

### Theses

Maurizio Villani  
Aliphatic hydrogen bonded oligomers and polymers from natural resources

Bahar Yeniad  
Synthesis and Enzymatic Post-Modification of Chiral Polymers

Yogesh Deshmukh  
Influence on hydrogen bonding efficiency of structural modification

### Scientific publications

J. A. W. Harings, Y. S. Deshmukh, M. R. Hansen, R. Graf and S. Rastogi  
*Processing of polyamides in the presence of water via hydrophobic hydration and ionic interactions*  
Macromolecules 45(14) 5789-5797

E. F. J. Rettler, M. V. Unger, R. Hoogenboom, H. W. Siesler and U. S. Schubert  
*Water uptake of poly(2-*n*-alkyl-2-oxazoline)s: Temperature-dependent fourier transform infrared (ft-ir) spectroscopy and two-dimensional correlation analysis (2dcos)*  
Applied Spectroscopy 66(10) 1145-1155

S. Jabbari-Farouji and P. van der Schoot  
*Theory of supramolecular co-polymerization in a two-component system*  
Journal of Chemical Physics 137(6)

C. von der Ehe, K. Kempe, M. Bauer, A. Baumgaertel, M. D. Hager, D. Fischer and U. S. Schubert  
*Star-shaped block copolymers by copper-catalyzed azide-alkyne cycloaddition for potential drug delivery applications*  
Macromolecular Chemistry and Physics 213(20) 2146-2156

L. Jasinska-Walc, M. Villani, D. Dudenko, O. van Asselen, E. Klop, S. Rastogi, M. R. Hansen and C. E. Koning  
*Local conformation and cocrystallization phenomena in renewable diaminoisoidide-based polyamides studied by ft-ir, solid state nmr, and waxd*  
Macromolecules 45(6) 2796-2808

H.G. Naik, B. Yeniad, C.E. Koning, and A. Heise  
*Investigation of asymmetric alcohol dehydrogenase (ADH) reduction of acetophenone derivatives: effect of charge density*  
Organic and Biomolecular Chemistry, 10, 4961-4967

V. Dmitrovic, G. J. M. Habraken, M. M. R. M. Hendrix, W. J. E. M. Habraken, A. Heise, G. de With and N. A. J. M. Sommerdijk  
*Random poly(amino acid)s synthesized by ring opening polymerization as additives in the biomimetic mineralization of caco3*  
Polymers 4(2) 1195-1210

### LARGE-AREA THIN-FILM ELECTRONICS

#### Projects

**#618:** Polymer light-emitting diodes with doped charge transport layers

**#640:** Engineering the morphology of organic (semi)-conductor layers

**#659:** Crosslinkable Semiconductors for Robust Polymer Electronics

**#663:** Initiated-chemical vapor deposition of polymer interlayers for ultra-high moisture

**#665:** Composite stacked organic semi-conductors: materials processing towards large area organic electronics

**#704:** Forming processes in metal oxide organic light-emitting diodes

**#733:** Solution processed multilayer polymeric light-emitting diodes

**#734:** Predictive processing of polymer: fullerene solar cells

**#735:** Solution-processable low-temperature oxide semiconductors for large-area electronics

**#741:** Inkjet Printing of Suspensions

**#748:** Organic semiconductors blended into a crosslinkable insulator: Separating processability from optoelectronic functionality

**#752:** Looking down the rabbit hole: impact of porosity in the (in)organic layers on the performance of moisture permeation multi-layer barriers

## Theses

Berend Brasjen  
Coating and stability of thin liquid films on chemically patterned substrates

Liyang Yu  
Composited Stacked Organic Semiconductors: Materials and Processing Towards Large Area Organic Electronics

Gianfranco Aresta  
Chemical vapor deposition of (in)organic layers

## Scientific publications

B. F. Bory, H. L. Gomes, R. A. J. Janssen, D. M. de Leeuw and S. C. J. Meskers  
*Role of hole injection in electroforming of lif-polymer memory diodes*  
Journal of Physical Chemistry C 116(23) 12443-12447

