

# Past Present Future ...

Annual Report 2011





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## 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.

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# Foreword

## Past, Present, Future ...

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In 2012 the Dutch Polymer Institute (DPI) is celebrating its fifteenth anniversary as a successful public-private partnership. The platform is built on a tight professional network, the DPI community.

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“DPI matches up to the best international research institutes”

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DPI TEAM – First row: Marc Ruis, Christianne Bastiaens, Leo Robben, Monique Bruining, Jan Stamhuis, John van Haare, Harold Gankema and Peter Nossin. Second row: Jacques Joosten, Martien Cohen Stuart, Peter Kuppens, Miranda Heuvelmans and Jeanne van Asperdt. Third row: Annemarie Steinmann, Renée Hoogers, Sherida Koenders, Shila de Vries and Johan Tiesnitsch.

The basic principle behind this success is that DPI provides a platform in which different, often competing, companies can work together on research themes of common interest. The companies share the knowledge that is created and then use it themselves to innovate and to improve their products and processes. The formula for success is a mix of vision, courage and resources. The vision is that public-private partnerships accelerate the innovation process. The courage lies in daring to draw up a plan, persuading companies and knowledge institutes to invest in it, and then submitting the plan to the government. A plan that the government found so convincing that it agreed to subsidise it, and continues to subsidise it fifteen years later. It is a form of collaboration that has now become the basis for the Netherlands' new industrial policy.

### Researchers

One of our most important 'products' is a constant stream of highly qualified scientists. Our ability to 'deliver' these researchers is one of the most important justifications for our existence. There is an enormous demand in the corporate sector for researchers who speak the same language as the industry and who understand what knowledge is required for joint innovation in the field of polymers. An adequate stream of highly qualified researchers is absolutely essential for the success of the Dutch government's industrial policy. DPI makes a substantial contribution to meeting that need in the chemical sector.

### Scientific excellence

Naturally, this accomplishment is also due to the proper guidance and monitoring of the quality of the research we perform. That process starts with the screening of the quality of the researchers who apply to join DPI. The quality and output of the research is then constantly monitored, for example by the Scientific Chairmen of the various research areas and by our Scientific Reference Committee. The sustained quality of our research is reflected in the findings of the annual independent appraisal of our scientific output and the number of citations from DPI publications. The articles appear in leading scientific journals with a huge impact, including Chemical Society Review, Nature Materials, Nature Nanotechnology and Biomacromolecules. In 2011 we reached a citation impact factor of 2.04 and an average journal impact factor of 4.55. In that regard, DPI matches up to the best international research institutes. This scientific excellence enables us to attract better scientists, who produce better research and better publications, and that in turn attracts wider attention from international research institutes and companies.

### Valorisation

An important lesson we have learned in recent years is that we generate very little income from patents derived from DPI research. The original idea was that patents would create a source of financing for research, but that proved over-optimistic. It is too expensive, in terms of time and money, to register and maintain patents in different countries. Accordingly, we decided to assign patents to participants in our network as soon as possible. If they are not interested, we assign the rights to our partner organisation, DPI Value Centre, whose principal task is to initiate and promote innovation in the field of polymers. We believe this approach is the most cost-effective way of maximising our contribution to the creation of new business activity.

DPI Value Centre not only exploits the knowledge and patents generated by DPI's research, but also develops ideas



DPI VALUE CENTRE TEAM – First row: Bart van den Berg, Evelien ter Hoeven, Arie Brouwer and Martin van Dord. Second row: Karin Molenveld, Eelco Rietveld, Lonneke de Graaff, Judith Tesser and Coco Lenssen. Third row: Femke Markhorst, Johan Tiesnitsch, Jos Lobée and Louis Jetten. Absent in this picture: Peter Nossin.

“DPI is rapidly becoming a recognised global leader”

originating in companies in the networks of DPI and DPI Value Centre. A number of new and successful companies have emerged from this model of open innovation in practice.

#### Centre of Excellence

DPI is rapidly becoming a recognised global leader, an International Centre of Excellence in Polymers. At the same time, we want to continue driving innovation in Western Europe. The presence of DPI and similar organisations, greatly enhances the Netherlands’ appeal as a location for international R&D laboratories. Teijin Aramid, a manufacturer of fibres, chose to establish its worldwide R&D centre and production facilities in the Netherlands and plans to invest around one billion euros in the country. DPI’s network and the quality of its work are important – and perhaps even decisive – factors in that type of investment decision.

#### New materials

The demand for new materials is growing faster than ever. One of the developments paving the way for the global transition to a sustainable society is the use of renewable raw materials, which calls for new methods and processes to produce those materials. At the same time, the market wants multifunctional materials that incorporate different properties, such as a combination of electrical conductivity and an anti-microbial effect. The switch from fossil feedstock to renewable raw materials is prompting a change in the methods of processing these raw materials: from chemical to biotechnological production, from the use of chemical catalysts to enzymes. To make this transition, a lot of new knowledge and expertise will be required and hence we will need new partners. DPI is already laying the groundwork for a sustainable polymer chain, which starts with renewable raw materials and effectively closes product life cycles.

#### Internationalisation

We intend to further intensify our international collaboration in the coming years, particularly with partners in the emerging

economies and with an emphasis on Brazil and China. Brazil is chosen because of its abundant supply of renewable raw materials and the associated technological developments. In that context, we can make use of existing contacts with companies in that country that have already been members of our network for a number of years. We recently signed a contract with National Council for Scientific and Technological Development (CNPq), which will provide the basis for intensifying and expanding the collaboration with Brazil. China is a crucial market because of its powerful economic growth and the corresponding growth in the demand for polymers, as well as its abundant supply of ambitious researchers. We constantly need new scientists and want to encourage more researchers to join us from China by actively recruiting there, especially because we will thereby increase the diversity in our teams and reduce the shortage of researchers in the Netherlands in the fields in which DPI and its industrial partners operate.

#### EU

DPI’s qualities and activities have not gone unnoticed in Brussels. The European Union has asked us to form a consortium dedicated to the subject of nanocomposites, which also includes Russian partners. The European programmes, such as the Seventh Framework Programme and, in the future, Horizon 2020, provide opportunities for DPI to expand its programme. We are now in a position to participate in these programmes when the subject and the conditions fit in with our strategy.

The Dutch government has rewarded our approach and again promised a subsidy for 2012 and 2013. DPI and its partners have the vision and the courage to make the long-term commitment required to remain a leading world player and regional driver of innovation. We hope that the government will display a similar vision and courage in its future industrial policy and will also make a commitment for the longer term. Only then can a public-private partnership have the necessary continuity and impact.

Jacques Joosten  
Managing Director



Martien Cohen Stuart  
Scientific Director





# Organisation 2011

## Supervisory Board

- **Dr. H.M.H. van Wechem**  
*Chairman*
- **Prof.dr. M. Dröschner**
- **Prof.dr. C.J. van Duijn**
- **Dr. F. Kuijpers**
- **Prof. K.C.A.M. Luyben**
- **Prof.dr. J. Put**

## 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,  
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*

## 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*
- **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



# Dutch Polymer Institute

DPI updated its strategy in 2010 to start a new growth curve and transform itself into an ‘**International Centre of Excellence in Polymers**’. To achieve this goal DPI expanded its pre-competitive research programme with programmes focussed on pre-commercial and societal themes.

## TRACK A - PRE-COMPETITIVE PROGRAMME

DPI Rules & regulations apply to all projects

Polyolefins	Performance Polymers	Functional Polymer Systems	Coatings Technology
<b>21 projects</b>	<b>15 projects</b>	<b>19 projects</b>	<b>11 projects</b>
<b>Industry</b> <ul style="list-style-type: none"> <li>• Borealis</li> <li>• Braskem</li> <li>• Dow Benelux</li> <li>• DSM</li> <li>• ExxonMobil</li> <li>• Lanxess</li> <li>• LyondellBasell</li> <li>• Petrobras</li> <li>• Sabic</li> <li>• Shell</li> <li>• Sinopec</li> <li>• Symyx</li> <li>• Teijin Aramid</li> <li>• Ticona</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>• Evonik</li> <li>• Lanxess</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 (ITRI), Taiwan</li> <li>• Merck</li> <li>• Philips</li> <li>• Sabic</li> <li>• Shell</li> <li>• Solvay</li> <li>• TNO</li> </ul>	<b>Industry</b> <ul style="list-style-type: none"> <li>• AkzoNobel</li> <li>• Altana</li> <li>• Bayer</li> <li>• DSM</li> <li>• Evonik</li> <li>• Saint Gobain</li> </ul>
<b>Academia</b> <ul style="list-style-type: none"> <li>• Deutsches Kunststoff Institut</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>• Queens University</li> <li>• Radboud University, Nijmegen</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 Twente</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• Deutsches Kunststoff Institut</li> <li>• Eindhoven University of Technology</li> <li>• ESPCI</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>• Stellenbosch University</li> <li>• University of Amsterdam</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>• Queen Mary &amp; Westfield College, University of London</li> <li>• University of Bayreuth</li> <li>• University of Cologne</li> <li>• University of Duisburg-Essen</li> <li>• University of Groningen</li> <li>• University of Münster</li> <li>• University of Ulm</li> <li>• University of Wuppertal</li> <li>• Wageningen University</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>• University of Amsterdam</li> <li>• University of Groningen</li> <li>• University of Haute-Alsace</li> <li>• Wageningen University</li> </ul>
Expenditure € 2.54 million FTEs 28.5 (41 researchers)	Expenditure € 2.20 million FTEs 24.5 (35 researchers)	Expenditure € 2.72 million FTEs 26.9 (41 researchers)	Expenditure € 1.09 million FTEs 9.4 (15 researchers)

## Track A Pre-competitive research programmes

Currently, nine technology areas are embedded in DPI's pre-competitive research programme. Companies and knowledge institutes can participate in one or more of these areas, which all consist of several projects. The participating companies jointly define the content and projects of the specific technology area(s) in which they participate. PhD students and post docs from the partici-

pating knowledge institutes execute the research in close collaboration with scientists from the industrial partners. Shaping the collaboration between industry and academia is key to building a community that delivers the desired high quality research results and prepares our scientists for their future (industrial) careers.

The interaction between academic researchers and industrial scientists is organised in various ways. Each project team submits quarterly reports to DPI and additionally all researchers report

bi-annually in the form of a presentation to all partners in the specific technology area. In this way the researchers can highlight and explain their research results. This enables DPI to monitor, evaluate and steer the projects. The research results are shared within the technology area, and all partners are free to use the knowledge gained, except knowledge that is part of an invention. When an invention is reported and partners are interested in using the knowledge, a patent application will be filed by DPI. The industrial partners involved in the specific technology area have the first right to take over the patent application.

### DPI Rules & regulations apply to all projects

High-Throughput Experimentation	Bio-Inspired Polymers	Large-Area Thin-Film Electronics	Emerging Technologies	Corporate Research
16 projects	12 projects	8 projects	2 projects	28 projects
<b>Industry</b> <ul style="list-style-type: none"> <li>• Chemspeed Technologies</li> <li>• Evonik</li> <li>• Forschungs Gesellschaft Kunststoffe</li> <li>• Michelin</li> <li>• Microdrop Technologies</li> <li>• Waters Technologies Corporation</li> </ul>	<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>• Evonik</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>• All DPI partner companies take part in Corporate Research</li> </ul>
<b>Academia</b> <ul style="list-style-type: none"> <li>• Deutsches Kunststoff Institut</li> <li>• Eindhoven University of Technology</li> <li>• Friedrich-Schiller University, Jena</li> <li>• Innovent</li> <li>• University of Amsterdam</li> <li>• University of Liverpool</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> <li>• Loughborough University</li> <li>• Max-Planck Institut für Polymerforschung</li> <li>• Polymer Technology Group, Eindhoven</li> <li>• University of Maastricht</li> <li>• University of Leeds</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Eindhoven University of Technology</li> <li>• Imperial College London</li> <li>• University of Algarve</li> <li>• University of Cologne</li> <li>• University of Groningen</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• University of Groningen</li> </ul>	<b>Academia</b> <ul style="list-style-type: none"> <li>• Delft University of Technology</li> <li>• Deutsches Kunststoff Institut</li> <li>• Eindhoven University of Technology</li> <li>• ESRF, Grenoble</li> <li>• FOM, Utrecht</li> <li>• Leibniz-Institut für Polymerforschung, Dresden</li> <li>• Radboud University, Nijmegen</li> <li>• TI Food and Nutrition, Wageningen</li> <li>• University of Amsterdam</li> <li>• University of Groningen</li> <li>• University of Naples Federico II</li> <li>• University of Twente</li> <li>• Wageningen University</li> </ul>
Expenditure € 1.51 million FTEs 16.9 (32 researchers)	Expenditure € 1.09 million FTEs 8.8 (16 researchers)	Expenditure € 1.05 million FTEs 11.8 (18 researchers)	Expenditure € 0.22 million FTEs 1.7 (2 researchers)	Expenditure € 1.92 million FTEs 16.7 (24 researchers)

## Track B

### Industrial pre-commercial programmes

The pre-commercial programme offers companies and/or research institutes the possibility to set up innovation projects in which different parties collaborate either along the chain of knowledge or along the value chain. Each partner in the project must play an active role and the innovation must be aimed at development. The projects should 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 the participating organisations to establish the collaboration and to design the project. Especially when SMEs are involved, DPI works together with the DPI Value Centre. Furthermore, DPI can play the role of coordinator in the project.

DPI provides a model framework for the collaboration, but the detailed rules are to be agreed upon by the collaborating parties. The starting point regarding intellectual property is that the knowledge created during the course of the project (foreground knowledge) is the property of the inventing party. Any knowledge contributed to the project as background will remain the property of the party that provided it. Other parties will have access to the knowledge contributed and/or generated during the project, but only to the extent necessary for developments in the project. Specific agreements will be made for commercial application of the knowledge outside the project.

## TRACK B - PRE-COMMERCIAL PROGRAMME

Model framework for collaboration	
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>Future project</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>	Partners along the chain of knowledge  Or  Partners along the value chain
Budget €2.2 million (€1.5 million EU subsidy)	

### Bekaert

Participates in Performance Polymers

“Polymers are playing an increasingly important role in Bekaert’s product portfolio. Examples range from coated wires to steel-cord-reinforced composites. We joined DPI to gain first-hand access not only to research results but also to scientists from leading polymer research institutes. The knowledge gained through participation in DPI projects will enable us to develop new products and improve our production processes. Most importantly, however, we believe that bringing academic researchers, polymer producers and polymer users together in the DPI framework generates an ideal environment for open innovation in Bekaert’s ‘better together’ spirit.”

### Saint-Gobain

Participates in Coatings Technology

“Saint-Gobain joined DPI at the end of 2010, in the Coatings technology area. Our motivation was to share our innovation focus on sustainability for materials, but as an end-user company, whereas most industrial partners are chemical companies. DPI offers us a unique opportunity to exchange thoughts with the chemical industry, our suppliers, in a very early/ pre-competitive stage in order to steer academic research in a direction that is of industrial end-user interest. Networking with both industrial and academic partners is an additional benefit.”

## Track C Projects driven by societal themes

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

### Sinopec

Participates in Polyolefins

"As a new member of DPI, Sinopec has gained favourable experiences working with members from both industry and research institutes over the past year. DPI provides a high level research platform that enables us to participate in project selection and evaluation, to share our perspectives and visions with colleagues from other top companies and institutes, and to forge the future of the industry. We also benefit from DPI as a communication platform in many of the informative discussions at DPI meetings and project tracking. We believe SINOPEC will further benefit from DPI, as a platform to work with other world class polyolefin players."

## TRACK C - SOCIETAL PROGRAMME

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

**Start 1 September 2012**

- Industry
- Knowledge institutes
- Retailers
- NGOs

### SNF

Participates in Emerging Technologies

"SNF joined the DPI programme thanks to Shell's invitation. After almost two years, we are enthusiastic about the opportunities that the DPI project on 'polymers for transport' has brought to our research group. Generally, most industrial companies have to be very secretive about focused research work that can generate revenue in a foreseeable future. Due to confidentiality and conflicting economic interests, they have to take care not to disclose valuable advances to their customers too early. This significantly inhibits the width and depth of their research efforts.

"Within the DPI framework, with its cost and IP sharing approach, research results can be evaluated more systematically, put to the academic test and openly shared early between potential producers and users. In this way, it sooner becomes clear why a system may or may not be scaled up and implemented, while a blue-sky research approach in the water soluble polymer area is still possible.

"The open sharing of advances during well-organised review meetings can provide all participants with inspiration for their own development work. In addition, in-kind contributions promote active participation and help provide direction to the efforts. Ultimately, this should benefit all and reduce the cost per unit of recovering oil using polymers and enlarge the footprint of these EOR technologies."

### LANXESS

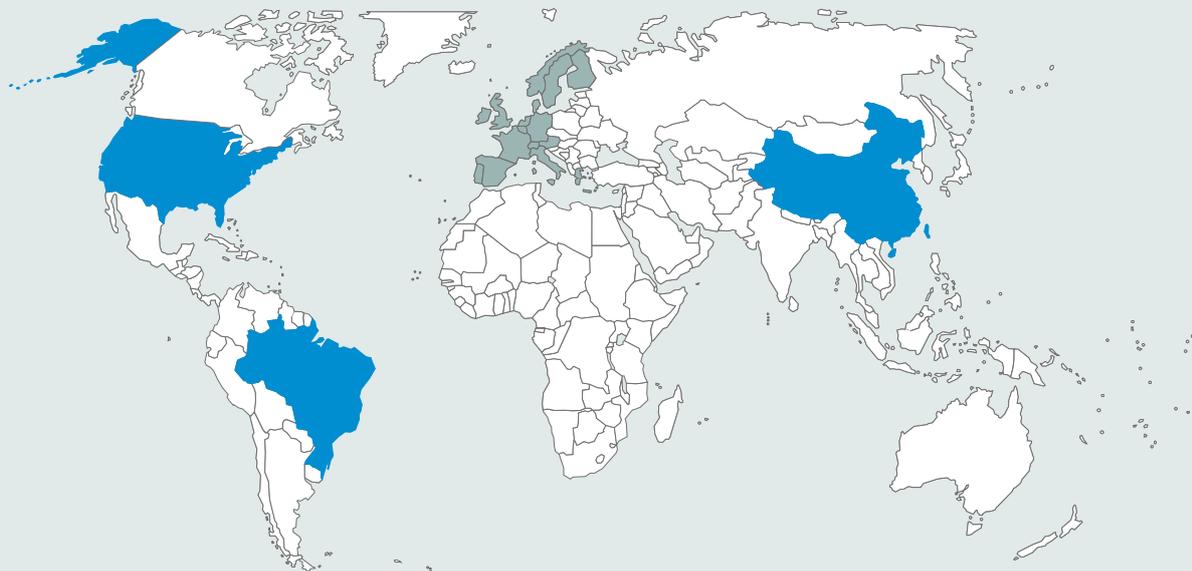
Participates in Polyolefins and in Performance Polymers

"LANXESS Elastomers joined DPI as a direct result of the sale of DSM Elastomers BV, one of the founding partners of DPI, to LANXESS last year. Right from the start, DSM Elastomers was very actively involved in DPI in both the Polyolefins and the Performance Polymers technology areas. When DSM announced its intention to divest the Elastomers business group, the Elastomers R&D department immediately decided that it would like to continue its membership in both technology areas. This was acknowledged by the top management of LANXESS, since innovation is very high on the agenda of this dynamic company with a growth mission.

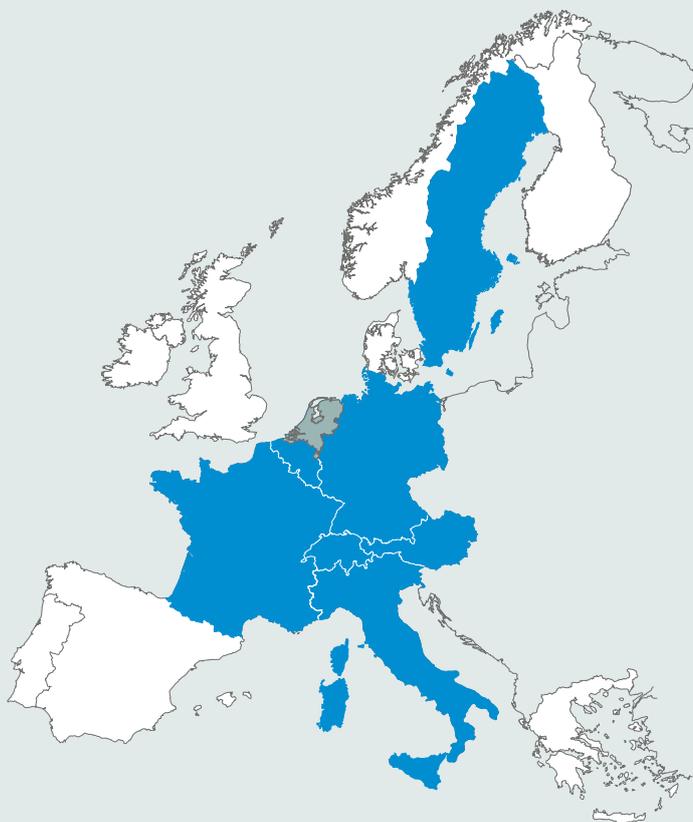
"The pre-competitive research programme is very useful – in an indirect way – for our internal R&D programme, and it supports this programme. Our researchers are in close contact with the project leaders, PhD students and postdocs and can discuss fundamental and explorative research. This nicely complements our internal business R&D, which is more focused on implementation and commercialisation. We highly appreciate the contacts with the top academia and other companies within the DPI network."

# Partners Industry 2011

## North and South America Asia



## Europe



	Altana (new per 2011)
	BASF
	Bayer
	Bekaert (new per 2011)
	Borealis
	Celanese
	Chemspeed Technologies
	Evonik
	Forschungsgesellschaft Kunststoffe



Braskem



ExxonMobil



Industrial Technology Research  
Institute Taiwan



Petrobras



Sinopec (new per 2011)



Symyx

Waters

Waters Technologies Corporation  
(left in 2011)

## The Netherlands



AkzoNobel



Dow Benelux



DSM



ECN



Food and Biobased Research  
Wageningen UR



FrieslandCampina



Lanxess Elastomers (new per 2011)



Philips



Sabic



Shell



Teijin Aramid



TNO



LyondellBasell



Merck



Michelin



Microdrop Technologies



Saint-Gobain



SKF



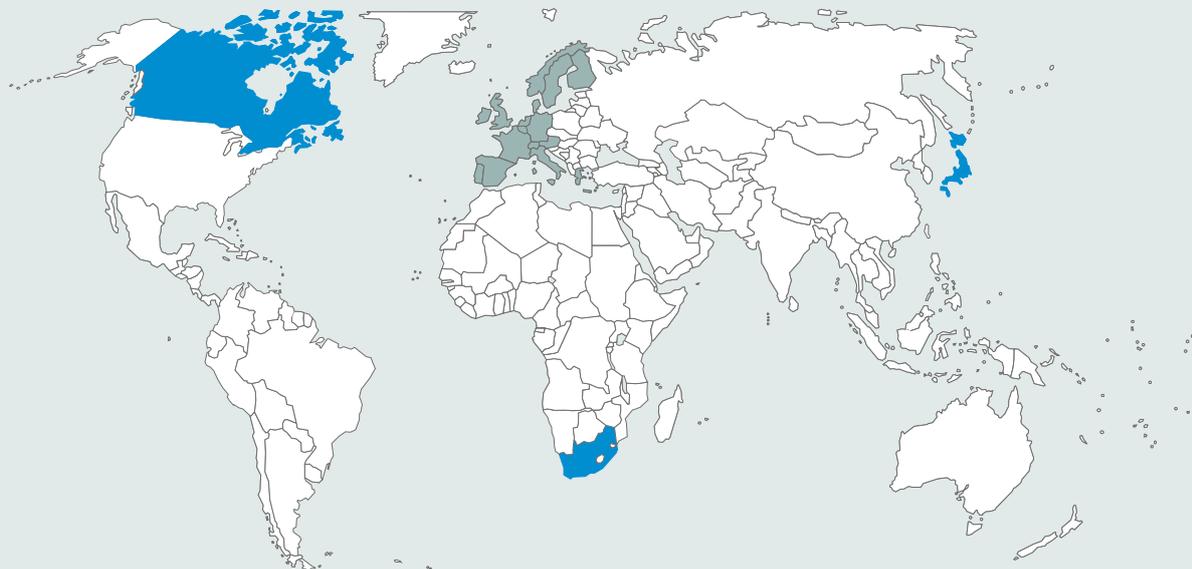
SNF Floerger



Solvay

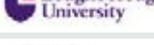
# Partners Knowledge institutes 2011

North America  
Africa  
Asia



Europe



	Deutsches Kunststoff Institut
	ESCPE-Lyon
	ESPCI
	Forschungsinstitut für Pigmente und Lacke
	Friedrich-Schiller-University Jena
	Imperial College London
	Innovent
	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
	Queen Mary & Westfield College, University of London
	University of Algarve



	Japan Advanced Institute of Science and Technology
	Queens University
	Stellenbosch University (no research projects in 2011)
	University of Manitoba
	University of Ottawa

## The Netherlands



	University of Bayreuth
	University of Cambridge (no research projects in 2011)
	University of Cologne
	University of Duisburg-Essen
	University of Glasgow (no research projects in 2011)
	University of Haute-Alsace
	University of Leeds
	University of Liverpool (no research projects in 2011)
	University of Münster (no research projects in 2011)
	University of Naples Federico II
	University of Perugia
	University of Salerno
	University of Ulm (no research projects in 2011)
	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
	TNO (no research projects in 2011)
	University Maastricht
	University of Amsterdam
	University of Groningen
	University of Leiden (no research projects in 2011)
	University of Twente
	Utrecht University (no research projects in 2011)
	Wageningen University

# Summary of financial data 2011

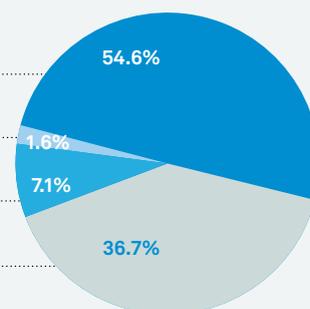
## Income

	(x EUR million)	%
Contributions from industrial partners	4.85	17.1
In-kind contributions from industrial partners	10.04	35.4
Revenue Patents	0.00	0.0
Revenue DPI Value Centre	0.44	1.6
Contributions from knowledge institutes	3.87	13.6
Contributions from Ministry of EA&I	9.00	31.7
Industrial pre-commercial research programme	0.16	0.6
<b>Total income</b>	<b>28.36</b>	<b>100</b>

## Expenditure (x EUR million)

### By nature

Personnel costs	15.07
Depreciation	0.43
Other costs	1.95
In-kind contribution	10.14
<b>Total expenditure</b>	<b>27.59</b>



### By Technology Area

Polyolefins	2.54	9.2%
Performance Polymers	2.20	7.9%
Functional Polymer Systems	2.72	9.8%
Coating Technology	1.09	4.0%
High-Throughput Experimentation	1.51	5.5%
Bio-Inspired Polymers	1.05	3.8%
Large-Area Thin-Film Electronics	1.09	4.0%
Emerging Technologies	0.22	0.8%
Corporate Research	1.92	6.9%
Knowledge Workers Scheme	0.74	
Knowledge Transfer	0.52	
Organisation and support	1.19	
Support to DPI Value Centre	0.44	
In-kind contribution	10.14	
Industrial pre-commercial research programme	0.17	
Societal theme	0.05	
<b>Total expenditure</b>	<b>27.59</b>	

# Key Performance Indicators 2011

## Number of industrial partners



## European governmental funding (% of total funding)



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



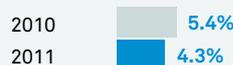
## Participation of foreign knowledge institutes as % of total expenditure



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



## Overhead costs as % of total expenditure



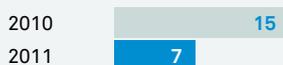
## Contribution Ministry of Economic Affairs as % of total income



## Expenditure for knowledge transfer



## Number of patents filed by DPI



## Track record DPI researchers

Left in total	62
Employed by partner knowledge institute	32
Employed by non-partner knowledge institute	10
Employed by partner industrial company	5
Employed by non-partner industrial company or start-up	10
Unknown	5

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



## Research output

	2010	2011
Scientific publications	141	157
PhD theses	5	14

Interest shown by industrial partners	2
Interest shown by university partners	1
Interest shown by DPI Value Centre	19

## Number of patents to be transferred 22

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# DPI Value Centre

## Innovation in polymers

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DPI first unveiled its plans to establish what is now the DPI Value Centre in 2006. Innovation and new business were the main drivers. The basic principle was that start-ups and small and medium-sized enterprises would drive innovation in polymers. They could develop the knowledge created in research institutes and universities and then commercialise it, in other words convert that knowledge into business and money.

By 2007 the plans had been finalised. Thanks to regional funding by Brainport, DPI Value Centre could be launched. DPI Value Centre and DPI complement one another, with DPI focusing on fundamental research and DPI Value Centre valorising the polymer-related research. Their networks also reinforce one another. DPI's network consists mainly of multinationals and research institutes, while DPI Value Centre's network is made up mainly of start-ups and SMEs. These companies are concentrated mainly in the Netherlands and parts of Belgium and Germany, whereas DPI's target group comprises organisations engaged in research into polymers worldwide. In short, DPI Value Centre and DPI each have their own focus and together form a valuable combination.

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trade fair 'Kunststoffen' in Veldhoven (the Netherlands), where we will be among the SMEs in the plastics sector, precisely where our added value lies.

### Cooperation in the chain

Innovation in polymers starts with knowledge. That knowledge is created by universities and through the partnership with DPI it is matched to the programmes and ambitions of companies. DPI Value Centre uses the results to promote innovation in the sector. Making the transition from DPI output to application takes time and money. During the Polymer Innovation Day 2011, for example, Erin Clark of ImagineOptix demonstrated a pocket beamer that is used in mobile telephones, a product that was developed thanks to DPI research and further licensed by DPI Value Centre. However, not all results of research lend themselves to further development by the target group.

### DPI Value Centre: from start-up to grown-up

Many companies that call on us are unaware that DPI Value Centre has itself emerged from the start-up phase only recently. We will be celebrating our fifth anniversary in 2012 during the plastics

### Investment

At the prompting of DPI Value Centre, in recent years the Dutch Ministry of Economic Affairs, Agriculture and Innovation has helped to promote innovation in the plastics sector by investing in feasibility studies, innovation projects and

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POCKET BEAMER – At the Polymer Innovation Day 2011, Erin Clark of ImagineOptix demonstrated a pocket beamer that is used in mobile telephones.





consortia. Up to now 128 companies have received subsidies for feasibility studies and innovation projects. Ten consortia have been formed, involving more than fifty companies. The DPI Value Centre team has been able to catalyze these collaborative relationships because it is highly familiar with both the individual companies and the overall sector. Companies invest their own time and money in innovation, while the government assumes part of the risk they take. The result is that we create new business activity in this sector in the Netherlands. The challenge lies in raising funds for the 'proof of concept' phase. It takes a long time to progress from the development of technology to its application, too long for regular investors, such as banks, who have a shorter return-on-investment horizon.

#### Knowledge transfer

Every year we organise more than twenty sparring sessions to explore opportunities with interested companies. For example, during the popular Bio Market Days (which in 2011 were held in Zelzate in Belgium and at the Chemelot site in Geleen in the Netherlands) suppliers and customers of bio polymers were able to meet and discuss possibilities face to face. At the end of 2011, in association with Wageningen University and Research Centre we

published a booklet on 'bio plastics'.

Written for the industry, it describes the current state of play regarding the possibilities of bio plastics. Sustainability is an important priority in our projects.

The Cradle to Cradle network has grown steadily since it was established in 2009. New projects have been launched; for example, a Life Cycle Analysis working group emerged from among the participants in the C2C network. The award winning Factory of the Future project that we started in 2010 with five partners is continuing. In November, we signed the 'green deal' with the 'companies and biodiversity' consortium. And for the fourth time we organised a workshop during the Dutch Design Week, during which we informed product designers of the latest developments in potential applications for the materials they use.

#### Teamwork

DPI Value Centre has a well-balanced team. The innovation coaches generally work part-time and they all have a specific area of expertise and their own network, ensuring that clients can receive comprehensive answers to their enquiries. New business is another priority, whether it involves coaching start-ups and growers or commercialising intellectual property. If additional expertise is needed, we can call on outside experts.

POLYMER INNOVATION DAY 2011

[Business market](#)

#### From start-up to grower

Our methods are appreciated. The Dutch government has designated the chemical industry as a leading sector and will incorporate the activities of DPI Value Centre in its plans for that sector. The aim is to promote intensive collaboration with sister organisations, technology transfer offices of universities and campuses like that of Chemelot as well as collaboration with other sectors such as textiles. With the DPI Value Centre approach we generate a lot of dynamism. We will continue our efforts for innovation in the sector. The challenge for the coming years is to reap what we have sown till now. It is up to innovative companies to do the sowing, and we will continue to give them tailor-made support.



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# The evolution of DPI's IP policy...

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At the start of DPI in 1997, the founding fathers -in total nine companies- agreed on the principles of the policy regarding Intellectual Property (IP). DPI would be responsible for securing the IP rights resulting from the research programme, and the companies would have a lifelong option to a license from DPI.

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But when the first research successes started to emerge, the limits of this policy soon became apparent. The first patentable results became visible after a few years, and from the year 2000 onwards, the patent portfolio slowly but steadily started to grow out of proportion. On the one hand, the time and money spent on the portfolio no longer corresponded with the research budget and the goals of a pre-competitive research institute, and on the other hand, the portfolio wasn't in the right hands at our institute; much rather, it should be in the hands of those who were actually using the technology resulting from the DPI research programme and turn it into business: the companies.

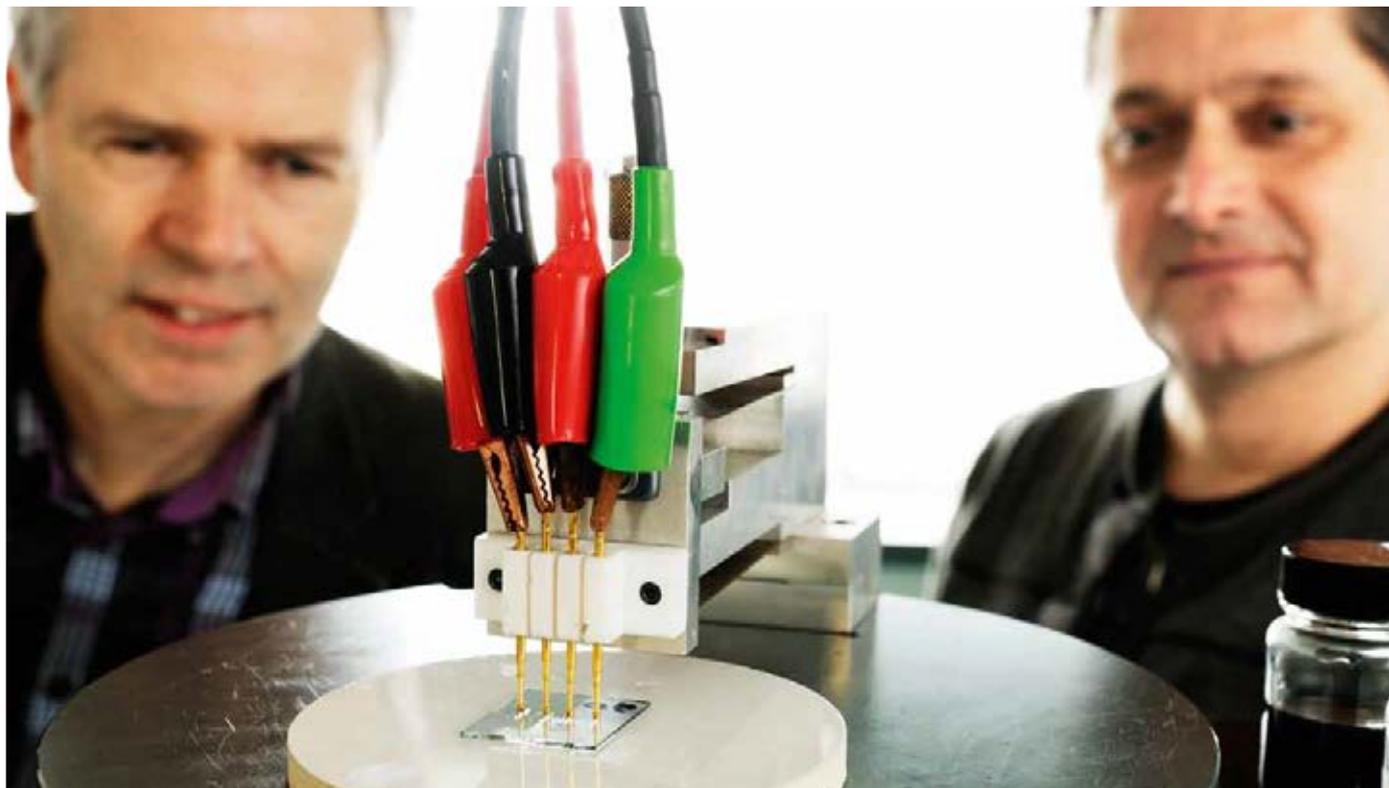
In 2006 the new -and currently still effective- IP policy was implemented. DPI is still responsible for filing patent applications on behalf of its partners, but within 2.5 years the patent applications have to be transferred to either a DPI partner company, the partner knowledge institute, or a third party. If no interested party is found within thirty months after first filing, the patent application is abandoned. DPI has made several deals with its partner companies for licenses and patent transfers. And we have been able to keep the patent portfolio in a healthy balance with our research portfolio.

Additionally the DPI Value Centre was founded in 2007, one of its tasks being to valorise DPI patents. Today the DPI Value Centre is our preferred partner for bringing DPI patents to the market 'outside the DPI community'. Arie Brouwer, Managing Director of the DPI Value Centre, describes the work they do in this area as the process of shaping rough diamonds. "Most of the patents originating from the DPI programme concern early stage technologies; you could picture them as rough diamonds. It is our mission to cut and polish these diamonds until they shine enough to be sold in the market place. Of course it also happens that they break down during shaping, proving that the technology wasn't strong enough."

## **...into tangible results in collaboration with the DPI Value Centre!**

An excellent example of this cooperation, of transforming a 'rough patent' into a 'shining prototype', started within the DPI technology areas Performance Polymers and Functional Polymer Systems. The respective partner companies selected two interconnected projects on the subject of dispersing Carbon Nanotubes into polymer matrices to be performed at Eindhoven University of Technology, one of DPI's partner knowledge institutes. The projects had a multidisciplinary approach. One part was executed within Prof. Cor Koning's group at the department of Chemical Engineering and focused on polymer chemistry. The other part, reflecting a theoretical physics perspective, was provided by Paul van der Schoot's group at the department of Applied Physics.

The research was executed by PhD students Nadia Grossiord and Marie-Claire Hermant (together with Joachim Loos, Oren Regev, Jan Meuldijk, Bert Klumperman and Paul van der Schoot) and resulted in a number of DPI patent applications. Once it turned out that neither the partner companies of the technology areas, nor any of the other companies outside DPI could use the technology at this stage at that particular



time for their business processes, DPI offered this set of patent applications to the DPI Value Centre.

- **DPI 03.002 Arabian Nanotubes**  
International Publication Number  
WO/2004/072159
- **DPI 05.013 Broad Nanotubes**  
International Publication Number  
WO/2007/121847
- **DPI 07.004 Surftron**  
International Publication Number  
WO2009/033933

In the meantime, the researchers continued their work on this subject, and developed films composed of Carbon Nanotubes and latex particles as a replacement for IndiumTinOxide (ITO), which they published in Nature Nanotechnology. ITO is a scarce material used as a conductive and transparent layer in touchscreens for mobile phones and other flat displays, as well as in solar cells.

But - together with the DPI Value Centre - they discovered that, in order to turn this principle into a tangible business opportunity, more work had to be done. DPI Value Centre provided the funds to bridge this

development project from 'proof of principle' to 'proof of concept' and the Polymer Technology Group Eindhoven, a 100% subsidiary of Eindhoven University of Technology, executed the project. A different production technology was developed, and a prototype film was produced that met the minimum conductivity and transparency requirements for the envisioned application.

This prototype film resulting from the development project initiated by DPI Value Centre, together with the patents originating from the DPI, is the perfect package deal to transfer the technology to companies. This way they can show 'proof of product' and eventually 'proof of sales', thereby completing the four stages of successful valorisation.

REPLACEMENT FOR INDIUMTINOXIDE  
4-point conductivity measurement of the new transparent conducting film developed by prof. Cor Koning (left) and prof. Paul van der Schoot (right). The black pot contains a dispersion of carbon nanotubes in water, and the white pot contains the conducting latex.  
Photo: TU/e.

# IP results 2011

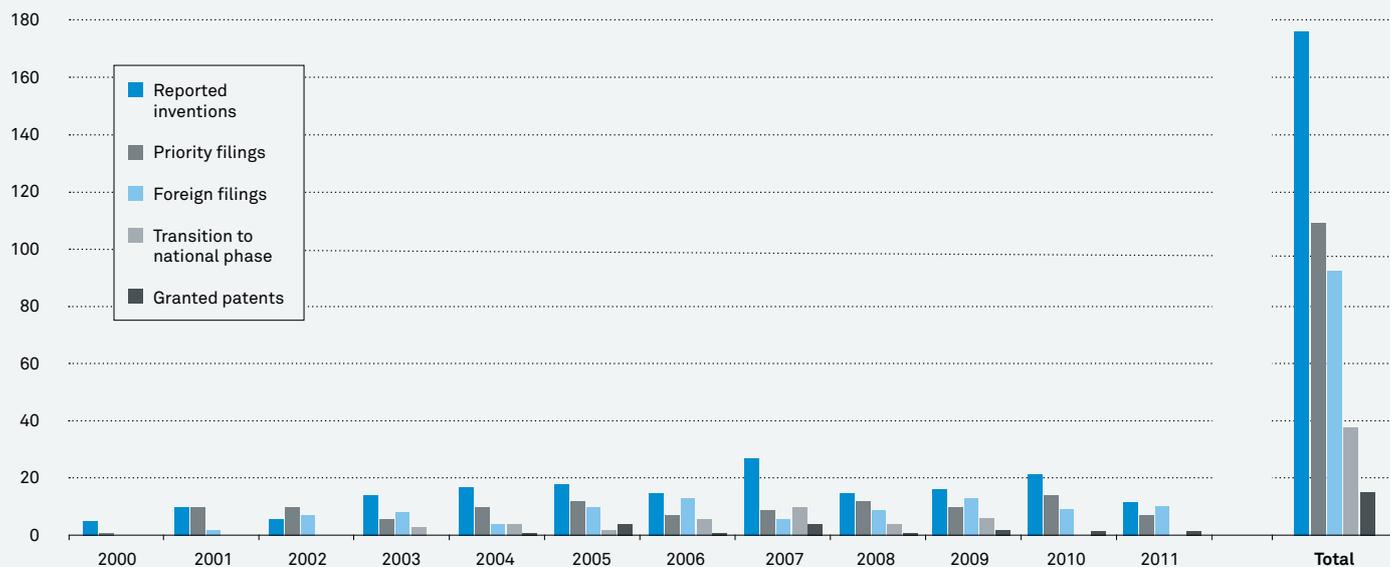
In 2011 DPI filed seven patent applications, on the basis of twelve reported inventions. These numbers are below average, as a natural result of the high numbers from the previous year.

In 2011 the technology areas Performance Polymers, Coating Technology and Functional Polymer Systems produced the highest number of inventions. The emerging technology area Polymers for Enhanced Oil Recovery has produced its first patent application. It is remarkable that the Corporate Research technology area also generated a number of

inventions and patent applications that were of interest to specific partner companies. The rights to results of the Corporate Research technology area reside with all partner companies of DPI, and since the links between the companies and the researchers are different compared to the other technology areas (which the companies have actively chosen to participate in), we are now putting extra effort into strengthening these links, among other things by presenting inventions from the Corporate Research technology area to the partner companies in a more pro-active way.

Furthermore, in order to honour the researchers who made an invention that proved to be of interest to our partners, we once again granted Certificates of Invention during our Annual Meeting in 2011. We granted a total of 55 Certificates of Invention to the inventors of 13 patent applications filed within the academic year 2010-2011. On page 26 you can find further information on the third DPI Invention Award that was presented to one of DPI's outstanding inventors – Prof. Cor Koning – at the European Polymer Congress in Granada, Spain on 29 June 2011.

## DPI patents 2000-2011



### Statistics per TA 2011

	PO	PP	FPS	CT	HTE	BIO	LATFE	EMT	Corp	Total
Reported inventions		3	3	3	1				2	12
Priority filings	1	1	2				1	1	1	7
foreign filings	1,5	1,5	1	2	1					11

# Overview 2011



# From molecular chemistry to material performance

## DPI Workshop on modelling polymers

Polymers are versatile materials whose properties can be optimised for all kinds of applications. In practice, the choice of a particular material is usually determined by trial and error and reasoned guesswork. That process would benefit if mechanical properties could be directly related to chemical and structural properties. Both in microscopic and in macroscopic regimes, models exist to predict polymer behaviour, but the big question is how to connect them. This question was addressed during a DPI workshop on modelling polymers, held 27 January 2011.

Models can address different length and time scales, from angstroms and picoseconds in quantum-mechanical models to millimetres and seconds in finite-element models (see Figure). In simple materials like metals and crystals the positions of the atoms are more or less fixed. The material can be divided into small quantities, grains, having the same properties and the same interaction with

each other. This allows for integration over macroscopic dimensions and thus macroscopic properties can be related to microscopic parameters. But can this method (known as coarse graining) also provide relevant answers for soft matter like polymers and biological materials? The size of the molecules and the interaction between them cannot straightforwardly be described with mean force fields. Relaxation of the molecules after a small disturbance must be described with transient forces. Different parts of polymers interact in a different manner. Molecular dynamics plays a role. But how to relate all this to macroscopic behaviour such as rheology, friction and aging? To start finding answers to these questions, several speakers and poster presenters at the workshop addressed different aspects.

### Interaction

The panel discussion after these presentations made it clear that there is a

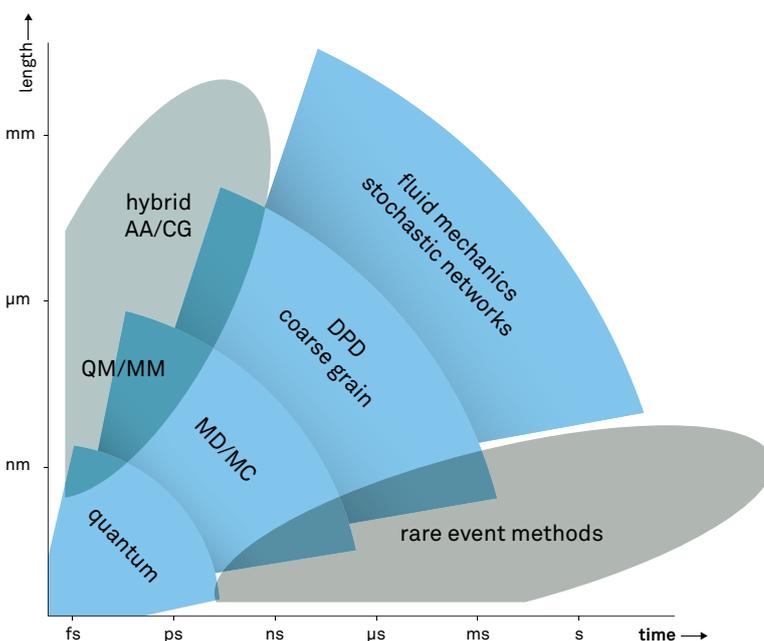
need for more interaction on this topic. Simulations can help to assess whether approximations in models, for instance representing molecules by hard spheres, are valid. Simulations should give us an understanding of what is going on at a microscopic level and predict general principles of material behaviour, especially in cases where we cannot calculate this behaviour by solving simple analytical equations. One such phenomenon that is important for applications and cannot be calculated is the aging of polymer materials.

With computing power becoming cheaper, the possibilities for simulations and modelling are increasing, but it is important to know what others are doing and to work together in a coherent manner. People working with top-down and bottom-up models, based on either structural or energy-related parameters, will benefit from each other's insights. Can we develop generic models or does every polymer system require an ad-hoc approach?

Is there a best coarse-grained method? How do we connect models in the different time and length scale regimes? It would be nice to have a model that could be used to zoom in on interesting microstructural properties and chemical detail in direct relation to macro-structural material performance. And sharing both the software and hardware would help to meet the increasing demands on the infrastructure.

In closing the workshop, DPI's Scientific Director Martien Cohen Stuart proposed the establishment of a think tank to build on the conclusions of the workshop and to prepare the issuing of a call for proposals. There is clearly a need for more research in this field. If he had learned one thing today, he said, it was that "simulation cannot provide all the answers".

MODELLING LANDSCAPE (Source: Peter Bolhuis)



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## New scientific chairman Performance Polymers

In 2011 the DPI Executive Board appointed Prof. Costantino Creton (ESPCI Paris) as the new Scientific Chairman for the Performance Polymers area.

Prof. Creton graduated from the Ecole Polytechnique Federale of Lausanne (Switzerland) in 1985 and earned his PhD at Cornell University NY. After postdoctoral research in the US he joined ESPCI, where he became research director in 2001. His research interests cover the mechanical properties of polymer materials, interfaces, and fracture. He has received several prizes (e.g., Prix Dedale, Wake Medal, J. Polymer Physics award 2008)

for his work on adhesion and is generally seen as a leading scientist in the area. We are proud that he has taken up the challenge to lead our Performance Polymers area in the years to come.

The chairmanship was handed over in June when the leaving chairmen, Jacques Noordermeer and Richard Van den Hof, stepped down.



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## Vincent Monteil laureate of Bronze CNRS Medal

Vincent Monteil, CNRS researcher in the Chemistry, Catalysis, Polymers and Processes laboratory (C2P2) at CPE Lyon, is a 2011 laureate of the Bronze Medal of the CNRS. His research activities focus on the (catalytic) polymerisation of olefins and especially their copolymerisation with polar vinyl monomers using hybrid radical/catalytic mechanisms. The Bronze medal rewards the initial work of a young researcher and represents an encouragement from the CNRS to pursue the research which has begun so successfully. Monteil is project leader of several research projects in the DPI Polyolefins technology area.

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## Knowledge institutes DPI and Eindhoven University of Technology collaborate with Brazil

In February 2011 the Dutch Polymer Institute (DPI) and Eindhoven University of Technology (TU/e) entered into a collaboration agreement with the National Council for Scientific and Technological Development (CNPq) of Brazil by signing a Letter of Understanding to this effect. This heralded the commencement of a three-year R&D cooperation in the area of nanotechnology and (bio-)polymers. It was agreed that ten PhD candidates would be appointed.

The chief goal of the cooperation between TU/e, DPI and CNPq is to set up a network to make better use of each other's strengths and to further develop these strengths. For this purpose joint research projects will be set up. The transfer of knowledge and experience will be stimulated through the exchange of ten PhD students (doctoral candidates). There will be five researchers from Brazil, three from DPI and two from TU/e. Six of them will join the DPI programme and four will join the

TU/e programme. If the evaluation to be made in two years shows that this cooperation is successful, the numbers will be doubled to a total of twenty doctoral candidates.