M. T. Lu, P. de Bruyn, H. T. Nicolai, G. J. A. H. Wetzelaer and P. W. M. Blom  
*Hole-enhanced electron injection from zno in inverted polymer light-emitting diodes*  
Organic Electronics 13(9) 1693-1699

## ENHANCED OIL RECOVERY

### Projects

**#716:** Design of new chemical products (polymers and amphiphilics) for EOR

**#736:** Relating Polymer Rheology to Apparent Viscosity in Pore Media

**#778:** Strategies towards industrial production of new (branched) polyacrylamide structures for EOR

## Scientific publication

D. A. Z. Wever, P. Raffa, F. Picchioni and A. A. Broekhuis  
*Acrylamide homopolymers and acrylamide-n-isopropylacrylamide block copolymers by atomic transfer radical polymerization in water*  
Macromolecules 45(10) 4040-4045

## Reported invention

**#716:** D.A.Z. Wever, F. Picchioni and A.A. Broekhuis  
Hydres-brPAM

## EMERGING TECHNOLOGIES

### Project

Advanced Composites  
**#761:** Reactive Liquid Crystal Oligomers as Precursors Towards Composite Resins

## CORPORATE TECHNOLOGY

### Projects

**#596:** Chemically improved polysaccharides-detailed structure-property relationships

**#598:** Application of time resolved X-ray diffraction techniques for study on structural and morphological changes during polymerization and processing

**#601:** Synthesis of well-defined branched architectures for method development in polymer characterization

**#615:** 3-D tomographic reconstruction of local morphology and properties of polymer systems with nanometric resolutions by means of TEM and AFM

**#643:** Development of High-Temperature 2-Dimensional Liquid Chromatography for the Characterization of Polyolefins

**#691:** Behind state of the art: Scanning Transmission Electron Microscopy (STEM) for analysis of polymer systems

**#693:** Elastin-Functionalized Silica Particles

**#694:** Modelling of draw resonance and related instabilities in polymer processes

**#695:** Optical microscopy for nanoscale imaging

**#698:** Designer Polypeptides for Self-Assembled Delivery Vehicles

**#699:** Artificial flagella: Nature-inspired micro-object manipulation using responsive polymers

**#700:** The Ultimate Stabilizer-Free Emulsion Polymerization

**#701:** Understanding the visco-elasticity of elastomer-based nanocomposites

**#705:** Light Scattering for soft matter and meso-structural materials

**#715:** Novel Polyimide Architectures: Towards Membranes with Tunable Transport Properties

**#717:** All-aromatic heterocyclic liquid crystal polymers for photovoltaic applications

**#718:** High Tg Liquid Crystal Thermosetting Resins: A New Generation High-performance Polymers for Advanced Composites

**#719:** Unravelling the lipid-amylose inclusion complex formation

**#720:** Nanomechanical characterization of supramolecular protein structures using atomic force microscopy

**#721:** Revealing the interplay between  $\beta$ -lactoglobulin unfolding, aggregation and cross-linking

**#722:** Exploring Structure and Interactions of Bio-Macromolecules with Conventional Raman, Confocal Raman, and Tip-Enhanced Raman Spectroscopy (TERS) Imaging

**#723:** Multiscale Structure and Mechanics of Collagenous Materials

**#724:** Molecular control over amyloid protein assembly by polyphenols

**#725:** Hybrid networks

**#726:** Cross-linked food proteins as hierarchical biopolymers

**#727:** Improved characterization techniques for branched polymers

## Theses

Elena Uliyanchenko  
Ultra-performance polymer separations

Danqing Liu  
Responsive surface topographies

## Scientific publications

K. Szendrei, M. Speirs, W. Gomulya, D. Jarzab, M. Manca, O. V. Mikhnenko, M. Yarema, B. J. Kooi, W. Heiss and M. A. Loi  
*Exploring the origin of the temperature-dependent behavior of pbs nanocrystal thin films and solar cells*  
Advanced Functional Materials 22(8) 1598-1605