Dr. Jacques Joosten, Managing Director of DPI, radiates enthusiasm about the collaboration between DPI, TU/e and Brazil. "We want to turn DPI into an International Centre of Excellence in Polymers. To that end we are expanding our network, focusing in particular on rapidly growing economies such as Brazil and China. This collaboration with the Brazilian Council for Scientific and Technological Development provides ample opportunities to enter into more alliances with Latin American parties in the future. Working with both industry and academia, as DPI does, is new to the Brazilian party." TU/e, too, sees opportunities for more joint ventures, particularly because Bio-based Materials is an area of special focus in the TU/e Department of Chemical Engineering and Chemistry.

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## Prof. Cor Koning wins DPI Invention Award

During the European Polymer Congress 2011 in Granada, Spain, on 29 June 2011, the Dutch Polymer Institute (DPI) presented the DPI Invention Award to Prof. Cor E. Koning. Cor Koning worked at the Eindhoven University of Technology and is currently employed by DSM. He received this award for his important contribution to the innovative capabilities of DPI.

Cor Koning is one of the major inventors at DPI and as such has contributed substantially to the technological areas of Performance Polymers, Coatings Technology and Bio-Inspired Polymers. The patents resulting from his work have among other things contributed to the creation of new projects and new business activities. Dr. Jacques Joosten, Managing

Director of DPI: "Cor Koning plays a crucial part within the DPI community. His working methods match the DPI strategy, which strives for excellent scientific research in combination with industrial relevance. That is why he wholly deserves this award."

The DPI Invention Award is presented on a biennial basis to a researcher from the DPI network in order to highlight the importance of inventions. The most important criteria are the number of inventions made in combination with scientific level and industrial relevance. Earlier winners of the award were: D.J. Broer, C.W.M. Bastiaansen and U.S. Schubert. The DPI Invention Award 2013 will be presented during the European Polymer Congress in Pisa, Italy.

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## Gilles Holst Medal granted to Prof. Dick Broer

On 31 October Dick Broer, Professor of Functional Organic Materials at Eindhoven University of Technology Department of Chemical Engineering & Chemistry, was presented the Gilles Holst Medal 2011 in Amsterdam (the Netherlands). He received the award for his research in the field of crystalline materials. According to the board of the Royal Dutch Academy of Sciences (KNAW), Broer's work led to numerous innovations such as LCD screens, biosensors, and the controlled administration of medicine.

Prof. Dick Broer is an active member of the DPI community and a lot of his research is part of DPI projects.

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## European projects

In 2010 DPI organised a workshop on hybrid materials that brought together end users, material suppliers and academia from all over Europe. They discussed the future possibilities of hybrid materials in the areas of automotive, solar energy, solid-state lighting, civil engineering and aviation and aerospace. The organisation of this workshop, in collaboration with SusChem and with support from the European Commission, was an important step towards collaboration projects in Europe within the FP7 framework.

The first DPI project in this framework is the CompNanoComp project, which started in October. The goal of the CompNanoComp project is to develop a multiscale simulation methodology and software for predicting the morphology (spatial distribution and state of aggregation of nanoparticles), thermal properties (glass temperature), mechanical properties (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.

This ground-breaking modelling methodology should significantly improve the reliable design and processability of nanocomposites, which will contribute to several EU Grand Challenges (reduction of CO<sub>2</sub> emissions, energy savings by lightweight 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 of nanocomposites and will have an immediate industrial, economic and environmental impact.

The CompNanoComp initiative consists of two collaborative projects being implemented by an EU consortium (8 partners) and a Russian consortium (4 partners) under the FP7 framework and the Federal Russian government. DPI acts as the coordinator of the project and John van Haare is the Project Leader of the CompNanoComp project.

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# Richard van den Hof

## retired from DPI

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Richard van den Hof retired from the Dutch Polymer Institute in 2011. In the spring of 2011 he handed over his duties as scientific chairman of Performance Polymers to Prof. Costantino Creton and on 1 October he officially retired.

Richard van den Hof made a valuable and crucial contribution to the Dutch Polymer Institute over the years. Since DPI's foundation he contributed a great deal to the Institute's growth and success. He played an essential role in the innovation of DPI's activities. DPI is very grateful to Richard van den Hof for his long term commitment and efforts.

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### **Richard van den Hof announced his retirement in a personal note:**

After more than 13 years' involvement in DPI I will leave for retirement on 1 October 2011. My involvement dates back from before the actual start of DPI. In my research position at DSM in many discussions then, mainly with Leen Struik, I was able to emphasise the importance of incorporating polymer processing research and soon after that I was asked to help realise this in a position as Industrial Contact Person, supporting the PC representative from DSM. That went well enough apparently to be nominated as PC member for DSM in the Engineering Plastics cluster. This eventually culminated in my becoming Programme Manager for that area, in which capacity I of course refrained from exercising voting rights for DSM. On a temporary basis I also fulfilled the role of Programme Manager for the Corporate Research Programme and the newly started Bio-Inspired Polymers cluster. A very busy but interesting period.

With the further growth of DPI, the current Technology Area structure emerged, and with that came a new challenge for me: Scientific Chairman of the Engineering Plastics area. After the merger with the Rubber Technology Area I kept that role for the engineering polymers, while Prof. Jacques Noordermeer took care of rubber technology. In the Spring of 2011 our chairmanships were taken over by Prof. Costantino Creton.

The DPI formula of an industry driven programme as the basis for fundamental research has proven to work very well. Industry relevant disciplines and cooperation were kept or built with sufficient critical mass, many well-educated people found their way into academia or industry, the scientific quality of the research surpasses that of non-industry-driven research in the same area and a vast and thriving network of people in industry and academia became the backbone of DPI as a whole.

I am very pleased to have been able to contribute to this formula, from both industry and DPI management positions. In the cooperation with industry partners and researchers I met full trust that we were working well on the right things, even when, no doubt, competitive issues played a role as well.

I would like to thank everyone for this trust and for their good cooperation and I wish DPI a bright future. The formula may need modification in changing situations but the core of industry driven fundamental research deserves continuation and growth.

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On behalf of the entire DPI community we would like to thank Richard van den Hof, a true DPI icon, for his efforts to make DPI the successful institute it is today. We wish him well in his future pursuits.

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# DPI Annual Meeting

On 15 and 16 November 2011 DPI organised its Annual Meeting in Zeist, the Netherlands. The event was hosted by Teijin Aramid and AkzoNobel and drew 160 DPI participants.

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## Young DPI

Prior to the Annual Meeting DPI organised the annual Young DPI day. This is an event for all PhD and postdoc students who started on a DPI project in the past academic year. The goal of the day is to get to know each other and to get to know DPI. This year's Young DPI day ended with a course on 'the art of letting go'.

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## Polymer Innovation Day

On Wednesday 16 November DPI organised the third Polymer Innovation Day together with DPI Value Centre. This year the theme was, 'Join the polymer innovation highway'. Around 300 people gathered to share their stories about this theme.

During the meeting several presentations were given around the theme 'Towards new polymer materials'. All of them were of excellent scientific quality. The speakers of 15 November were:

- **Martien Cohen Stuart** - Scientific Director of DPI
- **Jacques Joosten** - Managing Director of DPI
- **Costantino Creton** - Professor of Material Science at ESPCI
- **Joris Sprakel** - Assistant professor at Wageningen University
- **Sanjay Rastogi** - Principal Scientist at Teijin Aramid
- **Lambert van Breemen** - Assistant professor at Eindhoven University of Technology
- **Doros Theodorou** - Professor of Computational Polymer Science at National Technical University of Athens
- **Marc Lemmers** - PhD student in Physical Chemistry at Wageningen University
- **Gareth Crapper** - Innovation Manager at AkzoNobel

Their presentations can be found on the DPI intranet.

### Prizes

During the afternoon session three outstanding presentations were given by the three nominees of the Golden Thesis Award: Anna Khalyavina, Inge van der Meulen and Paulina Skrzczeska. After the presentations the jury deliberated and chose Anna Khalyavina as the winner of the Golden Thesis Award.

The poster prizes were granted during the conference dinner at Slot Zeist (Zeist Castle). The first poster prize was granted to the runner up of the past two years, Nicole Franssen. Second prize went to Jorge Vieyra and Vladimir Dimitrovic was granted the third prize. Putting together a Top Three was a very difficult task for the jury, as all the posters were of excellent quality. During the evening, Certificates of Invention were granted to 42 researchers.

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YOUNG DPI 2011



GOLDEN THESIS AWARD 2011  
Martien Cohen Stuart and  
Anna Khalyavina, the winner of the  
Golden Thesis Award 2011



HOSTS ANNUAL MEETING 2011  
Jan Roos of Teijin Aramid and  
Dick van Beelen of AkzoNobel both  
received a painting as a token of  
appreciation for hosting the Annual  
Meeting 2011



POSTER PRIZE 2011  
Poster prize winners Vladimir Dimitrovic,  
Nicole Franssen, Jorge Vieyra and  
Claus Eisenbach, chairman of the  
poster jury



# Green plastic powered by FOM, Michelin, SKF and DPI

## Partnership begins research project on polymer reinforcement

The FOM Foundation has formed a partnership with Michelin, SKF and Dutch Polymer Institute (DPI) to gain a better fundamental understanding of how polymers are reinforced by adding fillers. On 28 November 2011 the partners signed the contract for this new FOM Industrial Partnership Programme, which has a budget of 1.6 million euros. Nearly all 'plastic' objects around us consist of polymers that have been reinforced with fillers to improve their physical properties. The researchers have set their sights high: they want to be the first to make a quantitative connection between the macroscale properties and performances of these reinforced materials and their structure at the molecular level. The partners will jointly deploy a wide range of advanced techniques to study the network structures at the mesoscale.

## Filled polymers

Filled polymers are used for many applications, for example in tyres (Michelin), sealing solutions in bearing applications (SKF) and a range of other types of plastic or rubber (DPI). Yet at a fundamental level, we still do not know how fillers reinforce the polymer network. This is the key question to be answered during the next four years by the FOM researchers at the University of Amsterdam, the FOM institute AMOLF, Eindhoven University of Technology and the University of Glasgow, together with researchers from the participating companies.

## Unique training

The research programme will give five PhD students and one postdoc researcher the opportunity to work on a fundamental problem of major industrial relevance. These young researchers will work in university laboratories but will also have access to the research facilities at SKF and Michelin. The unique combination of many different state-of-the-art experimental techniques makes this programme particularly interesting for young talented researchers.

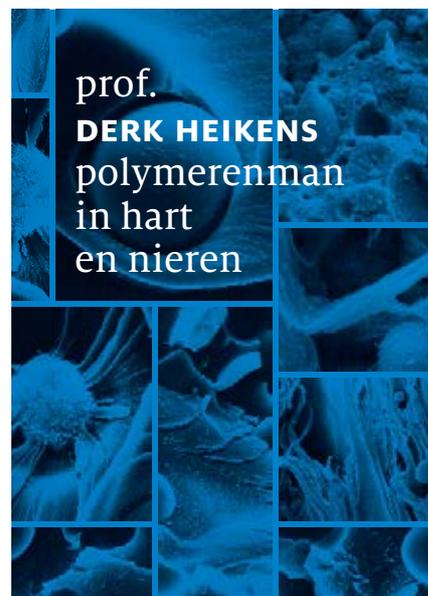
Programme leader Professor Daniel Bonn from the University of Amsterdam is enthusiastic about the new Industrial Partnership Programme that has now been given the green light: "Although many researchers are or have been working on this problem, we have yet to gain a better understanding of the relationship between the microstructure and the mechanical properties. It's great that we can now use a large number of highly advanced image-processing techniques to try to establish a quantitative link between the micro- and macroscales for the first time. Achieving that would really be a significant breakthrough. Fortunately FOM, DPI and the industrial partners share our goals!"

## Green tyres, seals and energy saving

Using various types of fillers, researchers are trying to change the mechanical properties (and, to a certain extent, the control) of a wide range of polymer systems. Michelin and SKF both have an interest in these systems. In the tyre industry, carbon black is still the most widely used filler substance. Nowadays the trend is towards 'green tyres' and carbon black is gradually being replaced by silica as a filler. Such a polymer-silica system is easier to control and characterise than the old polymer-carbon black system. This has opened up possibilities for research into the various physical processes that underlie the reinforcement of polymers by fillers. The most important challenge is linking the microstructure of the filled polymer to the macroscopic (non-linear) elasticity of the materials. Understanding such a relationship would help SKF, for example, to produce even more energy-efficient bearings by controlling the properties of sealing materials. These are typically silica-filled elastomers, which can be responsible for at least half of the friction produced within a bearing.

## Prof. Derk Heikens celebrates 90th birthday

In January 2011 emeritus professor Derk Heikens celebrated his 90th birthday. Heikens is one of the founding fathers of polymer science and research in the Netherlands and therefore DPI brought together several of his former colleagues and students in March 2011 to discuss the highlights of Heikens' career and what these highlights have meant for polymer research in the Netherlands and the rest of the world. The outcome of this lively discussion has been published in the form of a booklet (in Dutch), which was presented to Prof. Heikens in December. Copies are available via the DPI office.



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# Plastic Marine Litter

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## DPI on national TV

The increasing internationalisation of DPI is the main reason for DPI to collaborate with International Top Talent, an agency specialising in the recruitment and selection of Chinese professionals for European companies and knowledge institutions. In 2011 they selected about ten candidates for DPI vacancies in Europe.

This whole process was followed by a film crew from the Dutch investigative TV programme 'Tegenlicht'. The result, a 50-minute documentary entitled 'Holland gets talent' was broadcast by Dutch national television channel Nederland 2 on Monday 14 November 2011 at 8.55pm.

The documentary can be viewed (in Dutch) on <http://tegenlicht.vpro.nl>

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## Gianfranco Aresta granted AVS award

PhD student Gianfranco Aresta, working on project #663, received the Graduate Student award from the Thin Film Division of the American Vacuum Society for his submission for the Annual Symposium in November 2011 in Nashville, TN, USA.

DPI and DPI Value Centre are in the process of setting up a research programme with the aim of preventing Plastic Marine Litter, a challenging societal problem. Our solid knowledge base and experience in the field of polymer science and technology will hopefully enable us to help prevent this problem from becoming even bigger. However, we cannot do this by ourselves. Together with a number of partners we have formulated an initial project, 'closing the cycle of 0.5-liter plastic drinking bottles', which focuses on developing concepts of closed cycles for disposable packaging. We believe that the utilisation of closed loops is a very important mechanism to prevent plastic litter from ending up in a marine environment. Our future efforts will be focused on the execution of this project and on initiating more relevant projects on this topic together with partners in the value chain (from material producer to retailers).

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Water is the basis of life on Earth. Through water, all life on Earth is in some way or another connected to seas and oceans. People around the North Sea profit in many ways from the richness of the sea: eating its fish for food, enjoying the beautiful beaches, and using it as a medium for global transportation. Like many seas around the world the North Sea is under increasing stress from a multitude of human activities such as shipping, fishing, oil and gas production, and intensive agriculture. Plastic litter has recently moved centre stage as another stress factor for the marine environment.

Plastic, being a versatile, strong and lightweight material, benefits society in many ways. The negative side effects of society's growing dependence on plastic, however, are not equally shared. Due to its extreme persistence, disposed and abandoned plastic does not fully degrade. In the marine environment it only breaks down into smaller particles, thus making them available for ingestion to an ever-larger group of species. Plastic does not only spread over the surface of the waters, it also ends up on the seafloor, in sediments, is ingested by sea animals and stranded on beaches. Plastics can contain





additives, sometimes up to half of their weight, and some of these additives are toxic. These additives, embedded in the plastic, also find their way to the marine environment. Moreover, plastics particles can attract already present chemicals from the seawater and thus have the potential to concentrate toxicants.

Plastic marine litter directly harms marine species like seabirds and mammals. Hundreds of species have been reported to ingest or become entangled in plastic marine debris. The indirect effects include the potential impacts from micro plastics. Currently too little is known on pathways and impacts: these issues require further assessment. Due to these uncertainties it can, however, not be ruled out that (micro) plastics have an impact on various food web levels in such a way that human food consumption of marine resources becomes a risk. Similarly, there is a hypothetical possibility that plastic ingestion by lantern fishes, one of the most common fish species of the open ocean, negatively affects the biological pump that influences the uptake of carbon dioxide by the oceans.

Many effects have been known to exist for quite some time. As plastic production and plastic consumption are predicted to triple until 2050, without additional measures to reduce plastic waste the impact on the marine environment will increase. This justifies immediate action to mitigate and remedy the issue. As fragmentation of larger particles appears to be a major

source of micro plastics, general measures to reduce large plastic items benefits the micro plastic issue. Uncertainties over the indirect effects can therefore be no excuse for delaying action.

Thus far, addressing the problem has proved to be hard. Plastic marine litter originates from many sources and is a multi-faceted issue. Collaboration between scientists, industry, environmental organisations and governments is required to find solutions for all phases of the plastic life cycle. The unsustainable usage of plastic as a material is at the root of the problem and as such is part of society's general resource and waste problems. A transition to a circular, zero-waste economy is the only viable alternative and requires solutions for the manufacturing, usage, and end-of-life stages of plastic products.

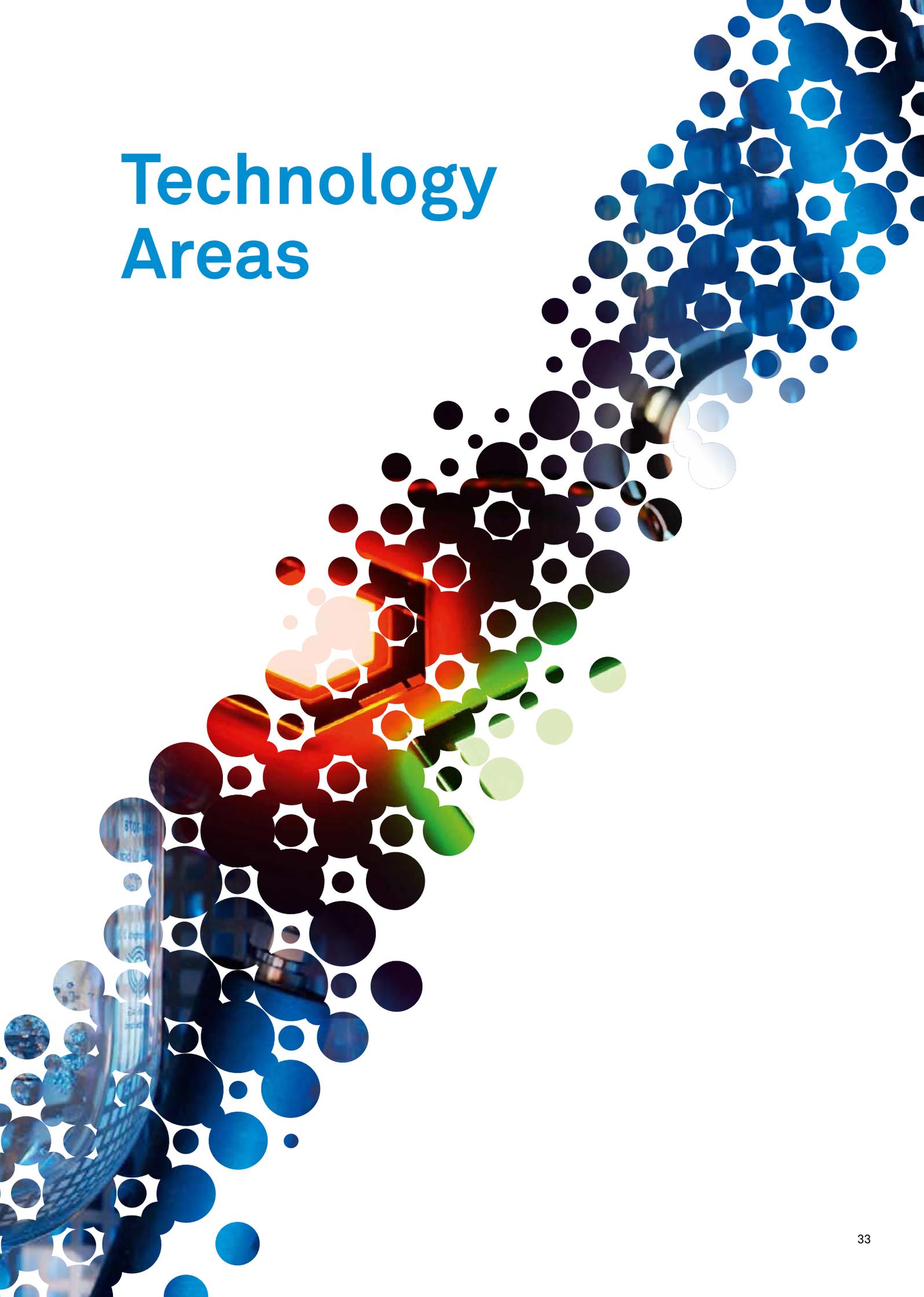
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Source of the text: Wurpel, G., Van den Akker, J., Pors, J. & Ten Wolde, A. (2011). *Plastics do not belong in the oceans. Towards a roadmap for a clean North Sea.* IMSA Amsterdam.

The report can be downloaded from: <http://www.plasticmarinelitter.eu/media/publications>



# Technology Areas



“DPI is probably the only network where people involved in polyolefins keep each other up to date.”



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# Wouter van Meerendonk

## A close link between research and production

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### POLYOLEFINS

Polyolefins (PO) are the only class of 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.

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**The production of polyolefins may be a mature field, but the many variables in the process and the wish to make it more environment-friendly mean that it still requires a lot of research effort. Even in the factory.**

“Tonight we will start up a test run in the EPDM factory. Together with the operators I will start up the improved production process,” says Wouter van Meerendonk, group leader at LANXESS’ Pilot Plant for EPDM (ethylene propylene diene monomer, a synthetic rubber) when we interview him at his current place of work. “The operators know all about the present catalyst technology, of course, but if a new technology has to be introduced the research department is involved as well. We advise them on how to vary the controls.” Starting up a factory is not his daily work as the project leader responsible for the EPDM pilot plant. But for a researcher who has the explicit ambition to work in an environment where he sees concrete applications of his work, it is, of course, a satisfying activity. “It is hard work, but also a lot of fun. In the pilot plant our team of seven – four operators, two scientists and myself as the project leader – can start a test

run, but in starting up a factory you need more people, including some people with a research background. Of course, as a researcher you primarily work on the long-term prospects but you are sometimes involved in solving day-to-day problems. I like it when things get a bit more concrete and applications come in sight,” says Van Meerendonk.

### New catalysts

Van Meerendonk was first introduced to polymers at the University of Groningen, where he studied chemistry. His graduation thesis was about organometal complexes that others in his group used as catalysts in a polymerisation set-up. After his graduation Van Meerendonk was offered a position as a PhD student in the sub-team of Cor Koning’s polymer chemistry group engaged in catalyst research. “If you come fresh from university, it is not only exciting but also very stimulating to present your project before a room full of interested people from other universities and industry. It gives an extra push to do your utmost if people are waiting for the results that you have in store for them,” says Van Meerendonk about the time when he started his DPI project. That project concerned the synthesis of polycarbonates with CO<sub>2</sub> as one of the feedstocks. The industrial routes to polycarbonate involve either hazardous ingredients, such as phosgene, or high temperatures. The advantages of preventing the use of both, as can be done with a CO<sub>2</sub>-based process, are obvious.

Van Meerendonk investigated the kinetics of the polymerisation reaction and the role of the commonly used catalysts. In addition, he proposed using new catalysts and new monomers to react with CO<sub>2</sub> to produce the polycarbonates. The project was successful, but he does not know whether his results were used directly in an industrial process in one of the factories of the industrial partners involved in his project. At the university, however, his work has been pursued and his polymers



were tested in bio-based coatings by Bart Noordover (see page 47 of this annual report). When DSM was to enter into a collaboration project with Novomer Inc. in 2010 to jointly develop a process for the production of CO<sub>2</sub>-based resins, the people involved in that process tracked Van Meerendonk down in the company and appealed to his experience with and knowledge of polycarbonate made with a CO<sub>2</sub>-based polymerisation technique. So DSM is involved in that type of polymers, but whether that is a direct result of Van Meerendonk's DPI project, he does not know.

His PhD project finished in 2005 and Van Meerendonk briefly worked for a start-up company, Dolphys Medical, on a temporary contract. In the meantime he kept looking for a permanent position, which he found with DSM, one of the industrial partners in his PhD project. His boss at DSM told him that one of the reasons why he got the job was that DSM knew who they would be dealing with if they were to employ him. "It is not so much what you have done – my first job with DSM had nothing to do with my PhD project – but rather how you have done it. They know you from your presentations, from the questions that you ask when others present their results," says Van Meerendonk. His first job at DSM was at the research department involved

in ultra-high molecular weight polyethylene (UHMWPE). After two years he moved to the research department of the Elastomers business group and since then he has been involved in the production of synthetic rubbers (EPDM). He became the group leader of the EPDM pilot plant, which is now owned by LANXESS because DSM sold its Elastomers unit to that company in May 2011.

#### Scouting

DPI continues to play a role in Van Meerendonk's working life. The transfer of his department from DSM to LANXESS in May 2011 has not altered that. At the moment he is not directly involved in a project as an industrial contact person (in the past he was involved in several projects), but he follows everything in the Polyolefins technology area. LANXESS is very well represented in that area. He explains why: "For us it is an important and effective way to stay in touch with research groups in the field, both at universities and in other industries. It is also a good network to use for scouting. You see researchers at work, you see how they present their results, and if I or one of my colleagues have a vacancy for a researcher, we always look whether we can approach someone in the DPI community for it. And of course I am also interested in the research results

themselves, not to use them immediately, but for the longer-term perspective. For my personal career, too, it is a useful network that I want to maintain. I am perfectly happy with my job right now, but circumstances may change and maybe I will be looking around for another job some time in the future. I currently have no idea what my position will be in five to ten years, although it will probably be in a research or production-related environment"

In the Polyolefins technology area, DPI's role is particularly important, according to Van Meerendonk. It is a mature research area and increasingly universities do not consider it 'sexy' enough and consequently do not spend much effort in that area. "Hard-core polyolefins research is gradually disappearing from the universities. DPI is probably the only network where people involved in the field keep each other up to date. I hope that this model will continue to exist. Initially it was a Dutch initiative but by now everybody involved in polymers all over the world, certainly in the field of polyolefins, is involved in DPI. Hopefully, they can keep up the good work and can find sufficient funding for that," Van Meerendonk concludes.