E. Uliyanchenko, P. J. C. H. Cools, S. van der Wal and P. J. Schoenmakers  
*Comprehensive two-dimensional ultrahigh-pressure liquid chromatography for separations of polymers*  
Analytical Chemistry 84(18) 7802-7809

J. Ciric, J. Oostland, J. W. de Vries, A. J. J. Woortman and K. Loos  
*Size exclusion chromatography with multi-detection in combination with matrix-assisted laser desorption ionization-time-of-flight mass spectrometry as a tool for unraveling the mechanism of the enzymatic polymerization of polysaccharides*  
Analytical Chemistry 84(23) 10463-10470

D. Q. Liu, C. W. M. Bastiaansen, J. M. J. den Toonder and D. J. Broer  
*Photo-switchable surface topologies in chiral nematic coatings*  
Angewandte Chemie-International Edition 51(4) 892-896

R. Winkler, R. Berger, M. Manca, J. Hulliger, E. Weber, M. A. Loi and C. Botta  
*All organic host-guest crystals based on a dumb-bell-shaped conjugated host for light harvesting through resonant energy transfer*  
Chemphyschem 13(1) 96-98

D. Q. Liu, C. W. M. Bastiaansen, J. M. J. Toonder and D. J. Broer  
*Photo-responsive surface topology in chiral nematic media*  
Emerging Liquid Crystal Technologies Vii 8279(

Y. Saricay, S. K. Dhayal, P. A. Wierenga and R. de Vries  
*Protein cluster formation during enzymatic cross-linking of globular proteins*  
Faraday Discussions 158(51-63

C. van der Walt, M. A. Hulsen, A. C. B. Bogaerds, H. E. H. Meijer and M. J. H. Bulters  
*Stability of fiber spinning under filament pull-out conditions*  
Journal of Non-Newtonian Fluid Mechanics 175(25-37

A. Fall, F. Bertrand, G. Ovarlez and D. Bonn  
*Shear thickening of cornstarch suspensions*  
Journal of Rheology 56(3) 575-591

M. F. M. Engel, C. C. VandenAkker, M. Schleegeer, K. P. Velikov, G. H. Koenderink and M. Bonn  
*The polyphenol egcg inhibits amyloid formation less efficiently at phospholipid interfaces than in bulk solution*  
Journal of the American Chemical Society 134(36) 14781-14788

M. B. van Eldijk, J. C. Y. Wang, I. J. Minten, C. L. Li, A. Zlotnick, R. J. M. Nolte, J. J. L. M. Cornelissen and J. C. M. van Hest  
*Designing two self-assembly mechanisms into one viral capsid protein*  
Journal of the American Chemical Society 134(45) 18506-18509

S. H. M. Sontjens, T. A. P. Engels, T. H. Smit and L. E. Govaert  
*Time-dependent failure of amorphous poly-d,l-lactide: Influence of molecular weight*  
Journal of the Mechanical Behavior of Biomedical Materials 13(69-77

R. Chitta, A. Ginzburg, T. Macko, R. Brull and G. van Doremaele  
*Interactive liquid chromatography of olefin-based elastomers*  
Lc Gc Europe 25(7) 352-+

T. Macko, A. Ginzburg, K. Remerie and R. Bruell  
*Separation of high-impact polypropylene using interactive liquid chromatography*  
Macromolecular Chemistry and Physics 213(9) 937-944

C. Batistakis, A. V. Lyulin and M. A. J. Michels  
*Slowing down versus acceleration in the dynamics of confined polymer films*  
Macromolecules 45(17) 7282-7292

D. Q. Liu, C. W. M. Bastiaansen, J. M. J. den Toonder and D. J. Broer  
*Light-induced formation of dynamic and permanent surface topologies in chiral-nematic polymer networks*  
Macromolecules 45(19) 8005-8012