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## 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 of the polyolefin polymers. 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 yields new applications and reduces the manufacture and user eco-footprint. A recent example is the 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).

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## FACTS AND FIGURES

### Partners from industry

- Borealis
- Braskem
- Dow Benelux
- DSM
- ExxonMobil
- Lanxess
- LyondellBasell
- Petrobras
- Sabic
- Shell
- Sinopec
- Symyx
- Teijin Aramid
- Ticona

### Partners from the research world

- Deutsches Kunststoff Institut
- Eindhoven University of Technology
- ESCPE Lyon
- Japan Advanced Institute of Science and Technology
- Loughborough University
- Martin-Luther University of Halle-Wittenberg
- Queens University
- Radboud University, Nijmegen
- 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 Twente

### Budget and organisation

Expenditure in 2011 totalled € 2.54 million (budget: € 3.40 million). A total of k€ 49 was spent on equipment. The total number of FTEs allocated at year-end 2011 was 28.5 (41 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 17 reviewed papers and four theses; one patent application was filed.

For details, see page 71.

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## 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 cocatalysts and activators.

### Polymer structure, properties and processing

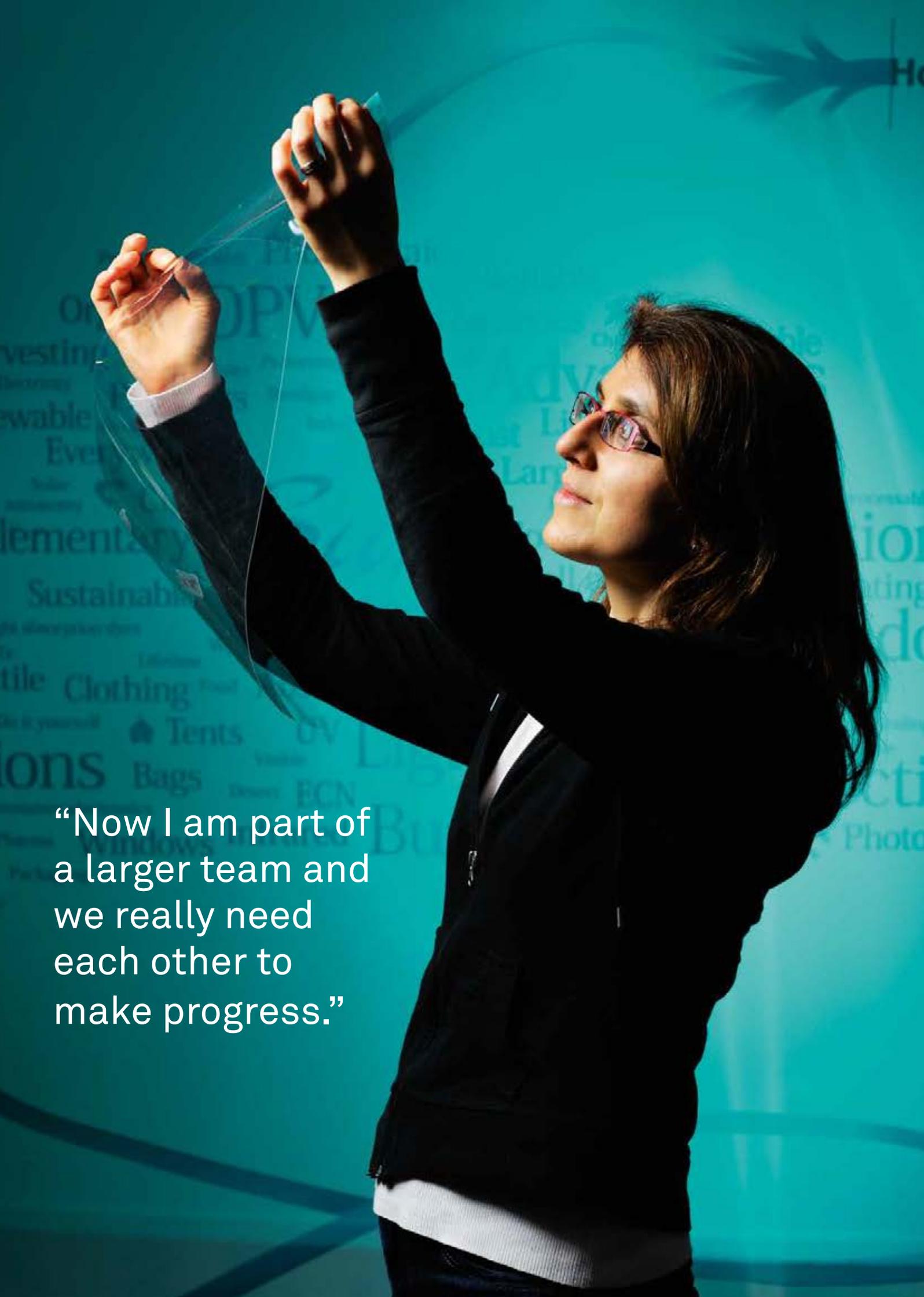
Understanding, modelling and predicting structure-processing property relationships in polyolefin-based polymer systems.

### 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.



“Now I am part of a larger team and we really need each other to make progress.”

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# Nadia Grossiord

## Working in a team

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### 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.

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**Nadia Grossiord started on her PhD project with DPI immediately after completing her Master's in polymer science in France. Only later did she realise how beneficial the DPI environment was to her career.**

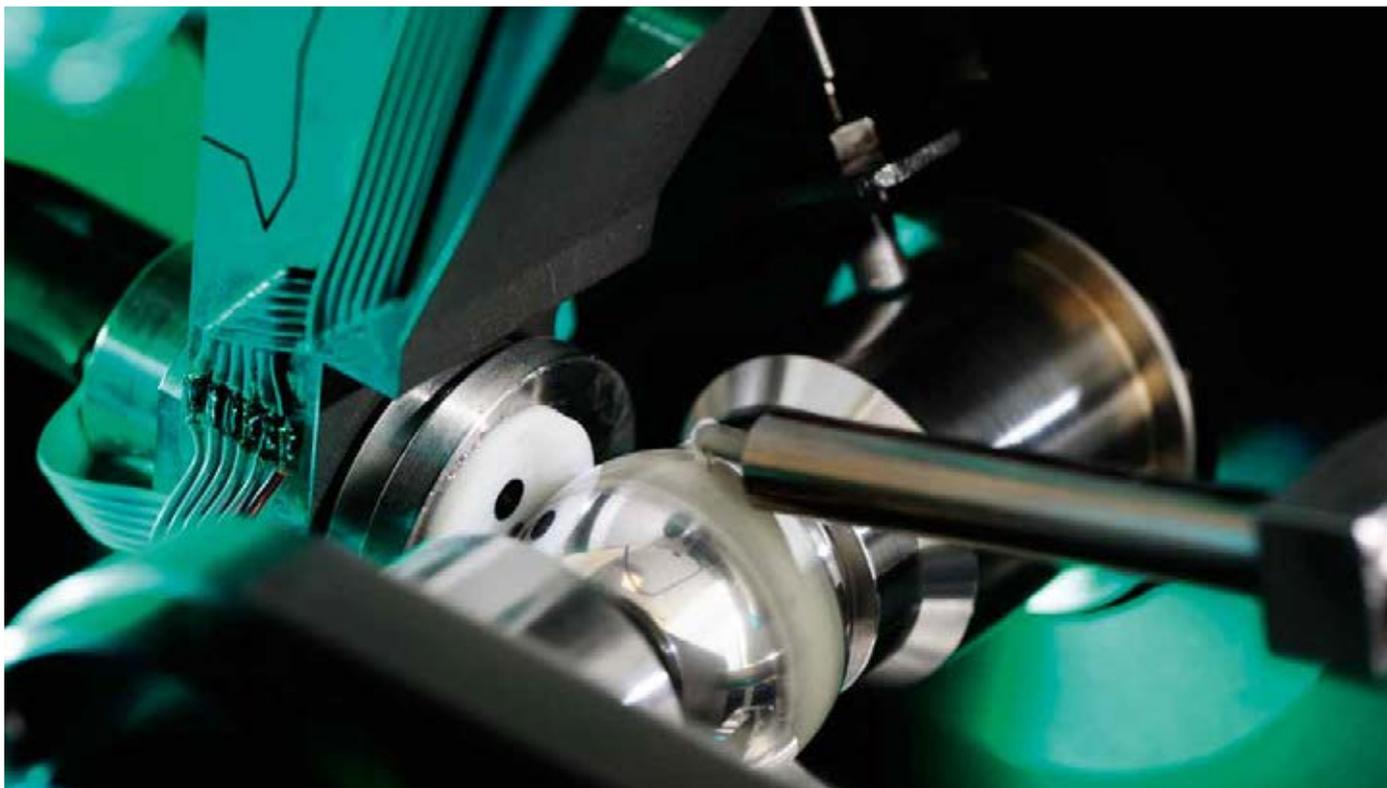
"When I came to the Netherlands for my PhD project within the DPI framework immediately after graduating, I had no idea how important and significant DPI would be for my career," says Nadia Grossiord, now researcher at the Holst Centre, when asked to look back on her career until now. After her studies in polymer chemistry in France, which included traineeships in Germany and Belgium, she wanted to do a PhD project abroad. Via a colleague she ended up in a DPI project at Eindhoven University of Technology. "The Netherlands was not my first choice, since I did not speak Dutch, but the project was interesting and everybody spoke English anyway." Grossiord investigated composites made of carbon nanotubes embedded in a polymer matrix. The amount of nanotubes in the composite determines its conductivity: a minimum critical concentration is needed to get conductivity. But the nanotubes also influence transparency: fewer nanotubes means higher transparency. For

applications such as electrodes in organic photovoltaics (OPV) and anti-static coatings cells, high conductivity and high transparency are required, so obviously an optimum needs to be found. She found several possibilities for robust processing that allowed for a check after each step to see whether things were still on track. This work was done in cooperation with the Massachusetts Institute of Technology in Boston (USA), the Ben Gurion University of the Negev (Israel) and the Free University of Brussels (Belgium), among others.

### Food

After defending her PhD thesis in December 2007, Grossiord went to the United Kingdom, where she worked for one year as a research fellow at Warwick University in the Midlands. "I wanted to go to an English-speaking country for a while. At Warwick I worked on emulsions for food. That may seem very different from my PhD work, but it wasn't. Both food emulsions and carbon nanotube-polymer blends are made by a subtle interplay of colloidal systems based on polymers, (nano-)particles and stabilisers," Grossiord says. She stayed in contact with DPI and came over for the annual meeting, she was the lucky one to receive DPI's Golden Thesis Award 2009. A year later she was back in the Netherlands, a bit unexpectedly. "My husband, who had also done a PhD funded by DPI, worked in Switzerland, so I went looking for a job there. When circumstances forced him to move back to the Netherlands, I changed my course as well and found my present job at the Holst Centre in Eindhoven."

Within the framework of her current job, Grossiord is in regular contact with people from DPI's Large-Area Thin-Film Electronics technology area. As part of a team she is involved in up scaling the process technology to make OPV cells, from the laboratory size of square millimetres and square centimetres to square meters. The aim is to replace the current, slow, batch-to-batch production process with one in which the necessary layers are printed roll-to-roll. "We have to take into account



all the restrictions that hold for a flexible plastic substrate. Curing at 300°C, for instance, is out of the question. Moreover, the printing speed, which is relatively low now, has to be raised to at least ten meters per minute to make it commercially viable. Imagine you have a rolled-up OPV cell that goes with your laptop. You roll it out in the sun and then it provides electricity for your computer,” Grossiord says about her present activities and their ultimate goal.

### **Dynamic**

The change of technology area – she was part of *Performance Polymers* during her PhD project – brought along changes in the way of working. “During my PhD project I had an overview of the whole process in a relatively well-defined system, with two components in direct interaction with each other. Now I am part of a larger team and we really need each other to make progress. I would not be able to do all the steps on my own. The system we are working on now has many unknown parameters. In an industrial product you have a lot of components, and these components can moreover vary between batches. We are seeing trends in the results, but it is very challenging to find the exact reasons for them, as it is not always possible to vary only one parameter like you do in a more controlled laboratory environment. But it is also

interesting to work with people with different backgrounds, with physicists and engineers. It is a completely different world,” she observes.

In DPI she is now playing the role that industrial partners played during her PhD project. She listens to the presentations of other PhD students. “Now I realise how important these presentations are for the industrial partners to get a regular update on the progress of the project. As a PhD student, you are totally absorbed by your subject. You know what you are doing and why, and you tend to forget that you need to keep others up to date,” Grossiord adds. She remembers yet another event that made her see DPI in a different light. “When I was in the UK, we had a meeting with new appointees in polymer science. There was one guy from the United States who was in the UK for a post doc at the time, and he mentioned DPI as the outstanding example of the kind of organisation needed to promote applied science. He said it would be fantastic to have such an organisation in for instance the UK as well. It opened my eyes, since for me that was the ‘normal’ situation.”

### **Writing**

Besides a thesis, several articles and two patents that resulted from Grossiord’s project, there is also the book that she

wrote together with her supervisor, Cor Koning, and her fellow PhD student, Marie Claire Hermant. At the request of a publisher, Pan Stanford Publishing, Hermant and Grossiord used their theses as a starting point and combined them into a new text. One reviewer wrote: “These authors are leading researchers and have done a great service to the community by capturing the current understanding of carbon nanotube polymer nanocomposites.” Grossiord recalls: “It was fantastic to see how complementary our work was. The two theses are not recognisable anymore; we completely rewrote the text. When we were busy with the book, I did not need to think about what I should do during the weekend. It was really a big effort, but it was a dream to be able to write a book.” It looks like she has caught the writing bug, because apart from the book, she was also involved in writing the executive report of the Holst Centre last year. Asked about her plans for the future, she says: “I can imagine myself doing a lot of things, as long as I find them interesting and as long as they are intellectually stimulating.”

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## 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.

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## 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**

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 viscoelastic 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.

### **Stability and long-term 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.

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## FACTS AND FIGURES

### **Partners from industry**

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

### **Partners from the research world**

- Delft University of Technology
- Deutsches Kunststoff Institut
- Eindhoven University of Technology
- ESPCI
- Leibniz-Institut für Polymerforschung, Dresden
- National Technical University of Athens
- Queen Mary & Westfield College, University of London
- Stellenbosch University
- University of Amsterdam
- University of Twente
- Wageningen University

### **Budget and organisation**

Expenditure in 2011 totalled € 2.20 million (budget: € 2.12 million). A total of k€ 15 was spent on equipment. The total number of FTEs allocated at year-end 2011 was 24.5 (35 researchers). With effect from June the two Scientific Chairmen Richard van den Hof MSc and Prof.dr. Jacques Noordermeer were succeeded by Prof.dr. Costantino Creton. Dr. Jan Stamhuis acted as Programme Area Coordinator of the Performance Polymers programme.

### **Publications and inventions**

This technology area generated a total of 29 reviewed papers and four theses; three inventions were reported and one patent application was filed.

For details, see page 72.



“I try to relate materials properties and physical processes to device behaviour and performance.”

# Jan Anton Koster

## The relationship between morphology and efficiency

### FUNCTIONAL POLYMER SYSTEMS

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

**Blends of polymers are complex systems – so complex that it is surprising that functioning devices such as solar cells or transistors can be made of them. By modelling these systems we can gain a deeper insight into their operation.**

“It was splendid teamwork. Whenever my colleague Valentin Michailetchi supplied me with data, I was absolutely sure that they were correct,” says Jan Anton Koster about his PhD project with DPI. A theoretical physicist by background, he soon found out that he was not born to be a lonely, hard-core elementary-particles man, so in 2002 he went looking for a position in which he could combine theoretical and experimental work. In his view doing experiments yourself is useful and perhaps necessary to understand what you are doing when you are modelling a system. He found this combination at his own university, the University of Groningen, the Netherlands, where he initially worked on hybrid organic/inorganic solar cells in Paul Blom’s Molecular Electronics group.

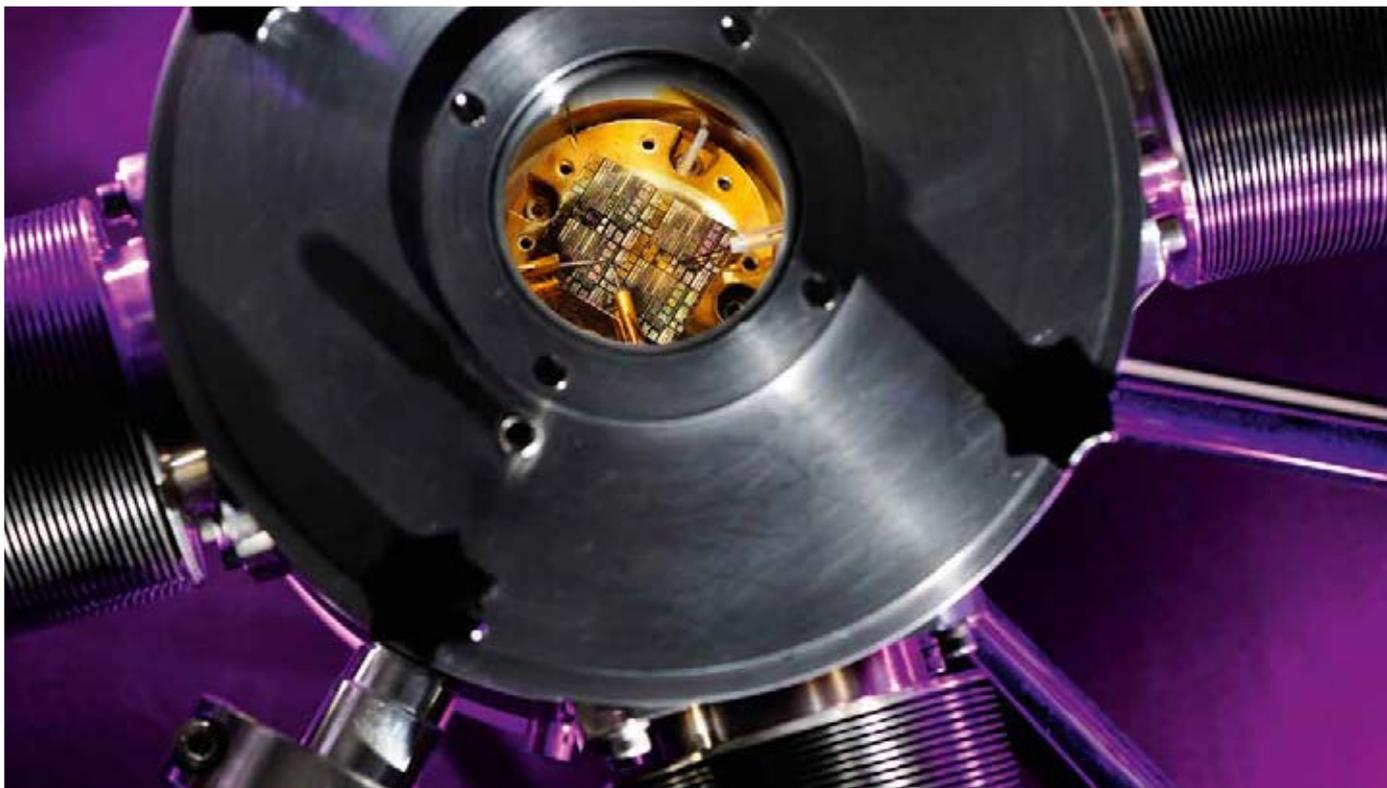
In hybrid solar cells, inorganic (for example, zinc oxide or titanium oxide) and organic (polymer) materials are combined. Such combinations would, in theory, result in high efficiencies. Koster combined experimental work (making and testing these combinations in solar cells) with theoretical work (developing a numerical

model to describe its operation). He also successfully applied his numerical model to all-organic solar cells made by his direct colleagues. It constituted the first consistent description of organic solar cells in terms of materials properties and basic physics.

### Cambridge

After his PhD Koster chose to temporarily leave the organic photovoltaic (OPV) research field as he wanted to widen his horizon. The experimental experience he had acquired while making the inorganic nano-particles was useful in his subsequent post doc position with Neil Greenham at the University of Cambridge. There he investigated charge transport in inorganic nano-particles that he synthesised himself. “I made a wide variety of particles and did a lot of electron microscopy and photolithography work. Like many of my Cambridge colleagues, I was initially overwhelmed by the idea that I could go to Cambridge, a university that has scooped up more Nobel Prizes on its own than entire countries such as France or Germany. Later on, I began to miss the OPV field in general and modelling work in particular. As my papers and thesis generated quite some interest in the field, I decided to move back to OPV and take up a post doc position at Eindhoven University of Technology with René Janssen. Thanks to my DPI network, I knew him well and was really looking forward to working in his group.”

In Eindhoven, in René Janssen’s group Molecular Materials and Nano Systems, he once again worked on organic solar cells, both theoretically and experimentally. Like the group in Groningen, Janssen’s group was working on hybrid cells with zinc oxide as the inorganic component. A DPI PhD student, Svetlana van Bavel, (see page 59 of this annual report), made very detailed 3D electron micro-tomography images, rich in contrast, of the complex morphology in these hybrid cells. Koster’s role in this project was to model the



exciton behaviour in three dimensions in such materials. “For a scientist the data sets based on such images, in which polymer and zinc oxide domains can be distinguished on a sub-nanometre scale, are pure gold. I related them to the efficiency of the cell,” Koster explains. His project was funded by the German Research Foundation (DFG).

Additionally, he developed a new experimental technique for quantifying charge recombination losses in organic solar cells. And even now (his post doc in Eindhoven came to an end late 2010), after having acquired a scholarship grant (VENI) from the Netherlands Organisation of Scientific Research at the University of Groningen, he is still exploiting these same data sets. His goal is to develop an optoelectronic model in which the 3D donor-acceptor morphology is related to the current-voltage characteristics and, hence, the efficiency of organic solar cells. The Eindhoven data set serves as a benchmark for the model. Besides this OPV modelling work, he now also works on light-emitting diodes and charge transport in organic materials. Within the Groningen FOM Focus Group ‘Next Generation OPV’ he has a similar role to play: relating materials properties to solar cell efficiency.

#### **Cross-fertilisation**

DPI has so far been a recurring element in Koster’s career. “When I wrote my proposal for the VENI grant during my Eindhoven period,” he says, “I got help from a few people of my DPI network.” He remembers that delivering the presentation before the deciding committee was more exacting than defending his thesis. But he received the grant and this has enabled him to be independent and pursue his own scientific interests, which range from solar cells to transistors, and from experiments to numerical simulations. In all instances, he aims to relate materials properties and physical processes to device behaviour and performance. By applying for additional funding he has managed to obtain his own PhD students.

What Koster appreciates very much is that DPI, in the person of the programme area coordinator, actively follows how a project progresses. It does so ‘from a distance’, and this detached view enables DPI to make suggestions for improvement that might otherwise have been overlooked by the project members themselves. He remembers that as a result of such suggestions the frequency of project meetings was increased and research groups started to exchange samples to get a better grip on the matter. Cross-fertilisation is an important aim. Koster also greatly

appreciates the fact that DPI keeps in touch with its researchers after their PhD (at least that is what happened in his case).

Koster is still involved in DPI as one of the co-investigators in a project within the Large-Area Thin-Film Electronics technology area. Its objective is to predict the optimal processing conditions of organic bulk heterojunction solar cells, leading to enhanced efficiencies and a drastically reduced optimisation time for large-area solar cells. It is well known that for instance the solvents used for spin casting have a dramatic influence on the morphology and thus on the efficiency of a solar cell. This project aims to identify how morphology formation can be tuned experimentally. Additionally, theoretical models will be used and extended in order to predict, from materials properties, what the resulting morphology looks like if a certain solvent (or solvent combination) is used. These predictions are then verified by electron microscopy studies. The final piece of the puzzle is to set up and verify a numerical model that can then predict solar cell efficiency based on the morphological information. This part of the project is done in Groningen by one of the four PhD students working within this DPI project. Koster supervises the Groningen PhD student, Davide Bartesaghi, who started his PhD in January 2012.

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## 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.

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## 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. Additionally, new materials are explored in the search for a significant improvement in the efficacy (lm/W) of polymer lighting applications. The research focuses on understanding materials and device performance, photo-physics and charge transport of white 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 bulk heterojunction PV. Polymer 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 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 response and/or large displacement upon an external electrical, magnetic, optical and/or chemical trigger. Other focal areas are new materials and devices for selective sensing of gases and bio-fluids as well as the actuating principles of rubber-like materials and corresponding devices.

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## FACTS AND FIGURES

### Partners from industry

- BASF
- DSM
- ECN
- Industrial Technology Research Institute (ITRI), Taiwan
- Merck
- Philips
- Sabic
- Shell
- Solvay
- TNO

### Partners from the research world

- Delft University of Technology
- ECN
- Eindhoven University of Technology
- Imperial College London
- Nanoforce Technology
- Queen Mary & Westfield College, University of London
- University of Bayreuth
- University of Cologne
- University of Duisburg-Essen
- University of Groningen
- University of Münster
- University of Ulm
- University of Wuppertal
- Wageningen University

### Budget and organisation

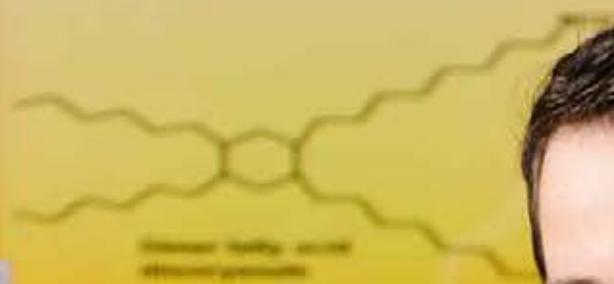
Expenditure in 2011 totalled € 2.72 million (budget: € 2.32 million). A total of € 72k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 26.9 (41 researchers). Prof.dr. Frans De Schryver acted as Scientific Chairman and Dr. John van Haare as Programme Area Coordinator.

### Publications and inventions

The research programme in this technology area generated a total of 41 reviewed papers and one thesis. Three inventions were reported and two patent applications were filed.

For details, see page 73.

## Bio-based polyurethane coatings



- preparation of NCO functional
- neutralization & dispersion
- chain extension with diamines
- high MW polyurethanes in water

/ Chemical Engineering and Chemistry

“The contacts with the partners during my PhD project were quite intense; I still benefit from them.”

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# Bart Noordover

## Waterborne coatings made from renewable resources

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### 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 preparing the coatings industry for future challenges.

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**A little over four years ago he finished his PhD project in the Coatings Technology area of DPI at Eindhoven University of Technology. After a few years in industry, Bart Noordover returned to Eindhoven and is now supervising DPI projects in Coatings Technology and other areas.**

In the DPI annual report of 2006 Bart Noordover, who at that time was completing his PhD project at Eindhoven University of Technology, expressed the wish to continue working with polymers. He preferred to do that in industry rather than at a university. But now, five years later, we find him at the same university in a different role, supervising no fewer than seven PhD projects (including three DPI ones). What happened to his plans to work in industry? "Oh, I have worked in a company," he hastens to say, "but after two years I missed the more scientific approach to polymer chemistry and the educational aspects of working at a university. And then my old group, who were working on step growth polymerisation, asked me whether I was interested in a vacancy in their staff. In the end I found that more appealing than continuing to work in industry."

#### **Open discussions**

At the end of his PhD project Noordover had job interviews with two of the companies involved in the project. A DPI project

always involves more than one industrial partner, he says, and the advantage is that you not only get input from multiple sides, but also have partners who are really committed to cooperation. Moreover, because of the open discussions, the partners get to know how you can be of value to them. He chose for Dow Chemical and worked there for two years, one year in Switzerland and one year in Terneuzen in the Netherlands. "In Switzerland I did several short projects in different research areas and the idea was that I would continue working there. However, due to changes in the organisation of that particular part of the company, I was transferred to Terneuzen. During that last year I was more involved in process technology and less in polymer chemistry, where my heart lies," Noordover says. "But I enjoyed working in a company and it was very instructive to see the differences with doing research at a university. In a company, researchers can be summoned to solve everyday problems, for example when the production process comes to a standstill. The conditions are not as well-defined as in a laboratory experiment, where we often work on a gram scale. Industrial production processes and product formulations need to be much more robust. Even when a mistake is made in the quantity of chemicals added to, for example, a polymerisation reaction, it still has to result in a useful product. These are the kind of things I learned there."

During his two years with Dow, Noordover kept in touch with his former colleagues in the group in Eindhoven in a natural way. Some of them still had to defend their theses and there were joint publications to finish. His contacts with the rest of the DPI community, however, were less frequent, mostly because the field he was working in was different. But after coming back to Eindhoven in 2010, he soon found out that his network was still intact. "The contacts with the partners during my PhD project had been quite intense; we really got to



know one another very well. I still benefit from this,” says Noordover.

The leader of Noordover’s group, Professor Cor Koning, is taking the opposite route; he recently decided to move back to industry and has reduced his activities at the university. Noordover took over the daily supervision of several of Koning’s PhD students. “We have a good group of people now. I want to consolidate that and build up a group of my own with a research portfolio that is interesting from both a scientific and an industrial perspective.”

### **Sustainable**

During his PhD project Noordover worked in the Coatings Technology area on polymeric coatings made from monomers from renewable resources. This involved the preparation and characterisation of linear and branched, fully bio-based polyester and polycarbonate resins. These polymers proved to have suitable chemical and thermal characteristics to be applied in powder coating formulations. To make such coatings, the polymer resins are ground into powders that, mixed with cross-linking agents and other additives, electrostatically adhere to a panel and are then cured in an oven. The polymer reacts with the cross-linker and forms a polymeric network with an extremely high molecular weight. Noordover investigated

whether the renewable resins could be used in toner for printing applications as well as in coatings. He cooperated closely with Agrotechnology and Food Innovations (A&F, currently known as Food and Bio-based Research, part of the Wageningen University and Research Centre), DSM and Océ during the project. The work progressed well and resulted in two patent applications and a number of scientific publications, some of which were written together with partners. Whether the results have turned up in a product in one of companies involved in his project, Noordover is unable to say. “We certainly made materials that DSM, Akzo and Océ were interested in. In some way my results will have had an influence on how these companies proceeded in this field, but it is not always easy to see how exactly research results contribute to further developments in a company.”

The DPI project in the Coatings Technology area that Noordover supervises is also related to biomass-based, sustainable coatings. It has to do with waterborne polyurethane dispersions based on renewable resources. These are non-toxic and non-flammable and contain no organic solvent, which means they are environmentally friendly. The PhD student working on this project, Yingyuan Li, is investigating several monomers from

renewable resources to prepare the polyurethanes. The reactivity and the polarity of the starting materials have to allow for making a dispersion of high molecular weight polymer in water. Noordover: “Recently, Yingyuan has succeeded in making polyurethanes with tunable properties that can indeed be dispersed in water. The molecular weight of the polymers in the dispersion is then increased by a process called chain extension. The resulting coatings show a good impact resistance and can be used for the protection of several types of surfaces in consumer and industrial applications.” The project will be completed next year.

In his new role of assistant professor, which he enjoys very much, Noordover is also involved in other DPI technology areas: Performance Polymers and Bio-Inspired Polymers, where the regular project review meetings are similarly organised and where attention is paid to both chemical and physical aspects of polymer science. He sees a certain amount of overlap between them: “Technology areas can learn from each other. Perhaps it is a good idea to organise more joint meetings where results of overlapping topics in the different technology areas are shared. At the DPI Annual Meeting there is not enough time for such an extensive exchange of information on a project basis.”

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## 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.

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## 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.

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## FACTS AND FIGURES

### **Partners from industry**

- AkzoNobel
- Altana
- Bayer
- DSM
- Evonik
- Saint-Gobain

### **Partners from the research world**

- Eindhoven University of Technology
- Food and Biobased Research, Wageningen UR
- University of Amsterdam
- University of Groningen
- University of Haute-Alsace
- Wageningen University

### **Budget and organisation**

Expenditure in 2011 totalled € 1.09 million (budget: € 1.28 million). A total of € 25k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 9.4 (15 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 four reviewed papers, one thesis and three inventions were reported.

For details, see page 75.

### **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.

“Seeing students grow and contributing to that is an aspect of my work that appeals to me very much.”



# Richard Hoogenboom

## Vehicle becomes research topic

### 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.

**Polyoxazolines, initially chosen as a vehicle to develop new synthetic methods, have stirred a renewed interest and are now one of the main research lines in Richard Hoogenboom's research group at Ghent University.**

"In two weeks' time I will be in San Diego, California," says professor Richard Hoogenboom, head of the Supramolecular Chemistry Group at Ghent University in Belgium. "At the American Chemical Society National Spring Meeting I am co-organising a sub-conference on poly(2-oxazoline)s. These polymers, discovered in the 1960s, fell into oblivion during the 1980s until we breathed new life into them about ten years ago. It so happened that we were using them to validate the *High-Throughput Experimentation* approach." During his PhD and a subsequent post doc position in the group of professor Ulrich S. Schubert at Eindhoven University of Technology, Hoogenboom was involved in getting the Chemspeed robots up and working to accelerate the synthesis of polymers, and poly(2-oxazoline)s were chosen as the vehicle to develop the synthesis methods. His PhD position was not on the payroll of DPI, but the *High-Throughput Experimentation* workflow and many of his direct co-workers were.

### Openness

"With the Chemspeed robots and microwave-assisted synthesis methods we were trying to design more efficient methods for synthesising polymers. If we found such methods, we would be able to synthesise A-B copolymers with different contents of A and B and analyse and optimise their properties. In that way we would be able to relate the properties to the structure of the polymers. We chose the poly(2-oxazoline)s because none of the participating companies in the project – which, besides Chemspeed, included materials companies such as BASF and Dow Chemical – had any business related to these polymers. This allowed the industrial partners to discuss their ideas in all openness," explains Hoogenboom. These poly(2-oxazoline)s appeared to be interesting materials with interesting properties. Now some twenty or thirty research groups all over the world, including four or five industrial ones, are heavily investigating them. At the conference one hundred participants will attend about fifty presentations devoted to these versatile materials. Poly(2-oxazoline)s result from a living polymerisation method. For a long time, there was little interest in them because of their long reaction times, but when these were shortened enormously by microwave-assisted synthesis, their potential use as biomaterials and thermo-responsive materials brought a revival. Although it is an (initially) unintended result of his work with DPI, Hoogenboom can rightly be proud of it.

During his post doc in Schubert's group Hoogenboom spent part of his time in a start-up biomedical company, Dolphys Medical, as a senior product developer. He found the experience useful, but in the end preferred an academic career. In 2008 another post doc period as a Humboldt Fellow at the RWTH in Aachen followed. After that, Hoogenboom got a Veni grant from NWO, the Netherlands Organisation for scientific Research, at the University of Nijmegen, but after eighteen months of



the three year-grant, he received a phone call from Ghent University in Belgium, where six new positions for research group leaders had been established. Professor Filip du Prez, head of the Department of Organic Chemistry, thought that Hoogenboom stood a good chance of getting one of these. He was proved right: Hoogenboom finished first out of 150 candidates. This meant, however, that he had to leave Nijmegen. "The opportunity to set up a research group with complete academic freedom and responsibility for all its ins and outs, was too tempting to resist," says Hoogenboom. When you are appointed to a position as assistant professor in Belgium you have complete freedom to organise your research work. This implies that you have to deal with all aspects, including the financial ones. The money the university receives from the Belgian government is not divided over the faculties in some predisposed way. Research leaders have to submit proposals. "We are not doing badly in that respect," reflects Hoogenboom.

In his research group at Ghent University the poly(2-oxazoline)s research is one of the three research lines. The others are responsive polymers that react to an external trigger, for instance temperature, and supramolecular materials. After eighteen months, his group now consists

of five PhD students and five Master's students. Two more PhD students and two post docs will follow soon. Hoogenboom does not want the group to grow much larger. "I want to walk through the labs and see what everybody is doing, give them some advice and discuss things with them on a regular basis. To be able to do that, the group should not be larger than twenty people. Even in the short time that I have been in Ghent I have seen students grow in their project, contributing to that is an aspect of my work here that appeals to me very much, besides doing interesting research projects." He remains involved in DPI as supervisor for some of the PhD projects in Schubert's group, now part of the University in Jena (Germany). Moreover, thanks to his DPI network he now has a not too expensive, second-hand, but completely refurbished Chemspeed robot at his disposal for the synthesis of polymers.

#### **Building bridges**

Hoogenboom thinks that the DPI scheme of generating research funding is a very efficient way to do not only that but also to contribute to building bridges between universities and companies. The quarters of the project budget that will be contributed by the university and the participating companies together and the doubling of the amount by the government is a way to ensure that everyone is committed. There

are, of course, differences between companies in this respect. The cultural diversity of the people involved in DPI and the different points of view they bring up, on the other hand, is an aspect in DPI that he really values. In summing up where his colleagues of Schubert's group, with whom he still cooperates on an ad hoc basis, ended up, he mentions a large part of Europe. Most of them are professors or assistant professors at universities. Apparently, the large number of publications that each of them has written, thanks to the *High-Throughput Experimentation* research facilities, has increased their chance of getting a position as a professor.

Looking for future research projects Hoogenboom turns to nature to find inspiration for making complex functional assemblies from a limited number of building blocks. Asked for an example, he mentions smart polymers that show self-healing functions in the same way that peptides in the blood ensure that a cut in our finger heals. Smart polymers that have recently been developed in Ghent respond to the amount of sugars present in a solution and can be used as a sensor to continuously measure the sugar content in blood. When such materials are coupled to a system that releases a medicine, for instance insulin for diabetics, biomedical applications come into sight.

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## 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.

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## 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.

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## FACTS AND FIGURES

### Partners from industry

- Chemspeed Technologies
- Evonik
- Forschungs Gesellschaft Kunststoffe
- Michelin
- Microdrop Technologies
- Waters Technologies Corporation

### Partners from the research world

- Deutsches Kunststoff Institut
- Eindhoven University of Technology
- Friedrich-Schiller University, Jena
- Innovent
- University of Amsterdam
- University of Liverpool

### Budget and organisation

Expenditure in 2011 totalled €1.51 million (budget: € 1.59 million). A total of € 79k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 16.9 (32 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 48 reviewed papers and one invention was reported.

For details, see page 75.



“As a researcher in DPI you gain insight into things that are important in industry.”

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# Jules Harings

## The chain of knowledge

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### 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.

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**During his PhD project with DPI, Jules Harings acquired a broad outlook on the whole process leading from scientific research to a commercial product. This experience has certainly had a positive influence on his career.**

The first DPI annual report to mention Jules Harings, now R&D scientist with Teijin Aramid in Arnhem (the Netherlands), was that of 2007. In that year, Harings was two years into his PhD Project at Eindhoven University of Technology. He looks back on this period with pleasure. The project went well and he acquired a lot of experience that turns out to be very beneficial to his present career. He explains what the project was about: “We investigated how polyamides (nylons) can be processed from an aqueous solution with the ultimate goal of making high-performance fibres. High strength and high stiffness go hand in hand with long, crystallised and well-aligned polymer chains. Hydrogen bonding between the polymer chains co-determines these parameters. In the processing phase, however, you do not want any formation of hydrogen bonds in order to prevent the formation of chain-folded polyamide crystals that cannot be unravelled. Nylons can dissolve in water at a high temperature and a high pressure. We were looking for a way to prevent the formation of hydrogen bonds during the cooling down of an aqueous solution by selectively removing the water and the ions, so that the polymers adopt the

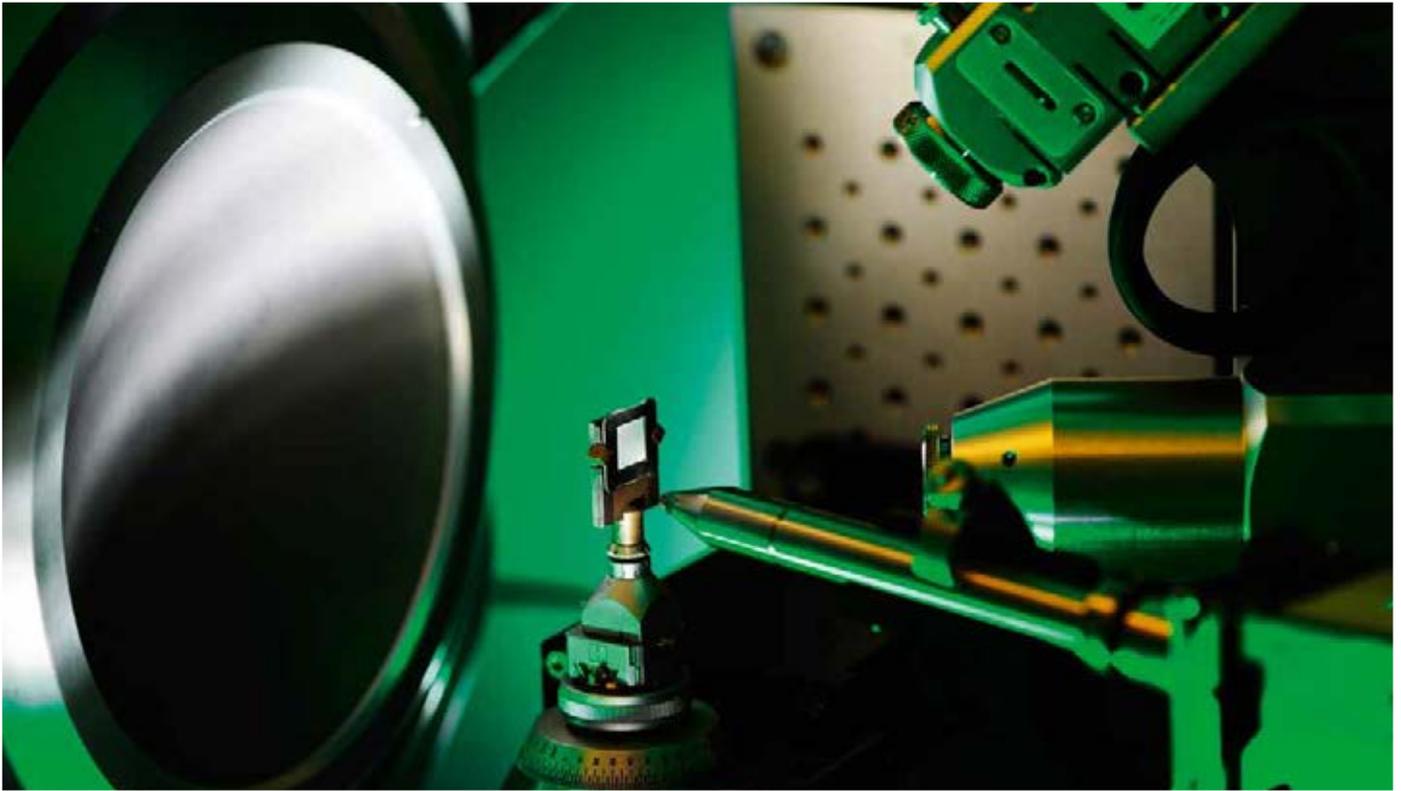
desired crystallised state and form a strong fibre.”

#### Patent

The model systems Harings used did not yet result in a new technology, but gave sufficient insight into the process for the next step to be made in that direction by his successor, Yogesh Deshmukh. A concrete result was a patent that DPI obtained and followed through. Whether this patent will be used directly in one of the companies involved in the project or will be capitalised via DPI Value Centre, he does not know. “Companies are probably not very willing to communicate about that. I can imagine that a company active in the field of polyamides or polymeric fibres would not tell everybody about it, and I would probably be the last person they would talk to, since I am working for one of their competitors and can deduce even from minor details what products they are developing,” says Harings.

It is not only the scientific content of his project that Harings looks back on with pleasure. He greatly values the problem approach and the way of working he learned at the time. He still benefits from it. “In a PhD project you are, of course, focused on one subject, but in Piet Lemstra’s group we were taught to approach a problem in conjunction with what he called the ‘chain of knowledge’. He meant that you had to consider the whole process, from the synthesis of a polymer to the end product made of it. This approach fits an organisation such as DPI like a glove, but that can hardly be a surprise,” Harings laughs. Piet Lemstra is, after all, co-founder of DPI. “The DPI network is a very nice environment to do research because the work is industrially relevant. As a researcher you gain insight into things that are important in industry.”

In his present job at Teijin Aramid, a business unit of Teijin Limited that produces high-performance materials, Harings builds on this view and can use his experience to the full. “I try to keep in touch with the whole process. I can contribute



to discussions on the polymerisation up to and including those on the composite level. This is what I was looking for when I decided to go for a job in an industrial environment after my PhD project.” Harings wanted to work in a team, develop his communicative and organisational skills and at the same time exploit his scientific experience. His idea was that he could make far better use of this combination in an industrial environment than at a university. And he appears to have been right, judging from his career until now. He started as senior researcher working at the interface of two groups, Fibre Physics and New Product Development. In his first year with Teijin he contributed to the development of a new high-performance tape called Endumax® that was recently introduced in the market. In the course of 2012 he will move more towards R&D management. But whatever the future has in store for him, the scientific content of a job must be significant. Harings really wants to be involved in scientific problems and utterly enjoys solving them. “It is very satisfactory when the penny drops and you know that you have taken the right route to solve a problem. I certainly do not want to miss that aspect in a future job. At the same time it is also very rewarding to see the results of your work in a successful product, which is something you definitely miss when you work at a university.”

#### **Award**

Harings’ DPI past was instrumental in finding a job in industry. “For a researcher in a DPI project, the doors to the companies participating in the project are wide open. The companies can take a clear-cut decision about a candidate employee after seeing him or her function for four years. I was invited to give a presentation about my project with DSM and during the project I worked intensively with people from Teijin. Both companies asked me to send in my CV. Maybe the companies have even been more eager and active than I was,” Harings recalls. After considering both companies, Harings eventually chose for Teijin Aramid, a high-performance materials company. This was a logical choice, given his project experience, but that was not the only reason. He also liked the atmosphere and culture at Teijin. It proved to be a good choice for both the company and himself: at Teijin’s annual Research and Technology congress in Tokyo at the end of 2011 Harings received an award for the company’s best research project. “To me this award is a kind of confirmation that my way of working, considering the whole chain, in this case from polymer to composite, is valuable to the company,” Harings adds.

Harings is still involved in DPI, where he occasionally attends meetings in the

Bio-Inspired Polymers technology area. It is important to him to keep up to date with developments at DPI and with trends in its research and projects, and to absorb the knowledge generated there. Apart from that, the personal network is an aspect that plays a role too. “I know DPI well and know what I can get there, not just in *Bio-Inspired Polymers* but also in other technology areas. DPI is important to polymer research in Europe, and I cannot imagine that Teijin would not be involved in it,” says Harings.

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## 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.

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## 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
- Loughborough University
- Max-Planck Institut für Polymerforschung
- Polymer Technology Group, Eindhoven
- University of Maastricht
- University of Leeds

### Budget and organisation

Expenditure in 2011 totalled € 1.09 million (budget: € 1.49 million). A total of € 22k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 8.8 (16 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 eight reviewed papers and two theses.

For details, see page 78.

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.

A woman with short dark hair and glasses, wearing a white button-down shirt, stands in a laboratory. The background is a bright red wall with various pieces of scientific equipment, including what appears to be a distillation or filtration apparatus. The lighting is dramatic, with a strong red glow from the background.

“The 3D morphology of the active layer determines the solar cell efficiency to a large extent.”

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# Svetlana van Bavel

## Controlling morphology is the ultimate goal

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### 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. It is a perfect example of a highly interdisciplinary research area, extending from chemistry and physics to engineering.

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**She knew what she wanted when she came to the Netherlands with a bachelor's degree in chemistry: to be involved in the development of new technologies at a large multinational company. Ten years later, Svetlana van Bavel has attained that goal. Her PhD project with DPI was one of the steps to reach it.**

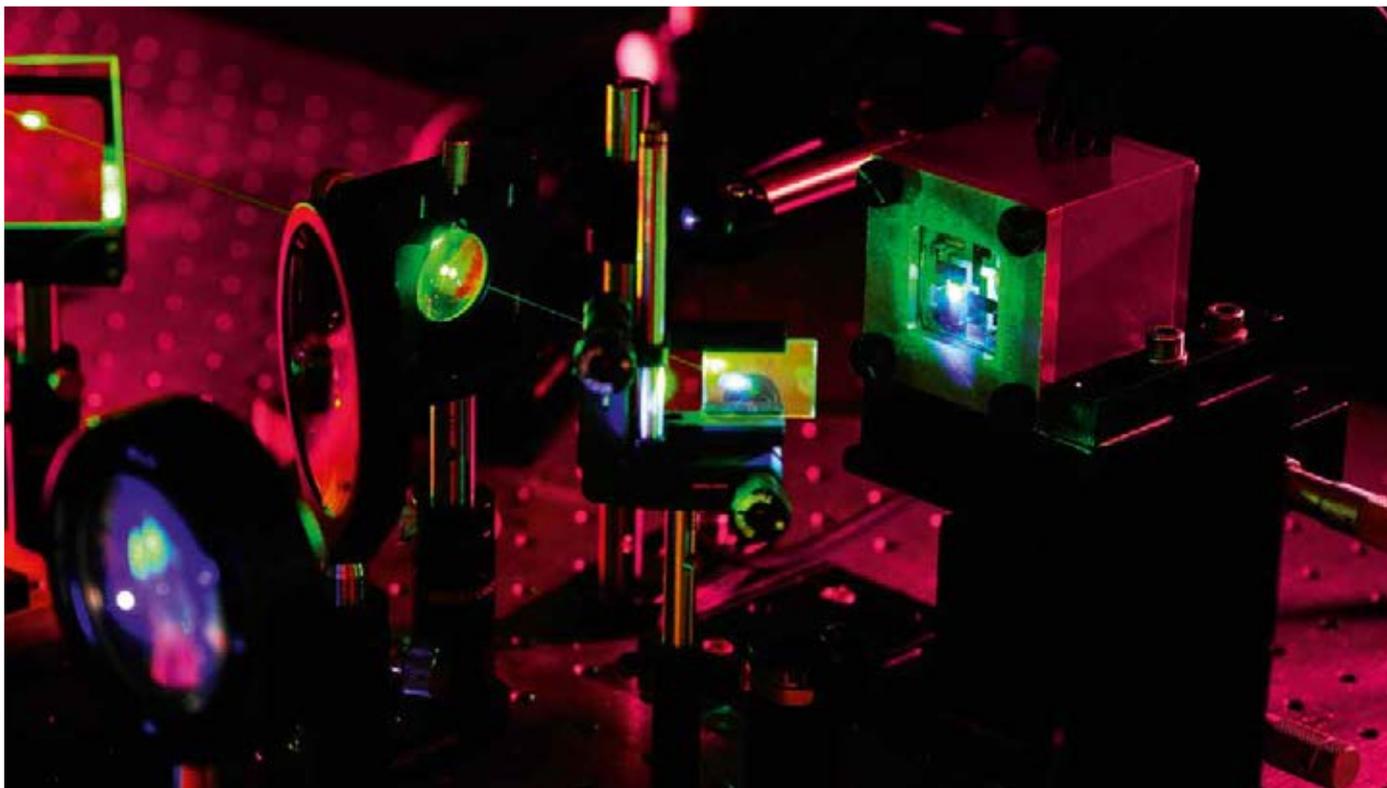
After completing her Bachelor's degree in chemistry in Moscow, Russia, and working in the marketing department of a Moscow-based ICT company for two years, Svetlana van Bavel came to the Netherlands in 2001. "I wanted to acquire experience abroad and I wanted to move back to chemistry. I worked for Océ Technologies for a short period but soon found out that I lacked the necessary experience: I didn't have the in-depth knowledge of a true academic and I didn't have the practical approach of a graduate from a polytechnic either." That is why she decided to continue her education by doing a Master's at Eindhoven University of Technology. Her Master's thesis (which was rated *cum laude*) focused on catalysts for ethylene polymerisation. She investigated whether it was possible to organise the catalysts at the surface instead of using them in solution. Attached to a surface, the catalysts could be more easily

reached by such analytical techniques as X-ray photoelectron spectroscopy and electron microscopy. Even before she finished her Master's, she was approached to do a PhD project with DPI and she accepted.