J. E. Fiscina, M. Pakpour, A. Fall, N. Vandewalle, C. Wagner and D. Bonn  
*Dissipation in quasistatically sheared wet and dry sand under confinement*  
Physical Review E 86(2)

E. Uliyanchenko, S. van der Wal and P. J. Schoenmakers  
*Challenges in polymer analysis by liquid chromatography*  
Polymer Chemistry 3(9) 2313-2335

M. Pakpour, M. Habibi, P. Moller and D. Bonn  
*How to construct the perfect sandcastle*  
Scientific Reports 2(

A. Hernandez-Garcia, M. W. T. Werten, M. C. Stuart, F. A. de Wolf and R. de Vries  
*Coating of single DNA molecules by genetically engineered protein diblock copolymers*  
Small 8(22) 3491-3501

A. Fall and D. Bonn  
*Shear thickening of laponite suspensions with poly(ethylene oxide)*  
Soft Matter 8(17) 4645-4651

M. Habibi, P. Moller, A. Fall, S. Rafai and D. Bonn  
*Pattern formation by dewetting and evaporating sedimenting suspensions*  
Soft Matter 8(17) 4682-4686

P. J. A. Janssen, M. D. Baron, P. D. Anderson, J. Blawdziewicz, M. Loewenberg and E. Wajnryb  
*Collective dynamics of confined rigid spheres and deformable drops*  
Soft Matter 8(28) 7495-7506

## Filed patent application

**#693:** M. van Eldijk, I. Minten, R. Nolte, J. Cornelissen and J. van Hest  
Self-assembly of nanocapsules from proteins

## Reported inventions

**#597:** E. Uliyanchenko and P. Schoenmakers  
Highspeed 2DLC

**#693:** M. van Eldijk, I. Minten, R. Nolte, J. Cornelissen and J. van Hest  
ELAFUSIL

**#693 :** M.B. van Eldijk, J.C. Thies and J.C.M. van Hest  
ELAFUSIL II

**#698:** A. Hernandez Garcia, F.A. de Wolf, R. de Vries and M.A. Cohen Stuart  
SynProt II

---

## DPI ...

DPI is a foundation funded by Dutch industry, universities and the government which was set up to perform exploratory research in the area of polymer materials.

DPI operates at the interface of universities and industry, linking the scientific skills of university research groups to the industrial need for innovation.

DPI carries out pre-competitive research projects to add value to the scientific community through scientific publications and to the industrial community through the creation of intellectual property.

DPI provides a unique platform for generating awareness of new technology, in which participating industrial companies, competitors in the market place, communicate on a pre-competitive basis to trigger innovation.

DPI integrates the scientific disciplines and know-how of universities into the 'chain of knowledge' needed to optimise the conditions for making breakthrough inventions and triggering industrial innovation.

DPI aims to combine scientific excellence with a genuinely innovative impact in industry, thereby creating a new mindset in both industrial and academic research.

DPI aims to fill the innovation gap between industry and universities and so resolve the Dutch Paradox of scientific excellence and lack of innovation.

Some 200 researchers (PhDs and Post-Docs) are currently involved in DPI projects at knowledge institutes throughout the world.

---

## COLOPHON

### Coordination

DPI Communications

### Design

Kade 05, Eindhoven

### Photography

Bart van Overbeeke Fotografie,  
Eindhoven

Bram Saeys Fotografie,  
Eindhoven

Phillip Hiersemann, Halle

### Interviews

1005 Tekstproducties, Geldrop

### Translation

Effective English, Den Haag

### Printing

Lecturis, Eindhoven





## Dutch Polymer Institute

### *Mail address*

P.O. Box 902  
5600 AX Eindhoven  
The Netherlands

### *Visiting address*

Kennispoort  
John F. Kennedylaan 2  
5612 AB Eindhoven

T +31 (0) 40 247 56 29

F +31 (0) 40 247 24 62

info@polymers.nl  
www.polymers.nl