### Morphology

Electron microscopy played an important role in the project. Van Bavel: "It was about organic photovoltaic cells and that always boils down to improving their efficiency and stability. The choice of the actual materials used in the active layer where the sunlight generates charge carriers plays a role. But the 3D morphology of the materials also determines the efficiency to a large extent. The morphology is in its turn linked to the processing method. For the roll-to-roll production of organic solar cells on a large scale, which is an attractive process because it makes fabrication faster, easier and less expensive, more knowledge about that relationship is needed. I studied this morphology with Transmission Electron Microscopy (more specifically, electron tomography) for several combinations of materials. I found, for instance, that in solar cells made of polythiophene and fullerenes, or 'bucky balls', the way the polymer crystallises is essential. If the polymer crystallises in fibrils a few micrometres in length and ten to twenty nanometres thick and forms a 3D network throughout the active layer, the transport of charge carriers is optimal and efficiency is high. Electron tomography allowed me to reconstruct the volume of a solar cell, that is, to clearly visualise the organisation of donor and acceptor materials in three dimensions, and then quantify the observed 3D structures/networks with the aim of better understanding the relationship between morphology and performance."

Van Bavel also studied hybrid (organic-inorganic) photovoltaic cells, and her 3D images were of great use for the model that Jan Anton Koster made for this type of cells (see page 43 of this annual report).



Van Bavel for her part benefited from Koster's models calculations. "It helped me understand what happened in this system. Together with Stefan Oosterhout, Jan Anton Koster and other researchers from TU Eindhoven, we also cooperated with mathematicians of the University of Ulm in Germany and wrote a few articles together. Things like that broaden your view and your experience. I am grateful to DPI that I had the opportunity to cooperate with so many interesting people. The extensive network of my co-supervisor Dr. Joachim Loos was also very valuable in that respect. All in all, my research and cooperation with others resulted in more than twenty joint papers."

#### **Workhorse**

Van Bavel was very pleased to have the opportunity to work with cutting-edge characterisation techniques; DPI had financed one of the two transmission electron microscopes (TEMs) that she used. "The FEI Tecnai microscope was my workhorse: it is relatively easy to use and it could be applied to solve many questions in my research. When more elaborate measurements were needed, I also used the FEI Titan microscope: one of the very best and elaborate TEMs out there. I was very lucky in this respect: many of my non-DPI colleagues in the department did not have such a generous

share of the available money for their instruments," says Van Bavel. Apart from that financial aspect, she also valued the way of working in DPI. The bi-annual meetings with discussions between academic researchers and industrial partners produced interesting questions and diverse points of view. "I was challenged by people coming from very diverse backgrounds, which was very instructive and valuable," says Van Bavel. "I also appreciated writing the quarterly reports: it takes time but helps to better focus and manage your project."

#### **Low-context country**

Even before defending her thesis (*cum laude*) in 2009, Van Bavel had decided to stay on in the Netherlands. "It is a low-context culture where people mean what they say and say what they mean and that suits me best," she explains. Van Bavel went looking for a research position in a large multinational company. She found a position with Shell, where she is now a Process Engineer Gas To Liquids (GTL) and investigates how natural gas is converted into liquid fuel, first via the formation of high-molecular weight paraffins in Fischer-Tropsch synthesis, followed by their cracking over a catalyst into such products as gas oil or kerosene. She is looking for new, more efficient catalysts and in addition provides technical support

to GTL units in Malaysia and Qatar. Shell is a market leader in GTL technology, which makes it very exciting to work in this field.

Van Bavel applied to Shell via an open application. There were Shell people involved in her DPI project and catching up with them helped her to form a better picture of what working for Shell would be like. "I think it's very important to hear from actual employees what it is like to work at that company; it certainly helps to make up one's mind. I was approached by other partners in my project who had jobs for me, so the DPI network can certainly be helpful in that respect."

The two years that she has now worked with Shell have brought Van Bavel what she expected. "Working in a company you see your results implemented much faster than at a university. In this respect, a company is a more dynamic environment," says Van Bavel. She wants to do her utmost in her job and in the future sees herself growing into a managerial position rather than into a technical expert. "I want to contribute to making the processes and applications that I work on more efficient, more safe and environment-friendly and (ideally) want to see the results of everything I do."

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## 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 of organic electronic devices.

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## FACTS AND FIGURES

### Partners from industry

- BASF
- Evonik
- Philips
- Solvay
- TNO

### Partners from the research world

- Eindhoven University of Technology
- Imperial College London
- University of Algarve
- University of Cologne
- University of Groningen

### Budget and organisation

Expenditure in 2011 totalled € 1.05 million (budget: € 1.70 million). A total of € 18k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 11.8 (18 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 seven reviewed papers and one patent application was filed.

For details, see page 78.

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## SUB-PROGRAMMES

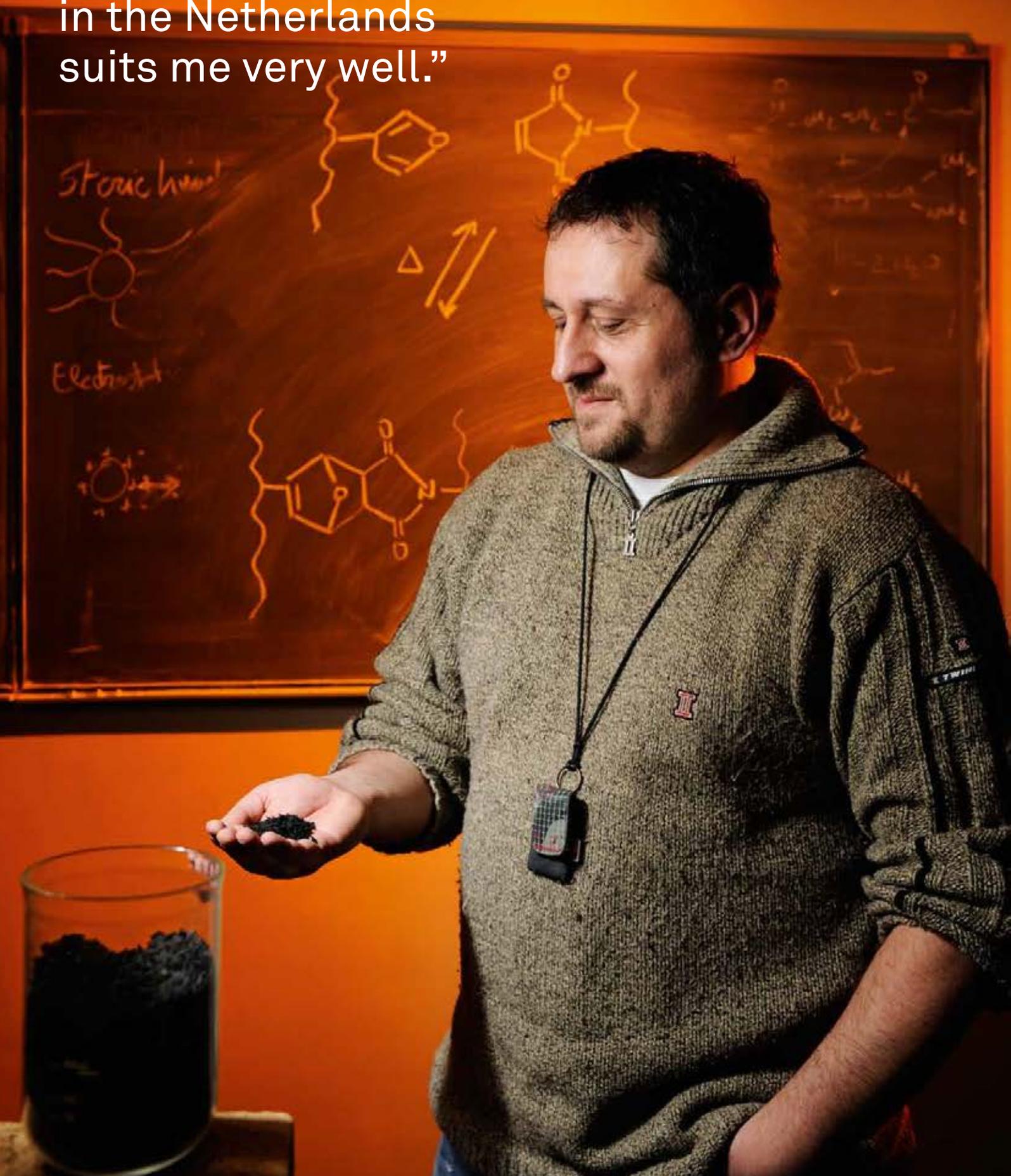
### Large-area material deposition using solution processing

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. Although lab-scale devices have superb performance, we lack the industrial processes and the fundamental knowledge about large-area material deposition from solution 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 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).

“The direct way in which people approach each other in the Netherlands suits me very well.”



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# Francesco Picchioni

## Scientific quality and industrial relevance

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### EMERGING TECHNOLOGIES

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

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**Teaching students and doing research with industrial applications are both aspects of chemical technology that appeal to Francesco Picchioni. DPI made him come from Italy to the Netherlands. He liked it and stayed.**

‘Scientific quality and industrial relevance’ is a combination of words that Francesco Picchioni often uses when talking about DPI. “DPI is a fantastically dynamic institution where scientific quality is combined with industrial relevance in a way that, to my knowledge anyway, is not found anywhere else in the world,” says Picchioni. “Twelve years ago I left Italy, and maybe things have changed in the meantime, but we did not have these consortia of companies and universities that, together with the government, take the financial responsibility to develop new technology and educate students.” His present involvement in DPI is limited to two projects, but he has a history with DPI and in the future he wants to tighten the bonds and submit more project proposals.

#### **Elevator pitch**

Contrary to what Italians do when they are eighteen – ‘staying with their *mamma*’ as Picchioni states – he left his native region, Umbria, to study polymer chemistry in

Pisa, in Tuscany, and did his PhD project at that same university. His project concerned the chemical modification of rubber with the aim of making the rubber better processable and at the same time improve its mechanical properties. It was a project that also involved an Italian company, so he had some experience with industrial cooperation before he came to the Netherlands.

He recalls how he ended up in the Netherlands, even further away from home. “That was a real elevator pitch,” he laughs. “After my PhD I helped to organise a conference in the north of Italy and stood in the elevator with a professor, who later turned out to be Piet Lemstra, the founder of DPI. That was in 1999. He asked me who I was and whether I had completed my thesis. The answers I gave during that short elevator ride, it was literally an elevator pitch, apparently were enough for him to say ‘Come to Eindhoven for a post doc’. My partner and I wanted to move to another country and when a PhD position for her became available in Bert Meijer’s group in Eindhoven, the choice was easy.”

In Lemstra’s group in Eindhoven, Picchioni was once again involved in process technology. He wanted to gain a better fundamental understanding of a process used to modify polypropylene, Hivalloy, to improve its processing properties and make it better suitable for the intended end applications. Three years and four publications later, the process was mastered. Whether this has led to changes in the process on a large scale, Picchioni does not know, but he values the experience gained. “It was really a new world for me,” he says, “and a dynamic one in which collaboration with people from more than one industrial company was the rule. I still had complete academic freedom, but in the discussions with people with different backgrounds and different interests, the suggestions that I received proved very



valuable. The direct way in which people approach each other in the Netherlands suits me very well.” Ten years ago big companies still had large research departments with people who approached a problem in a scientific manner, something that the company Picchioni had cooperated with in Italy did not have. In such consortia it is easier to find the scientific aspects in a request from an industrial partner.

#### **Tenure tracker**

The Netherlands appealed to Picchioni and his partner. They had initially planned to spend a couple of years here, but after his post doc and her PhD project they stayed on. In 2003 Picchioni moved to the University of Groningen, where he is now associate professor in the department of Chemical Technology. Although DPI did not play an active role in getting this position, it would not have happened if Picchioni had not been involved in DPI. He was approached by Professor Jan Teuben, whom he had met during one of the DPI annual meetings and who informed him that a position for a tenure tracker had been created in the Department Chemical Technology at the University of Groningen. At that time Picchioni also had a job offer from a company, but after some thought he applied for the job in Groningen and got selected. Groningen, with its old

buildings, appealed to him more than Eindhoven, he says.

He has never regretted it. “It was clear from the beginning that a lot of teaching was involved in this job, and that initially took a lot of my time. To start with, I had to improve my Dutch. But I really enjoy lecturing and contributing to the education of young people. It is not so much conveying the factual knowledge of chemistry; they can find that in text books. For me, teaching is getting across the attitude of someone with a science background, the way of reasoning that goes with that background. Teaching them the scientific method, that is what I hope to achieve with my students. After all, I received my education in the city where Galileo Galilei was born,” explains Picchioni. Judging from the awards for ‘best lecturer’ adorning the walls of his office, his teaching style seems to strike a chord.

#### **Cradle-to-cradle**

Apart from the lectures he has to give, he really appreciates the freedom that he has in his research projects. At this moment there are two DPI projects in which he is involved together with his boss, Ton Broekhuis. One is in the *Emerging Technology* area about the development of water-soluble polymers

to enhance oil recovery, the other has to do with modifying rubber to make it recyclable among other things – to use it really cradle-to-cradle. “We used a known concept to make a polymer recyclable. That result made it to the pages of the New York Times. Perhaps that same principle can also be used for rubbers. We have only recently started that project, and a PhD student will soon start working on it. Now that I am getting a bit more time, since my lectures no longer take up all the available hours, I want to start new projects with DPI,” says Picchioni.

Asked about his future plans, Picchioni laughs. “I am an Italian! So I am supposed not look beyond tomorrow, and tomorrow I will come here and do what I do today.” When his next evaluation as a tenure tracker turns out positive, he will become professor. At this moment he is associate professor. “But really, I will continue to do what I do now, whether I am professor or not.” He is not really worried about the evaluation, but he still crosses his fingers when talking about it!

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## OBJECTIVES

EMT projects are handled like any other DPI projects. However, after two years a decision will be made on whether the project will be extended for another two years. A condition that has to be met after the first two years is that, apart from the industrial party that started the project, at least one other industrial party is willing to participate. The intellectual property (IP) that is generated in the first two years is owned by all of DPI's partners, as is the case with projects in the Corporate Research technology area. After two years, the project can be absorbed into a separate technology area and IP is treated in the same way as in other technology areas. The focus areas that were identified for EMT in 2011 were Water-Soluble Polymers, Smart Packaging and Advanced Composites. Potential projects in these areas are presently being discussed with industry. However, other opportunities are emerging that would promote the mission of DPI: to study and develop new sustainable polymer technologies in cooperation with industry and academia.

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## FACTS AND FIGURES

### Partners from industry

- Shell
- SNF

### Partners from the research world

- University of Groningen

### Budget and organisation

Expenditure in 2011 totalled € 0.22 million (budget: € 0.43 million). A total of k€ 35 was spent on equipment. The total number of FTEs allocated at year-end 2011 was 1.7 (two researchers). 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 one reviewed paper and one patent application was filed.

For details, see page 79.

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## SUB-PROGRAMMES

The active project in EMT in 2011, involving water-soluble polymers to be used for Enhanced Oil Recovery (EOR) became part of a new technology area, Polymers for EOR. The project, which is being carried out at the University of Groningen, is designed to investigate structure-performance relationships and new polymer structures to improve oil recovery from new and existing reservoirs.

“DPI projects should lead to industrially applicable answers and well-trained researchers in a field useful to industry.”



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# Arjen Bogaerds

## Models for structure-property relationships

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### 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.

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**Facilitating research, including fundamental research, in a direction that is useful to industry – that is DPI’s task according to Arjen Bogaerds, one of the first DPI funded PhD students.**

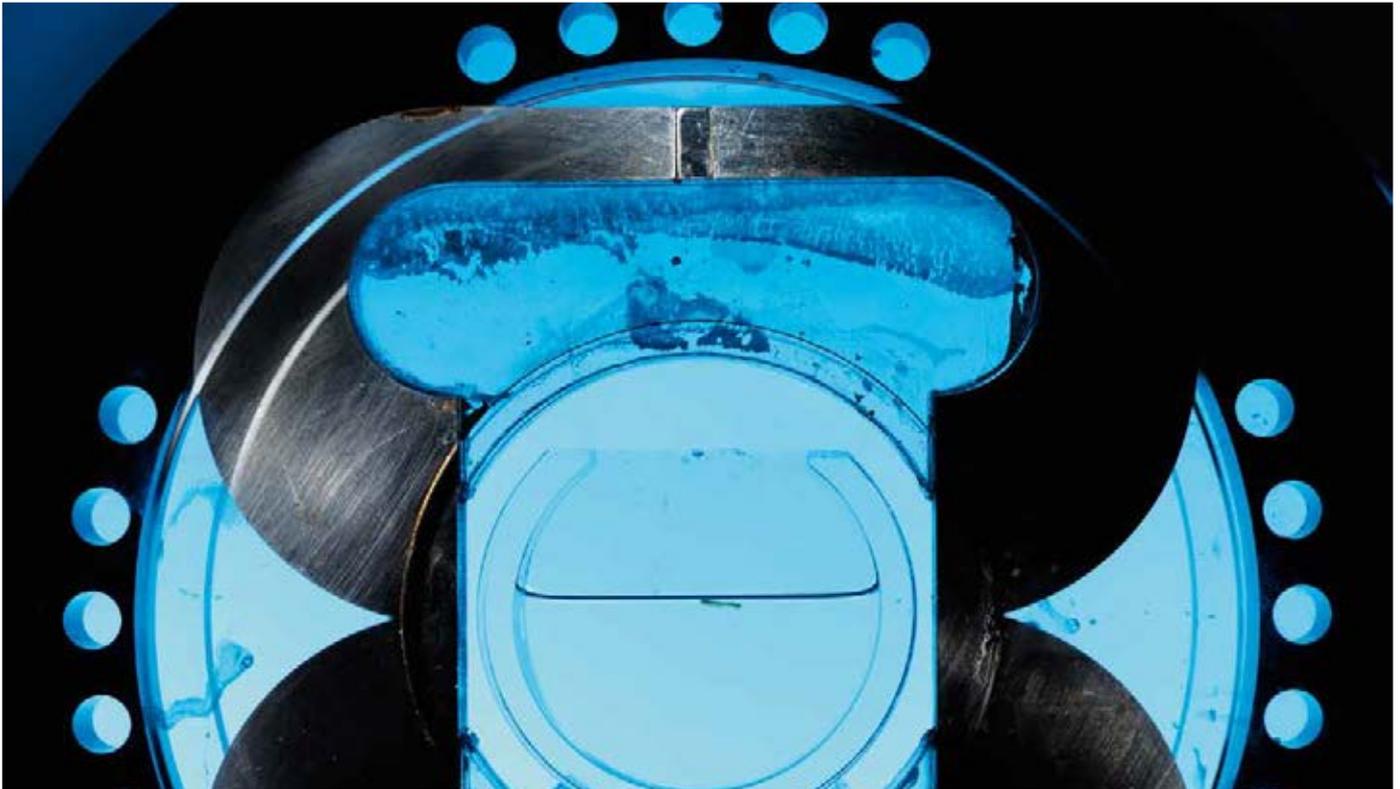
“I was one of DPI’s first PhD students, back in 1998,” remembers Arjen Bogaerds, now research scientist in computational rheology within DSM Ahead. “During my Master’s project in mechanical engineering in the group of Frank Baaijens and Han Meijer at Eindhoven University of Technology, I was involved in developing numerical models for the viscoelastic flow of polymers. When a DPI project was defined to analyse instabilities during the injection moulding of polymers, I was the obvious person to carry it out.” In the large machines used for injection moulding it is hardly possible, if at all, to conduct measurements or observations in the position where the front of the molten polymer leaves the nozzle. Laboratory scale models of such machines, made of for instance glass, can be used to try and retrieve important parameters, and forensic research on the processed products may help to find out what is actually happening. But particularly when the processing speed increases, instabilities occur. Moreover, polymers behave differently from other materials because of their structure, consisting of large chain molecules that deform and relax in the flow. Changing the chain length and the

molecular weight has an influence on the flow. Numerical analysis is one of the tools to address all these aspects in one go. It is not an easy field of research, which explains why it is a very thinly populated discipline.

### Peace

“During the first three years of my project I did not have much contact with the people from DSM who initiated it, but that was hardly surprising,” recalls Bogaerds. “Applicable results did not come into view until the last year. Still, the first three years are important to set the stage. The development of a mathematical model to describe an unstable process with all its details takes time, and not all stages are immediately interesting for the partners. A PhD project is the only period when you have the time and the peace to dive deeply into a subject, and as long as that subject eventually leads to industrially applicable answers and well-trained researchers in a field useful to industry, it is the way to go. For industry it is a way to get people who are knowledgeable in a certain field. I would never have been able to do what I do now if I had been educated in analytical chemistry, for instance.”

That his project succeeded in that respect appears from two things: the DPI Golden Thesis Award that Bogaerds received in 2003 and the fact that after defending his thesis (*cum laude*) he was offered a job with DSM to further develop his model and put it to use. It is a detailed phenomenological model that provides insight into the technology of processing polymers, but the real relationship between chemical structure and fluid dynamics or processing conditions is still unknown. Asked for an example of its use, Bogaerds mentions the high-speed coating of optical fibres with a polymeric resin. Thanks to the insight the model gave, the coating speed could be increased from approximately twelve metres per second to almost thirty metres per second.



## Fibers

After five years with DSM, Bogaerds went back to his university in Eindhoven in the role of assistant professor in the Cardiovascular Biomechanics research group of the BioMedical Technology faculty, where he was also active in the field of rheology. The behaviour of complex fluids is what interests him. He planned to devote part of his time to lecturing and educating students and reserve another part for doing research. Soon after returning to Eindhoven, Bogaerds also became a supervisor in a DPI project in Han Meijer's group. A PhD student, Carina van der Walt, in DPI's Corporate Research technology area is developing a numerical model for fibre spinning. Bogaerds explains what it is about: "Molten polymer is pushed through a small nozzle to form a fibre. If you pull the fibre at a higher velocity than the average velocity inside the nozzle, the fibre is extended as well as reduced in diameter. In this way you can create the fibre that you are aiming at. During this pulling a force is exerted to stretch the polymer chains and you would like to know how the flow properties are affected. All kinds of things may happen: The fibre may break if it is pulled too hard. When it doesn't break, a more interesting flow phenomenon called 'draw resonance' can occur. The result is a varying fibre diameter. The focus of this project is on this

flow instability but now related to a filament that is pulled so hard that the fibre does not start at the nozzle end but it is pulled inward into the nozzle. This changes the dynamics of draw resonance completely and we want to know and understand the limits of stability under this condition. As in the case of large injection moulding machines, it is difficult to directly measure the relevant parameters, so here, too, numerical models are the way to try to master the process."

## Attractive

Bogaerds has continued to supervise this and several other PhD projects at Eindhoven University of Technology since he went back to DSM towards the end of 2011. His motivation to go back to DSM was that the education part of his job in Eindhoven took the greater part of his time and too little time remained for doing research – but he was judged on his research results. "I could blame nobody but myself for my decision to aim for an academic career, but once I knew both sides of the medal, I could make a well-founded choice and went back to industry. DSM welcomed me back (after all, there aren't many experts in numerical modelling), and I could continue where I left off four years ago. A lot of the things I had been working on are still very relevant. The field progresses slowly, not surprising

when there are not so many people active in it," says Bogaerds. The problem is, apparently, to find good researchers and therefore Bogaerds more than once stresses that it is important to interest students not only in this type of work, but in polymer science in general. That should be done before they choose the subject of their academic study. "Maybe DPI should play a more active role in making it more attractive to study polymer science," he muses.

However, what Bogaerds sees as DPI's most important task is making sure that its research projects are attuned to industry's needs and, by doing so, making people with the right background available to work for that industry in the future. Only then will continued cooperation and transfer of project results between universities and industries be guaranteed. Apart from the above-mentioned project, Bogaerds is currently not involved in any other DPI activities, but for the future he expects cooperation between DSM and universities to continue, inside or outside of the framework of DPI.

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## 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.

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## 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.

### Reinforced Polymers

The FOM Foundation formed a partnership with Michelin, SKF and Dutch Polymer Institute (DPI) to gain a better fundamental understanding of how polymers are reinforced by adding fillers. In 2011 the partners signed the contract for this new FOM Industrial Partnership Programme that has a budget of 1.6 million euros. Nearly all 'plastic' objects around us consist of polymers that have been reinforced with fillers to improve their physical properties. The researchers have set their sights high: they want to be the first to make a quantitative connection between the macroscale properties and performances of these reinforced materials and their structure at the molecular level. The partners will jointly deploy a wide range of advanced techniques to study the network structures at the mesoscale.

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## FACTS AND FIGURES

### Partners from industry

- All DPI partners take part in Corporate Research

### Partners from Academia

- Delft University of Technology
- Deutsches Kunststoff Institut
- Eindhoven University of Technology
- ESRF, Grenoble
- Foundation for fundamental research on matter (FOM), Utrecht
- Leibniz-Institut für Polymerforschung, Dresden
- Radboud University, Nijmegen
- Stellenbosch University
- TI Food and Nutrition (TIFN), Wageningen
- University of Amsterdam
- University of Groningen
- University of Naples Federico II
- University of Twente
- Wageningen University

### Budget and organisation

Expenditure in 2011 totalled € 1.92 million (budget: € 2.23 million). A total of € 32k was spent on equipment. The total number of FTEs allocated at year-end 2011 was 16.7 (24 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 21 reviewed papers and two theses. Two inventions were reported and two patent applications were filed.

For details, see page 79.

# Output per area 2011



## POLYOLEFINES

### Projects

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

**#633:** Understanding structure/performance relationships for nonmetallocene olefin polymerization catalysts

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

**#636:** The study of the role of the support, support preparation and initial conditions on olefin polymerisation

**#637:** Role of entanglements on the flow behavior of polyolefins

**#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 VAL\_FIC a model for Flow Induced Crystallization

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

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

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

### Theses

W. Godlieb  
High Pressure Fluidization

J.A. Laverman  
On the hydrodynamics in gas polymerization reactors

A. Pandey  
Non linear viscoelastic response of a thermodynamic metastable polymer melt

E. Tioni  
Optimization of a tool to study the start-up of the gas phase olefin polymerization

### Scientific publications

S. Licciulli, K. Albahily, V. Fomitcheva, I. Korobkov, S. Gambarotta and R. Duchateau  
*A Chromium Ethylidene Complex as a Potent Catalyst for Selective Ethylene Trimerization*  
Angewandte Chemie-International Edition 50(10) 2346-2349

A.V. Chuchuryukin, R.B. Huang, E.E. van Faassen, G.P.M. van Klink, M. Lutz, J.C. Chadwick, A.L. Spek and G. van Koten  
*Mono N,C,N-pincer complexes of titanium, vanadium and niobium. Synthesis, structure and catalytic activity in olefin polymerisation*  
Dalton Transactions 40(35) 8887-8895

G.A. Shamov, G. Schreckenbach and P.H.M. Budzelaar  
*Stability of Hydrocarbons of the Polyhedrane Family Containing Bridged CH Groups: A Case of Failure of the Colle-Salvetti Correlation Density Functionals (vol 6, pg 3442, 2010)*

Journal of Chemical Theory and Computation 7(3) 804-806

T. Taniike, B.T. Nguyen, S. Takahashi, T.Q. Vu, M. Ikeya and M. Terano  
*Kinetic Elucidation of Comonomer-Induced Chemical and Physical Activation in Heterogeneous Ziegler-Natta Propylene Polymerization*  
Journal of Polymer Science Part a-Polymer Chemistry 49(18) 4005-4012

J. Giboz, A.B. Spoelstra, G. Portale, T. Copponnex, H.E.H. Meijer, G.W.M. Peters and P. Mele  
*On the Origin of the "Core-Free" Morphology in Microinjection-Molded HDPE*  
Journal of Polymer Science Part B-Polymer Physics 49(20) 1470-1478

W. Godlieb, N.G. Deen and J.A.M. Kuipers  
*Bubble Behaviour in Fluidised Beds at Elevated Pressures*  
Macromolecular Materials and Engineering 296(3-4) 270-277

A. Pandey, Y. Champouret and S. Rastogi  
*Heterogeneity in the Distribution of Entanglement Density during Polymerization in Disentangled Ultrahigh Molecular Weight Polyethylene*  
Macromolecules 44(12) 4952-4960

A. Pandey, A. Toda and S. Rastogi  
*Influence of Amorphous Component on Melting of Semicrystalline Polymers*  
Macromolecules 44(20) 8042-8055

L. Balzano, S. Rastogi and G. Peters  
*Self-Nucleation of Polymers with Flow: The Case of Bimodal Polyethylene*  
Macromolecules 44(8) 2926-2933

E. Novarino, I.G. Rios, S. van der Veer, A. Meetsma, B. Hessen and M.W. Bouwkamp  
*Catalyst Deactivation Reactions: The Role of Tertiary Amines Revisited*  
Organometallics 30(1) 92-99

A.V. Chuchuryukin, R.B. Huang, M. Lutz, J.C. Chadwick, A.L. Spek and G. van Koten  
*NCN-Pincer Metal Complexes (Ti, Cr, V, Zr, Hf, and Nb) of the Phebox Ligand (S,S)-2,6-Bis(4'-isopropyl-2'-oxazolonyl)phenyl*  
Organometallics 30(10) 2819-2830

G. Ciancaleoni, N. Fraldi, P.H.M. Budzelaar, V. Busico and A. Macchioni  
*Structure and Dynamics in Solution of Bis(phenoxy-amine)Zirconium Catalysts for Olefin Polymerization*  
Organometallics 30(11) 3096-3105

H. Xu, A. Lele and S. Rastogi  
*The influence of carbon-based nanofillers on the melt flow singularity of linear polyethylene*  
Polymer 52(14) 3163-3174

Z. Ma, R.J.A. Steenbakkens, J. Giboz and G.W.M. Peters  
*Using rheometry to determine nucleation density in a colored system containing a nucleating agent*  
Rheologica Acta 50(11-12) 909-915

A. Ginzburg, T. Macko and R. Brull  
*Characterization of Functionalized Polyolefins by High-Temperature Two-Dimensional Liquid Chromatography*  
American Laboratory 43(1) 11-13

A. Greiderer, L. Steeneken, T. Aalbers, G. Vivo-Truyols and P. Schoenmakers  
*Characterization of hydroxypropylmethyl-cellulose (HPMC) using comprehensive two-dimensional liquid chromatography*  
Journal of Chromatography A 1218(34) 5787-5793

M. Finger, J.N.H. Reek and B. de Bruin  
*Role of beta-H Elimination in Rhodium-Mediated Carbene Insertion Polymerization*  
Organometallics 30(5) 1094-1101

## Filed patent application

**#637:** A.V. Pandey, S. Rastogi, G.W.M. Peters, M.S.C. Singh  
Melt extrusion of UHMWPE

## PERFORMANCE POLYMERS

## Projects

**#616:** Flow of particle filled viscoelastic fluids in complex geometries

**#623:** Fundamental aspects of Nano-composites

**#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 grapheme nanosheets 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

**#696:** Self healing thermoplastic polymers based on in-situ solvent deployment

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

## Theses

D. Tang  
Biobased thermoplastic polyurethanes synthesized by isocyanate-based and isocyanate-free routes

R.H.J. Otten  
Self-Organisation of anisometric particles

Y.J. Choi  
Modelling Particulate Complex Flows using XFEM

A.J. Zielinska  
Cross-linking and modification of saturated elastomers using functionalized azides

## Scientific publications

S. Thiyagarajan, L. Gootjes, W. Vogelzang, J. van Haveren, M. Lutz and D.S. van Es  
*Renewable Rigid Diamines: Efficient, Stereospecific Synthesis of High Purity Isohexide Diamines*  
Chemsuschem 4(12) 1823-1829

J. Wu, P. Eduard, S. Thiyagarajan, J. van Haveren, D.S. van Es, C.E. Koning, M. Lutz and C.F. Guerra

*Isohexide Derivatives from Renewable Resources as Chiral Building Blocks*  
Chemsuschem 4(5) 599-603

A.J. Zielinska, J.W.M. Noordermeer, A.G. Talma and M. van Duin  
*Di-azides cross-linked, iPP/EPDM-based thermoplastic vulcanizates*  
European Polymer Journal 47(12) 2311-2320

R.J. Gaymans and A.W. van Swaaij  
*Enhancing the Drawability of a Polyester by Copolymerization with a Second Type of Crystallizable Block*  
Journal of Applied Polymer Science 119(1) 23-30

A.A. Verhoeff, R.H.J. Otten, P. van der Schoot and H.N.W. Lekkerkerker  
*Magnetic field effects on tactoids of plate-like colloids*  
Journal of Chemical Physics 134(4)

R.H.J. Otten and P. van der Schoot  
*Connectivity percolation of polydisperse anisotropic nanofillers*  
Journal of Chemical Physics 134(9)

A.V. Lyulin, D. Hudzinskyy, E. Janiaud and A. Chateauminois  
*Competition of time and spatial scales in polymer glassy dynamics: Rejuvenation and confinement effects*  
Journal of Non-Crystalline Solids 357(2) 567-574

M.G.H.M. Baltussen, Y.J. Choi, M.A. Hulsen and P.D. Anderson  
*Weakly-imposed Dirichlet boundary conditions for non-Newtonian fluid flow*  
Journal of Non-Newtonian Fluid Mechanics 166(17-18) 993-1003

R. Kochetov, A.V. Korobko, T. Andritsch, P.H.F. Morshuis, S.J. Picken and J.J. Smit  
*Modelling of the thermal conductivity in polymer nanocomposites and the impact of the interface between filler and matrix*  
Journal of Physics D-Applied Physics 44(39)

S.J. Picken, A.V. Korobko, E. Mendes, B. Norder, V.V. Makarova, G.B. Vasilyev, V.V. Karbushev and M.Y. Tolstykh  
*Mechanical and thermal properties of polymer micro- and nanocomposites*  
Journal of Polymer Engineering 31(2-3) 269-273

D.L. Tang, B.A.J. Noordover, R.J. Sablong and C.E. Koning  
*Metal-Free Synthesis of Novel Biobased Dihydroxyl-Terminated Aliphatic Polyesters as Building Blocks for Thermoplastic Polyurethanes*

Journal of Polymer Science Part a-Polymer Chemistry 49(13) 2959-2968

E. Janiaud, A. Chateauinois and C. Fretigny  
*Cyclic Nonlinear Behavior of a Glassy Polymer Using a Contact Method*

Journal of Polymer Science Part B-Polymer Physics 49(8) 599-610

L.C.A. van Breemen, E.T.J. Klompen, L.E. Govaert and H.E.H. Meijer  
*Extending the EGP constitutive model for polymer glasses to multiple relaxation times*  
Journal of the Mechanics and Physics of Solids 59(10) 2191-2207

Y.J. Choi and M.A. Hulsen  
*Simulation of extrudate swell using an extended finite element method*  
Korea-Australia Rheology Journal 23(3) 147-154

A.A. Verhoeff, I.A. Bakelaar, R.H.J. Otten, P. van der Schoot and H.N.W. Lekkerkerker  
*Tactoids of Plate-Like Particles: Size, Shape, and Director Field*  
Langmuir 27(1) 116-125

D.L. Tang, D.J. Mulder, B.A.J. Noordover and C.E. Koning  
*Well-defined Biobased Segmented Polyureas Synthesis via a TBD-catalyzed Isocyanate-free Route*  
Macromolecular Rapid Communications 32(17) 1379-1385

G.C. Sanders, T.J.J. Sciarone, H.M.L. Lambermont-Thijs, R. Duchateau and J.P.A. Heuts  
*Methacrylic Stereoblock Copolymers via the Combination of Catalytic Chain Transfer and Anionic Polymerization*  
Macromolecules 44(24) 9517-9528

D. Hudzinsky, A.V. Lyulin, A.R.C. Baljon, N.K. Balabaev and M.A.J. Michels  
*Effects of Strong Confinement on the Glass-Transition Temperature in Simulated Atactic Polystyrene Films*  
Macromolecules 44(7) 2299-2310

G. Galgali, E. Schlangen and S. van der Zwaag  
*Synthesis and characterization of silica microcapsules using a sustainable solvent system template*  
Materials Research Bulletin 46(12) 2445-2449

D. Hudzinsky and A.V. Lyulin  
*Confinement and shear effects for atactic polystyrene film structure and mechanics*  
Modelling and Simulation in Materials Science and Engineering 19(7)

M. Diepens and P. Gijsman  
*Outdoor and accelerated weathering studies of bisphenol A polycarbonate*  
Polymer Degradation and Stability 96(4) 649-652

R.J. Gaymans  
*Segmented copolymers with monodisperse crystallizable hard segments: Novel semi-crystalline materials*  
Progress in Polymer Science 36(6) 713-748

M. Shirazi and J.W.M. Noordermeer  
*Factors Influencing Reinforcement of Nr and Epdm Rubbers with Short Aramid Fibers*  
Rubber Chemistry and Technology 84(2) 187-199

A.J. Zielinska, J.W.M. Noordermeer, A.G. Talma and M. Van Duin  
*Crosslinking of Saturated Elastomers with Diazides. Part I: Mechanical Properties of Vulcanizates*  
Rubber Chemistry and Technology 84(2) 243-257

A.J. Zielinska, J.W.M. Noordermeer, A.G. Talma, R. Peters and M. Van Duin  
*Cross-Linking of Saturated Elastomers with Di-Azides. Part II: Mechanistic Study*  
Rubber Chemistry and Technology 84(2) 258-272

V.M. Litvinov, R.A. Orza, M. Kluppel, M. van Duin and P.C.M.M. Magusin  
*Rubber-Filler Interactions and Network Structure in Relation to Stress-Strain Behavior of Vulcanized, Carbon Black Filled EPDM*  
Macromolecules 44(12) 4887-4900

L. Jasinska, M. Villani, J. Wu, D. van Es, E. Klop, S. Rastogi and C.E. Koning  
*Novel, Fully Biobased Semicrystalline Polyamides*  
Macromolecules 44(9) 3458-3466

M. Finger, J.N.H. Reek and B. de Bruin  
*Role of beta-H Elimination in Rhodium-Mediated Carbene Insertion Polymerization*  
Organometallics 30(5) 1094-1101

S. Thiyagarajan, L. Gootjes, W. Vogelzang, J. Wu, J. van Haveren and D.S. van Es  
*Chiral building blocks from biomass: 2,5-diamino-2,5-dideoxy-1,4-3,6-dianhydroiditol*  
Tetrahedron 67(2) 383-3

### Filed patent application

#648: E.E. Tkalya, C.E. Koning, P.P.A.M. van der Schoot  
Conductive polymer composition

### Reported inventions

#648: E.E. Tkalya, C.E. Koning, P.P.A.M. van der Schoot  
Conductive polymer composition

#656: J. Wu, D.S. van Es, J. van Haveren, C.E. Koning  
Fully bio-based polyesters

#664: M. Shirazi, G.H.P. Ebberink, J.W.M. Noordermeer, A.J. Huis in 't Veld  
Chemical adhesion of aramid fibres to rubber matrices

### FUNCTIONAL POLYMER SYSTEMS

### Projects

#518: Singlet to triplet exciton formation in polymeric light-emitting diodes

#524: Polymer-fullerene solar cells and low band-gap donor materials for photovoltaics

#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 a 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

## Thesis

M.J. Spijkman  
Dual-gate thin-film transistors for logic and sensors

## Scientific publications

S.D. Oosterhout, L.J.A. Koster, S.S. van Bavel, J. Loos, O. Stenzel, R. Thiedmann, V. Schmidt, B. Campo, T.J. Cleij, L. Lutzen, D. Vanderzande, M.M. Wienk and R.A.J. Janssen  
*Controlling the Morphology and Efficiency of Hybrid ZnO:Polythiophene Solar Cells Via Side Chain Functionalization*  
Advanced Energy Materials 1(1) 90-96

M. Kuik, G.J.A.H. Wetzelaer, J.G. Ladde, H.T. Nicolai, J. Wildeman, J. Sweelssen and P.W.M. Blom  
*The Effect of Ketone Defects on the Charge Transport and Charge Recombination in Polyfluorenes*  
Advanced Functional Materials 21(23) 4502-4509

M.J. Spijkman, K. Myny, E.C.P. Smits, P. Heremans, P.W.M. Blom and D.M. de Leeuw  
*Dual-Gate Thin-Film Transistors, Integrated Circuits and Sensors*  
Advanced Materials 23(29) 3231-3242

C.A. Strassert, C.H. Chien, M.D.G. Lopez, D. Kourkoulos, D. Hertel, K. Meerholz and L. De Cola  
*Switching On Luminescence by the Self-Assembly of a Platinum(II) Complex into Gelling Nanofibers and Electroluminescent Films*  
Angewandte Chemie-International Edition 50(4) 946-950

O. Stenzel, H. Hassfeld, R. Thiedmann, L.J.A. Koster, S.D. Oosterhout, S.S. van Bavel, M.M. Wienk, J. Loos, R.A.J. Janssen and V. Schmidt  
*Spatial Modeling of the 3d Morphology of Hybrid Polymer-Zno Solar Cells, Based on Electron Tomography Data*  
Annals of Applied Statistics 5(3) 1920-1947

K. Asadi, P. de Bruyn, P.W.M. Blom and D.M. de Leeuw  
*Origin of the efficiency enhancement in ferroelectric functionalized organic solar cells*  
Applied Physics Letters 98(18) 3301

M. Spijkman, E.C.P. Smits, J.F.M. Cillessen, F. Biscarini, P.W.M. Blom and D.M. de Leeuw  
*Beyond the Nernst-limit with dual-gate ZnO ion-sensitive field-effect transistors*  
Applied Physics Letters 98(4) 3502

M. Kuik, H.T. Nicolai, M. Lenes, G.J.A.H. Wetzelaer, M.T. Lu and P.W.M. Blom  
*Determination of the trap-assisted recombination strength in polymer light emitting diodes*  
Applied Physics Letters 98(9) 3301

G.A.H. Wetzelaer, M. Kuik, M. Lenes and P.W.M. Blom  
*Origin of the dark-current ideality factor in polymer:fullerene bulk heterojunction solar cells*  
Applied Physics Letters 99(15) 3506

H.T. Nicolai, A.J. Hof, M. Lu, P.W.M. Blom, R.J. de Vries and R. Coehoorn  
*Quantitative analysis of the guest-concentration dependence of the mobility in a disordered fluorene-arylamine host-guest system in the guest-to-guest regime*  
Applied Physics Letters 99(20) 3303

M. Kemper, D. Spridon, L.J. van IJendoorn and M.W.J. Prins  
*Interaction of myoglobin with oxidized polystyrene surfaces studied using rotating particles probe*  
European Biophysics Journal with Biophysics Letters 40 50

S.L.M. van Mensfoort, J. Billen, M. Carvelli, S.I.E. Vulto, R.A.J. Janssen and R. Coehoorn  
*Predictive modeling of the current density and radiative recombination in blue polymer-based light-emitting diodes*  
Journal of Applied Physics 109(6) 4502

J.M. Ball, R.K.M. Bouwer, F.B. Kooistra, J.M. Frost, Y.B. Qi, E.B. Domingo, J. Smith, D.M. de Leeuw, J.C. Hummelen, J. Nelson, A. Kahn, N. Stingelin, D.D.C. Bradley and T.D. Anthopoulos  
*Soluble fullerene derivatives: The effect of electronic structure on transistor performance and air stability*  
Journal of Applied Physics 110(1) 4506

M. Carvelli, R.A.J. Janssen and R. Coehoorn  
*Spatial resolution of methods for measuring the light-emission profile in organic light-emitting diodes*  
Journal of Applied Physics 110(8) 4512

I. Stengel, A. Mishra, N. Pootrakulchote, S.J. Moon, S.M. Zakeeruddin, M. Gratzel and P. Bauerle  
*Click-chemistry approach in the design of 1,2,3-triazolyl-pyridine ligands and their Ru(II)-complexes for dye-sensitized solar cells*  
Journal of Materials Chemistry 21(11) 3726-3734

M. Dai, O.T. Picot, N.F. Hughes-Brittain, T. Peijs and C.W.M. Bastiaansen  
*Formation of relief structures on fibres by photo-embossing*  
Journal of Materials Chemistry 21(39) 15527-15531

I. Kanelidis, A. Vaneski, D. Lenkeit, S. Pelz, V. Elsner, R.M. Stewart, J. Rodriguez-Fernandez, A.A. Lutich, A.S. Sussha, R. Theissmann, S. Adamczyk, A.L. Rogach and E. Holder  
*Inorganic-organic nanocomposites of CdSe nanocrystals surface-modified with oligo- and poly(fluorene) moieties*  
Journal of Materials Chemistry 21(8) 2656-2662

S.A. Muntean, M. Kemper, L.J. van IJendoorn and A.V. Lyulin  
*Roughness and Ordering at the Interface of Oxidized Polystyrene and Water*  
Langmuir 27(14) 8678-8686

D.H.K. Murthy, T. Xu, W.H. Chen, A.J. Houtepen, T.J. Savenije, L.D.A. Siebbeles, J.P. Nys, C. Krzeminski, B. Grandidier, D. Stievenard, P. Pareige, F. Jomard, G. Patriarche and O.I. Lebedev  
*Efficient photogeneration of charge carriers in silicon nanowires with a radial doping gradient*  
Nanotechnology 22(31) 5710

A.V. Kyrlyuk, M.C. Hermant, T. Schilling, B. Klumperman, C.E. Koning and P. van der Schoot  
*Controlling electrical percolation in multicomponent carbon nanotube dispersions*  
Nature Nanotechnology 6(6) 364-369

T.M. de Jong, D.K.G. de Boer and C.W.M. Bastiaansen  
*Surface-relief and polarization gratings for solar concentrators*  
Optics Express 19(16) 15127-15142

O.V. Mikhnenko, P.W.M. Blom and M.A. Loi  
*Sensitive triplet exciton detection in polyfluorene using Pd-coordinated porphyrin*  
Physical Chemistry Chemical Physics 13(32) 14453-14456

G.A.H. Wetzelaer, M. Kuik, H.T. Nicolai and P.W.M. Blom  
*Trap-assisted and Langevin-type recombination in organic light-emitting diodes*  
Physical Review B 83(16) 5204

H.T. Nicolai, M.M. Mandoc and P.W.M. Blom  
*Electron traps in semiconducting polymers: Exponential versus Gaussian trap distribution*  
Physical Review B 83(19) 5204

M. Carvelli, R.A.J. Janssen and R. Coehoorn  
*Determination of the exciton singlet-to-triplet ratio in single-layer organic light-emitting diodes*  
Physical Review B 83(7) 5203

W.C. Germs, J.J.M. van der Holst, S.L.M. van Mensfoort, P.A. Bobbert and R. Coehoorn  
*Modeling of the transient mobility in disordered organic semiconductors with a Gaussian density of states*  
Physical Review B 84(16) 5210

G.A.H. Wetzelaer, L.J.A. Koster and P.W.M. Blom  
*Validity of the Einstein Relation in Disordered Organic Semiconductors*  
Physical Review Letters 107(6) 6605

F. Gholamrezaie, K. Asadi, R.A.H.J. Kicken, B.M.W. Langeveld-Voss, D.M. de Leeuw and P.W.M. Blom  
*Controlling charge injection by self-assembled monolayers in bottom-gate and top-gate organic field-effect transistors*  
Synthetic Metals 161(21-22) 2226-2229

### Filed patent applications

**#625:** A. Saha, K. Pacheco, R.P. Sijbesma, D.J. Broer, C.W.M. Bastiaansen  
Ketone sensor

**#679:** C.W.M. Bastiaansen, O.T. Picot, M. Dai, A.A. Peijs  
Substrate with a relief structure

### Reported inventions

**#679:** C.W.M. Bastiaansen, O.T. Picot, M. Dai, A.A. Peijs  
Substrate with a relief structure

**#625:** C-K Chang, C.W.M. Bastiaansen, D.J. Broer, H-L Kuo  
Sensor to discriminate between ethanol and methanol

**#679:** O.T. Picot, C.W.M. Bastiaansen, T. Reynolds, A.A. Peijs  
Optical strain sensor

## COATINGS TECHNOLOGY

### Projects

**#606:** Real-time 3D imaging of microscopic dynamics during film formation.

**#607:** Polycarbonate powder coatings

**#617:** Mobility of water and charge carriers in polymer/oxide/aluminium alloys

**#655:** Fully reversible coating networks

**#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

### Thesis

T.N. Raja  
Fluorescence Spectroscopy and Imaging of Dynamics and Microstructure of Acrylic Polymer Emulsions

### Scientific publications

P. Malanowski, R.A.T.M. van Benthem, L.G.J. van der Ven, J. Laven, S. Kisin and G. de With  
*Photo-degradation of poly(neopentyl isophthalate). Part II: Mechanism of cross-linking*  
Polymer Degradation and Stability 96(6) 1141-1148

M.B. Yagci, S. Bolca, J.P.A. Heuts, W. Ming and G. de With  
*Self-stratifying antimicrobial polyurethane coatings*  
Progress in Organic Coatings 72(3) 305-314

M.B. Yagci, S. Bolca, J.P.A. Heuts, W. Ming and G. de With

*Antimicrobial polyurethane coatings based on ionic liquid quaternary ammonium compounds*

Progress in Organic Coatings 72(3) 343-347

M. Lemmers, I.K. Voets, M.A.C. Stuart and J. van der Gucht  
*Transient network topology of interconnected polyelectrolyte complex micelles*  
Soft Matter 7(4) 1378-1389

### Reported inventions

**#672:** D. Ribena, L.G.J. van de Ven, N. Sommerdijk, G. de With  
N-stearoyldopamine based binders

**#655:** J.A. Loontjens, R. van Calck  
Fully reversible coatings

**#657:** M. Lemmers, M.A.C. Stuart  
Bridging particles by triblock copolymers

## 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

- #667:** Advanced copolymer analysis by MALDI TOF/TOF-MS/MS
- #668:** Microwave-assisted synthesis of polyamides from amines and carboxylic acids
- #669:** HT discovery of polymers for ambient temperature H<sub>2</sub> storage
- #670:** Mechanical screening method a films for combinatorial compounding
- #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
- Scientific publications**
- A. Teichler, R. Eckardt, S. Hoepfner, C. Friebe, J. Perelaer, A. Senes, M. Morana, C.J. Brabec and U.S. Schubert  
*Combinatorial Screening of Polymer: Fullerene Blends for Organic Solar Cells by Inkjet Printing*  
Advanced Energy Materials 1(1) 105-114
- A. Winter, S. Hoepfner, G.R. Newkome and U.S. Schubert  
*Terpyridine-Functionalized Surfaces: Redox-Active, Switchable, and Electroactive Nanoarchitectures*  
Advanced Materials 23(31) 3484-3498
- A. Winter, M.D. Hager, G.R. Newkome and U.S. Schubert  
*The Marriage of Terpyridines and Inorganic Nanoparticles: Synthetic Aspects, Characterization Techniques, and Potential Applications*  
Advanced Materials 23(48) 5728-5748
- A. Chojnacka, A. Ghaffar, A. Feilden, K. Treacher, H.G. Janssen and P. Schoenmakers  
*Pyrolysis-gas chromatography-mass spectrometry for studying N-vinyl-2-pyrrolidone-co-vinyl acetate copolymers and their dissolution behaviour*  
Analytica Chimica Acta 706(2) 305-311
- H.M.L. Lambermont-Thijs, M.W.M. Fijten, U.S. Schubert and R. Hoogenboom  
*Star-shaped Poly(2-oxazoline)s by Dendrimer Endcapping*  
Australian Journal of Chemistry 64(8) 1026-1032
- K. Babiuch, R. Wyrwa, K. Wagner, T. Seemann, S. Hoepfner, C.R. Becer, R. Linke, M. Gottschaldt, J. Weisser, M. Schnabelrauch and U.S. Schubert  
*Functionalized, Biocompatible Coating for Superparamagnetic Nanoparticles by Controlled Polymerization of a Thioglycosidic Monomer*  
Biomacromolecules 12(3) 681-691
- K. Kempe, C. Weber, K. Babiuch, M. Gottschaldt, R. Hoogenboom and U.S. Schubert  
*Responsive Glyco-poly(2-oxazoline)s: Synthesis, Cloud Point Tuning, and Lectin Binding*  
Biomacromolecules 12(7) 2591-2600
- M. Meiland, T. Liebert, A. Baumgaertel, U.S. Schubert and T. Heinze  
*Alkyl beta-D-cellulosides: non-reducing cellulose mimics*  
Cellulose 18(6) 1585-1598
- R. Siebert, F. Schlutter, A. Winter, M. Presselt, H. Gols, U.S. Schubert, B. Dietzek and J. Popp  
*Ruthenium(II)-bis(4'-(4-ethynylphenyl)-2,2':6';2''-terpyridine) - A versatile synthon in supramolecular chemistry. Synthesis and characterization*  
Central European Journal of Chemistry 9(6) 990-999
- A. Winter, G.R. Newkome and U.S. Schubert  
*Catalytic Applications of Terpyridines and their Transition Metal Complexes*  
Chemcatchem 3(9) 1384-1406
- C. Pietsch, U.S. Schubert and R. Hoogenboom  
*Aqueous polymeric sensors based on temperature-induced polymer phase transitions and solvatochromic dyes*  
Chemical Communications 47(31) 8750-8765
- M. Glassner, K. Kempe, U.S. Schubert, R. Hoogenboom and C. Barner-Kowollik  
*One-pot synthesis of cyclopentadienyl endcapped poly(2-ethyl-2-oxazoline) and subsequent ambient temperature Diels-Alder conjugations*  
Chemical Communications 47(38) 10620-10622
- A. Wild, A. Winter, F. Schlutter and U.S. Schubert  
*Advances in the field of pi-conjugated 2,2':6';2''-terpyridines*  
Chemical Society Reviews 40(3) 1459-1511
- F. Kloss, U. Kohn, B.O. Jahn, M.D. Hager, H. Gols and U.S. Schubert  
*Metal-Free 1,5-Regioselective Azide-Alkyne [3+2]-Cycloaddition*  
Chemistry-an Asian Journal 6(10) 2816-2824
- B. Happ, G.M. Pavlov, E. Altuntas, C. Friebe, M.D. Hager, A. Winter, H. Gols, W. Gunther and U.S. Schubert  
*Self-Assembly of 3,6-Bis(4-triazolyl)-pyridazine Ligands with Copper(I) and Silver(I) Ions: Time-Dependant 2D-NOESY and Ultracentrifuge Measurements*  
Chemistry-an Asian Journal 6(3) 873-880
- T.S. Druzhinina, N. Herzer, S. Hoepfner and U.S. Schubert  
*Formation of Iron Oxide Particles by Reduction with Hydrazine*  
Chemphyschem 12(4) 781-784
- V.V. Rajan, B. Steinhoff, I. Alig, R. Waber and J. Wieser  
*Online Monitoring of the Influence of the Chemical Structure of Hindered Amines on the Hydrolysis of Polycarbonate in a Polycarbonate/Poly(acrylonitrile-butadiene-styrene) Blend by Ultraviolet-Visible Spectroscopy*  
Journal of Applied Polymer Science 119(1) 491-499
- A. Baumgaertel, C. Weber, N. Fritz, G. Festag, E. Altuntas, K. Kempe, R. Hoogenboom and U.S. Schubert  
*Characterization of poly(2-oxazoline) homo- and copolymers by liquid chromatography at critical conditions*  
Journal of Chromatography A 1218(46) 8370-8378
- R. Edam, S. Eeltink, D.J.D. Vanhoutte, W.T. Kok and P.J. Schoenmakers  
*Hydrodynamic chromatography of macromolecules using polymer monolithic columns*  
Journal of Chromatography A 1218(48) 8638-8645
- T. Druzhinina, S. Hoepfner, N. Herzer and U.S. Schubert  
*Fabrication of ring structures by anodization lithography on self-assembled OTS monolayers*  
Journal of Materials Chemistry 21(24) 8532-8536
- R. Siebert, C. Hunger, J. Guthmuller, F. Schlutter, A. Winter, U.S. Schubert, L. Gonzalez, B. Dietzek and J. Popp  
*Direct Observation of Temperature-Dependent Excited-State Equilibrium in Dinuclear Ruthenium Terpyridine Complexes Bearing Electron-Poor Bridging Ligands*  
Journal of Physical Chemistry C 115(25) 12677-12688
- M.M. Bloksma, S. Rogers, U.S. Schubert and R. Hoogenboom  
*Main-Chain Chiral Poly(2-oxazoline)s: Influence of Alkyl Side-chain on Secondary Structure Formation in Solution*

- Journal of Polymer Science Part a-Polymer Chemistry 49(13) 2790-2801
- A. Can, S. Hoepfner, P. Guillet, J.F. Gohy, R. Hoogenboom and U.S. Schubert  
*Upper Critical Solution Temperature Switchable Micelles Based on Polystyrene-block-poly(methyl acrylate) Block Copolymers*  
Journal of Polymer Science Part a-Polymer Chemistry 49(17) 3681-3687
- M.A.M. Mballa, U.S. Schubert, J.P.A. Heuts and A.M. Van Herk  
*Automated Batch Emulsion Copolymerization of Styrene and Butyl Acrylate*  
Journal of Polymer Science Part a-Polymer Chemistry 49(2) 314-326
- F. Schlutter, G.M. Pavlov, J.F. Gohy, A. Winter, A. Wild, M.D. Hager, S. Hoepfner and U.S. Schubert  
*Synthesis, Characterization, and Micellization Studies of Coil-Rod-Coil and ABA Ruthenium(II) Terpyridine Assemblies with pi-Conjugated Electron Acceptor Systems*  
Journal of Polymer Science Part a-Polymer Chemistry 49(6) 1396-1408
- A.R. Liberski, J.T. Delaney, H. Schafer, J. Perelaer and U.S. Schubert  
*Organ Weaving: Woven Threads and Sheets As a Step Towards a New Strategy for Artificial Organ Development*  
Macromolecular Bioscience 11(11) 1491-1498
- K. Babiuch, C.R. Becer, M. Gottschaldt, J.T. Delaney, J. Weisser, B. Beer, R. Wyrwa, M. Schnabelrauch and U.S. Schubert  
*Adhesion of Preosteoblasts and Fibroblasts onto Poly(pentafluorostyrene)-Based Glycopolymers and their Biocompatibility*  
Macromolecular Bioscience 11(4) 535-548
- L. Tauhardt, K. Kempe, K. Knop, E. Altuntas, M. Jager, S. Schubert, D. Fischer and U.S. Schubert  
*Linear Polyethyleneimine: Optimized Synthesis and Characterization - On the Way to "Pharmagrade" Batches*  
Macromolecular Chemistry and Physics 212(17) 1918-1924
- S. Daus, K. Petzold-Welcke, M. Kotteritzsch, A. Baumgaertel, U.S. Schubert and T. Heinze  
*Homogeneous Sulfation of Xylan from Different Sources*  
Macromolecular Materials and Engineering 296(6) 551-561
- M.M. Bloksma, U.S. Schubert and R. Hoogenboom  
*Poly(cyclic imino ether)s Beyond 2-Substituted-2-oxazolines*  
Macromolecular Rapid Communications 32(18) 1419-1441
- K. Kempe, R. Hoogenboom and U.S. Schubert  
*A Green Approach for the Synthesis and Thiol-ene Modification of Alkene Functionalized Poly(2-oxazoline)s*  
Macromolecular Rapid Communications 32(18) 1484-1489
- M.M. Bloksma, C. Weber, I.Y. Perevyazko, A. Kuse, A. Baumgaertel, A. Vollrath, R. Hoogenboom and U.S. Schubert  
*Poly(2-cyclopropyl-2-oxazoline): From Rate Acceleration by Cyclopropyl to Thermo-responsive Properties*  
Macromolecules 44(11) 4057-4064
- H.M.L. Lambermont-Thijs, M.W.M. Fijten, A.J. van der Linden, B.M. van Lankvelt, M.M. Bloksma, U.S. Schubert and R. Hoogenboom  
*Efficient Cationic Ring-Opening Polymerization of Diverse Cyclic Imino Ethers: Unexpected Copolymerization Behavior*  
Macromolecules 44(11) 4320-4325
- K. Kempe, C.R. Becer and U.S. Schubert  
*Microwave-Assisted Polymerizations: Recent Status and Future Perspectives*  
Macromolecules 44(15) 5825-5842
- B. Happ, J. Schafer, R. Menzel, M.D. Hager, A. Winter, J. Popp, R. Beckert, B. Dietzek and U.S. Schubert  
*Synthesis and Resonance Energy Transfer Study on a Random Terpolymer Containing a 2-(Pyridine-2-yl)thiazole Donor-Type Ligand and a Luminescent [Ru(bpy)(2)(2-(triazol-4-yl)pyridine)](2+) Chromophore*  
Macromolecules 44(16) 6277-6287
- K. Kempe, R. Hoogenboom, M. Jaeger and U.S. Schubert  
*Three-Fold Metal-Free Efficient ("Click") Reactions onto a Multifunctional Poly(2-oxazoline) Designer Scaffold*  
Macromolecules 44(16) 6424-6432
- G.M. Pavlov, I.Y. Perevyazko, O.V. Okatova and U.S. Schubert  
*Conformation parameters of linear macromolecules from velocity sedimentation and other hydrodynamic methods*  
Methods 54(1) 124-135
- G.R. Whittell, M.D. Hager, U.S. Schubert and I. Manners  
*Functional soft materials from metallopolymers and metallosupramolecular polymers*  
Nature Materials 10(3) 176-188
- K. Albahily, Z. Ahmed, S. Gambarotta, E. Koc, R. Duchateau and I. Korobkov  
*New Iminophosphonamide Chromium(II) Complexes as Highly Active Polymer-Free Ethylene Oligomerization Catalysts*  
Organometallics 30(21) 6022-6027
- R. Siebert, A. Winter, U.S. Schubert, B. Dietzek and J. Popp  
*The molecular mechanism of dual emission in terpyridine transition metal complexes-ultrafast investigations of photoinduced dynamics*  
Physical Chemistry Chemical Physics 13(4) 1606-1617
- A. Baumgaertel, K. Scheubert, B. Pietsch, K. Kempe, A.C. Crecelius, S. Bocker and U.S. Schubert  
*Analysis of different synthetic homopolymers by the use of a new calculation software for tandem mass spectra*  
Rapid Communications in Mass Spectrometry 25(12) 1765-1778
- A.C. Crecelius, T. Alexandrov and U.S. Schubert  
*Application of matrix-assisted laser desorption/ionization mass spectrometric imaging to monitor surface changes of UV-irradiated poly(styrene) films*  
Rapid Communications in Mass Spectrometry 25(19) 2809-2814
- J.M. Kranenburg, M. Van Duin and U.S. Schubert  
*High-Throughput Kinetic Study of Peroxide Curing of Epdm Rubber*  
Rubber Chemistry and Technology 84(1) 101-113
- I.Y. Perevyazko, J.T. Delaney, A. Vollrath, G.M. Pavlov, S. Schubert and U.S. Schubert  
*Examination and optimization of the self-assembly of biocompatible, polymeric nanoparticles by high-throughput nanoprecipitation*  
Soft Matter 7(10) 5030-5035
- S. Schubert, J.T. Delaney and U.S. Schubert  
*Nanoprecipitation and nanoformulation of polymers: from history to powerful possibilities beyond poly(lactic acid)*  
Soft Matter 7(5) 1581-1588
- C. Guerrero-Sanchez, D. Wouters, S. Hoepfner, R. Hoogenboom and U.S. Schubert  
*Micellar dye shuttle between water and an ionic liquid*  
Soft Matter 7(8) 3827-3833
- A. Teichler, R. Eckardt, C. Friebe, J. Perelaer and U.S. Schubert  
*Film formation properties of inkjet printed poly(phenylene-ethynylene)-poly(phenylene-vinylene)s*  
Thin Solid Films 519(11) 3695-3702

E.F.J. Rettler, H.M.L. Lambermont-Thijs, J.M. Kranenburg, R. Hoogenboom, M.V. Unger, H.W. Siesler and U.S. Schubert  
*Water uptake of poly(2-N-alkyl-2-oxazoline)s: influence of crystallinity and hydrogen-bonding on the mechanical properties*  
Journal of Materials Chemistry 21(43) 17331-17337

## Reported invention

**#690:** U.S. Schubert, S. Hoepfner, U. Mansfeld  
Observation method by TEM or SEM

## BIO-INSPIRED POLYMERS

### Projects

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

**#602:** Collagen inspired self-organizing materials

**#604:** Biomimetic polymers for the encapsulation of functional entities

**#608:** High molecular weight aliphatic polyesters by enzymatic polymerization for medical applications

**#609:** Advanced materials based on cellulose via novel reaction processes

**#610:** Combined MESAB/MIMICKNAT proposal

**#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

## Theses

G.J.M. Habraken  
Functional Polypeptides Obtained by Living Ring Opening Polymerizations of N-Carboxyanhydrides

P.J. Skrzeseweska  
Collagen-inspired self-assembling materials

## Scientific publications

G.J.M. Habraken, M. Peeters, P.D. Thornton, C.E. Koning and A. Heise  
*Selective Enzymatic Degradation of Self-Assembled Particles from Amphiphilic Block Copolymers Obtained by the Combination of N-Carboxyanhydride and Nitroxide-Mediated Polymerization*  
Biomacromolecules 12(10) 3761-3769

I. van der Meulen, Y.Y. Li, R. Deumens, E.A.J. Joosten, C.E. Koning and A. Heise  
*Copolymers from Unsaturated Macrolactones: Toward the Design of Cross-Linked Biodegradable Polyesters*  
Biomacromolecules 12(3) 837-843

P.J. Skrzeseweska, L.N. Jong, F.A. de Wolf, M.A.C. Stuart and J. van der Gucht  
*Shape-Memory Effects in Biopolymer Networks with Collagen-Like Transient Nodes*  
Biomacromolecules 12(6) 2285-2292

B. Yeniad, H. Naik, R.J. Amir, C.E. Koning, C.J. Hawker and A. Heise  
*Encoded dendrimers with defined chiral composition via 'click' reaction of enantiopure building blocks*  
Chemical Communications 47(35) 9870-9872

I. van der Meulen, E. Gubbels, S. Huijser, R. Sablong, C.E. Koning, A. Heise and R. Duchateau  
*Catalytic Ring-Opening Polymerization of Renewable Macrolactones to High Molecular Weight Polyethylene-like Polymers*  
Macromolecules 44(11) 4301-4305

Z.W. Deng, G.J.M. Habraken, M. Peeters, A. Heise, G. de With and N.A.J.M. Sommerdijk  
*Fluorescein functionalized random amino acid copolymers in the biomimetic synthesis of CaCO<sub>3</sub>*  
Soft Matter 7(20) 9685-9694

L. Jasinska, M. Villani, J. Wu, D. van Es, E. Klop, S. Rastogi and C.E. Koning  
*Novel, Fully Biobased Semicrystalline Polyamides*  
Macromolecules 44(9) 3458-3466

E.F.J. Rettler, H.M.L. Lambermont-Thijs, J.M. Kranenburg, R. Hoogenboom, M.V. Unger, H.W. Siesler and U.S. Schubert  
*Water uptake of poly(2-N-alkyl-2-oxazoline)s: influence of crystallinity and hydrogen-bonding on the mechanical properties*  
Journal of Materials Chemistry 21(43) 17331-17337

## 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 diffusion barrier systems (POLYMOBAS).

**#665:** Composite stacked organic semiconductors: materials processing towards large area organic electronics.

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

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

**#735:** Solution-processable low-temperature oxide semiconductors for large area electronics (S-PLORE)

### Scientific publications

M.T. Lu, H.T. Nicolai, G.J.A.H. Wetzelaer and P.W.M. Blom  
*N-type doping of poly(p-phenylene vinylene) with air-stable dopants*  
Applied Physics Letters 99(17)

L. Yu, X. Li, E. Pavlica, M.A. Loth, J.E. Anthony, G. Bratina, C. Kjellander, G. Gelinck and N. Stingelin  
*Single-step solution processing of small-molecule organic semiconductor field-effect transistors at high yield*  
Applied Physics Letters 99, 263304

B.J. Brasjen, A.W. van Cuijk and A.A. Darhuber  
*Dip-coating of chemically patterned surfaces*  
Chemical Engineering and Processing 50(5-6) 565-568

J.A.V. Salas and A.A. Darhuber  
*Evaporation of liquids on chemically patterned surfaces*  
Chemical Engineering and Processing 50(5-6)  
583-588

R.Z. Rogowski, A. Dzwilewski, M. Kemerink and A.A. Darhuber  
*Solution Processing of Semiconducting Organic Molecules for Tailored Charge Transport Properties*  
Journal of Physical Chemistry C 115(23)  
11758-11762

M.T. Lu, H.T. Nicolai, G.J.A.H. Wetzelaer and P.W.M. Blom  
*Effect of n-type Doping on the Hole Transport in Poly(p-phenylene vinylene)*  
Journal of Polymer Science Part B-Polymer Physics 49(24) 1745-1749

M.T. Lu, H.T. Nicolai, M. Kuik, G.J.A.H. Wetzelaer, J. Wildeman, A. Palmaerts and P.W.M. Blom  
*Polymer light-emitting diodes with doped hole-transport layers*  
Physica Status Solidi a-Applications and Materials Science 208(10) 2482-2487

### Filed patent application

#640: A. A. Darhuber, P.R. Bloemen, J.M. van der Veen, J.A. Vieyra Salas  
Method for controlling deposition

### EMERGING TECHNOLOGIES

#### Projects

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

#736: Relating Polymer Rheology to Apparent Viscosity in Poreus Media

#### Scientific publication

D.A.Z. Wever, F. Picchioni and A.A. Broekhuis  
*Polymers for enhanced oil recovery: A paradigm for structure-property relationship in aqueous solution*  
Progress in Polymer Science 36(11)  
1558-1628

#### Filed patent application

#716: D.A.Z. Wever, F. Picchioni, A.A. Broekhuis  
Enhanced oil recovery using polyacrylamides

### CORPORATE TECHNOLOGY

#### Projects

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

#597: Ultra-performance polymer separations

#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

#692: Reading (Bio-) Macromolecules with Tip-Enhanced Raman Spectroscopy (TERS) Imaging: on the way to local sequencing

#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

#702: Immobilization of molecular catalysts on well-defined flat model surfaces

#715: Novel Polyimide Architectures: Towards Membranes with Tunable Transport Properties PEI-Mem

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

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

#727: Improved characterization SACCHAR techniques for branched polymers

### Bio-Related Materials Programme (In collaboration with FOM and TiFN)

#719: Unravelling the lipid-amylose inclusion complex formation

#720: Nano mechanical 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

### Theses

M. Al-Samman  
Development Well Defined Branched Architectures For Method Development in Polymer Characterization

A. Khalyavina  
Synthesis of Well Defined Branched Architectures for Method Development in Polymer Characterization

### Scientific publications

S.J. Mu, T. Al-Samman, V. Mohles and G. Gottstein  
*Cluster type grain interaction model including twinning for texture prediction: Application to magnesium alloys*  
Acta Materialia 59(18) 6938-6948

- J.J. Jonas, S.J. Mu, T. Al-Samman, G. Gottstein, L. Jiang and E. Martin  
*The role of strain accommodation during the variant selection of primary twins in magnesium*  
Acta Materialia 59(5) 2046-2056
- S.S. van Berkel, M.B. van Eldijk and J.C.M. van Hest  
*Staudinger Ligations as a Method for Bioconjugation*  
Angewandte Chemie-International Edition 50(38) 8806-8827
- E. Uliyanchenko, P.J. Schoenmakers and S. van der Wal  
*Fast and efficient size-based separations of polymers using ultra-high-pressure liquid chromatography*  
Journal of Chromatography A 1218(11) 1509-1518
- E. Uliyanchenko, S. van der Wal and P.J. Schoenmakers  
*Deformation and degradation of polymers in ultra-high-pressure liquid chromatography*  
Journal of Chromatography A 1218(39) 6930-6942
- P. Schon, S. Dutta, M. Shirazi, J. Noordermeer and G.J. Vancso  
*Quantitative mapping of surface elastic moduli in silica-reinforced rubbers and rubber blends across the length scales by AFM*  
Journal of Materials Science 46(10) 3507-3516
- S. Namdeo, S.N. Khaderi, J.M.J. den Toonder and P.R. Onck  
*Swimming direction reversal of flagella through ciliary motion of mastigonemes*  
Biomicrofluidics 5(3)
- L.J. Xue, W.Z. Li, G.G. Hoffmann, J.G.P. Goossens, J. Loos and G. de With  
*High-Resolution Chemical Identification of Polymer Blend Thin Films Using Tip-Enhanced Raman Mapping*  
Macromolecules 44(8) 2852-2858
- X. Li, C. Liu and T. Al-Samman  
*Microstructure and mechanical properties of Mg-2Gd-3Y-0.6Zr alloy upon conventional and hydrostatic extrusion*  
Materials Letters 65(11) 1726-1729
- X. Li, T. Al-Samman and G. Gottstein  
*Microstructure development and texture evolution of ME20 sheets processed by accumulative roll bonding*  
Materials Letters 65(12) 1907-1910
- T. Al-Samman and X. Li  
*Sheet texture modification in magnesium-based alloys by selective rare earth alloying*  
Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing 528(10-11) 3809-3822
- X. Li, T. Al-Samman, S. Mu and G. Gottstein  
*Texture and microstructure development during hot deformation of ME20 magnesium alloy: Experiments and simulations*  
Materials Science and Engineering a-Structural Materials Properties Microstructure and Processing 528(27) 7915-7925
- X.Y. Liu, S. Shen, Z. Ge, W.L. Lim, M. Dobrowolska, J.K. Furdyna and S. Lee  
*Scaling relations between anomalous Hall and longitudinal transport coefficients in metallic (Ga,Mn)As films*  
Physical Review B 83(14)
- M. Yildirim, S. March, R. Mathew, A. Gamouras, X. Liu, M. Dobrowolska, J.K. Furdyna and K.C. Hall  
*Electronic structure of Ga(1-x)Mn(x) As probed by four-wave mixing spectroscopy*  
Physical Review B 84(12)
- T.A.P. Engels, L.C.A. van Breemen, L.E. Govaert and H.E.H. Meijer  
*Criteria to predict the embrittlement of polycarbonate*  
Polymer 52(8) 1811-1819
- S.J. Picken, D.J. Sikkema, H. Boerstael, T.J. Dingemans and S. van der Zwaag  
*Liquid crystal main-chain polymers for high-performance fibre applications*  
Liquid Crystals 38(11-12) 1591-1605
- X. Liu, D.J. Smith, J. Fan, Y.H. Zhang, H. Cao, Y.P. Chen, J. Leiner, B.J. Kirby, M. Dobrowolska and J.K. Furdyna  
*Structural properties of Bi(2)Te(3) and Bi(2)Se(3) topological insulators grown by molecular beam epitaxy on GaAs(001) substrates*  
Applied Physics Letters 99(17)
- R. Matesanz, J. Rodriguez-Salarichs, B. Pera, A. Canales, J.M. Andreu, J. Jimenez-Barbero, W. Bras, A. Nogales, W.S. Fang and J.F. Diaz  
*Modulation of Microtubule Interprotofilament Interactions by Modified Taxanes*  
Biophysical Journal 101(12) 2970-2980
- A. Ginzburg, T. Macko and R. Brull  
*Characterization of Functionalized Polyolefins by High-Temperature Two-Dimensional Liquid Chromatography*  
American Laboratory 43(1) 11-13
- A. Greiderer, L. Steeneken, T. Aalbers, G. Vivo-Truyols and P. Schoenmakers  
*Characterization of hydroxypropylmethylcellulose (HPMC) using comprehensive two-dimensional liquid chromatography*  
Journal of Chromatography A 1218(34) 5787-5793
- V.M. Litvinov, R.A. Orza, M. Kluppel, M. van Duin and P.C.M.M. Magusin  
*Rubber-Filler Interactions and Network Structure in Relation to Stress-Strain Behavior of Vulcanized, Carbon Black Filled EPDM*  
Macromolecules 44(12) 4887-4900

### Filed patent application

#698: A. Garcia, F.A. de Wolf, R. de Vries  
Diblock copolymer

### Reported inventions

#692: G.G. Hoffmann, G. de With, L. Xue  
Scanning of sample surface with one AFM Head

#698: A. Garcia, F.A. de Wolf, R. de Vries  
Diblock copolymer

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# 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.

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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.

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Effective English, Den Haag

### Photography

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Eindhoven  
Bram Saeys Fotografie,  
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### Printing

Lecturis, Eindhoven





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