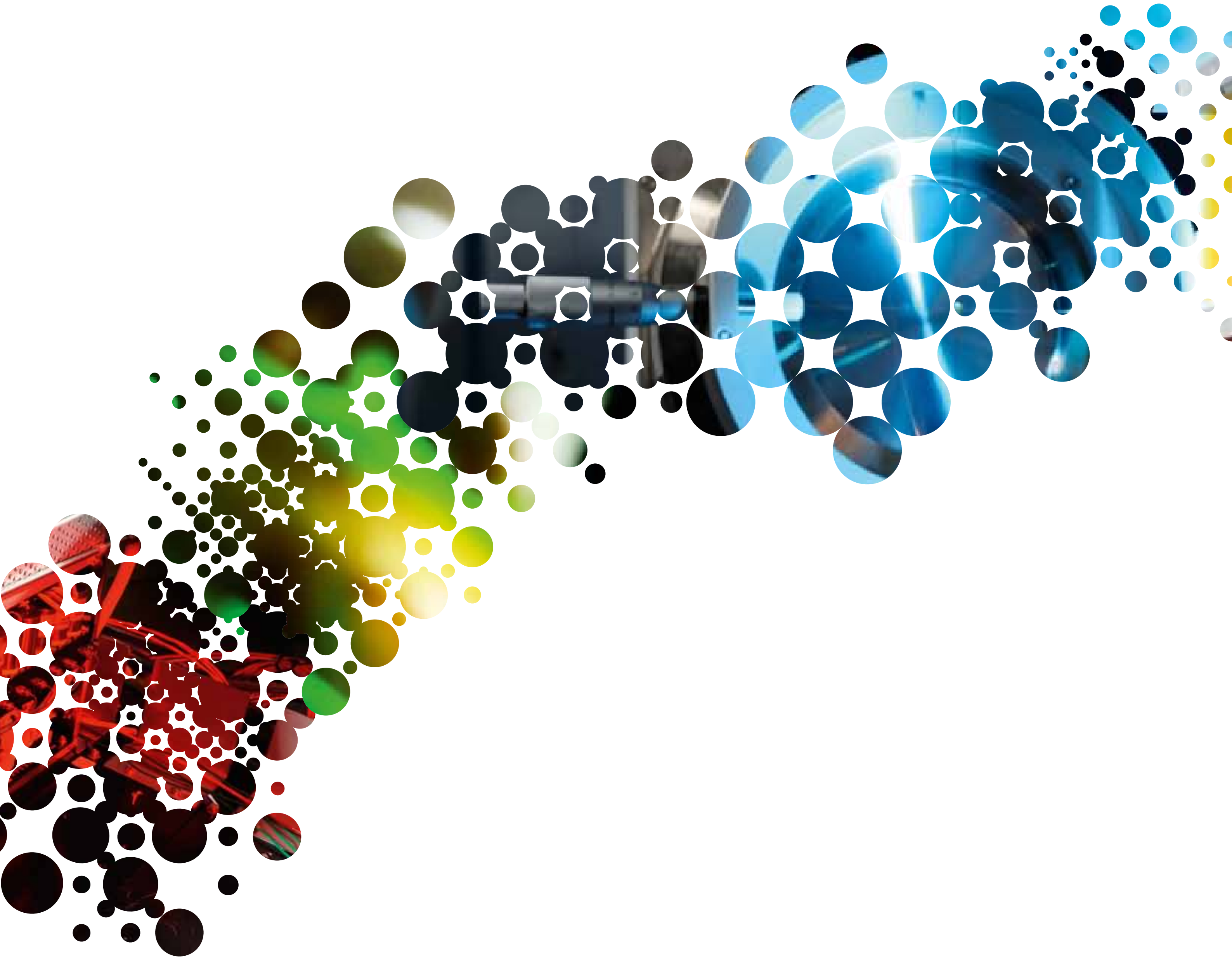
DPI
Dutch Polymer Institute


.... TOMORROW'S BUSINESS



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.

Foreword
'Today's science, tomorrow's business'

DPI is at a crucial juncture in its development. The changing environment calls for a change in our strategy. Our ambition is to evolve into a global Centre of Excellence in polymers and broaden our financial base. To achieve this, we will expand our partnership base by looking for partners across the entire polymer value chain and internationalising our activities, and we will continue our commitment to excellence.

Top sectors

Last year a new government was installed in the Netherlands and the contours of a new national industry and innovation policy are emerging. The present government wants to strengthen Dutch industry sectors that are already strong, among other things by concentrating scientific research on specific areas. Three of these 'top sectors' are very relevant for DPI: Chemicals, Agro Food and High Tech Systems & Materials.

At the same time, the government has decided that, unlike in previous years, no additional funds from the national gas revenues will be made available for investments in research. This means that the financing of a research project will increasingly depend on the project's added value for industry and industry's willingness to co-fund it. This is very much in line with the model with which DPI has enjoyed so much success since 1996. The Dutch government has high hopes for public-private R&D partnerships, in which knowledge institutes (universities and research institutes) and companies jointly carry out research on topics that are relevant for industry.

It is clear, however, that there are far fewer resources available than in previous years. It is therefore crucial for DPI to be involved in the 'knowledge agendas' that are being formulated for each of the top sectors in the spring of 2011. We should be able to do so, based on our excellent track record in creating and organising consortia and conducting research that is of strategic importance for industry and for which companies are willing to pay (demand-driven research).

In our new strategy, we have decided to broaden our horizons in order to generate more income from partnerships with the international polymer industry and become less dependent on government funding.

Opportunities for growth

DPI owes its growth in the last few years to its cooperation with mainly West European companies, but we need to expand our partnership base in the coming years. The BRIC countries (Brazil, Russia, India and China) offer particularly good prospects, because in these countries there is a huge demand for polymer knowledge and expertise and for training facilities for research scientists working for companies and research institutes. There is also a clear need for closer cooperation between universities and companies in these countries. This represents an excellent opportunity for us to transfer our expertise and knowledge and, in doing so, bring our partner companies into contact with potential suppliers of raw materials and potential customers for their products.

At the same time, DPI's existing corporate partners feel an increasing need to innovate, but the global financial crisis of recent years has made them more cost-conscious, and this cost-consciousness extends to their budgets for R&D. For DPI this means that we must focus even more sharply on subjects that will help these partners to innovate and enable them to remain internationally competitive. We will continue to pursue our proven strength: public-private cooperation in pre-competitive research. In our new strategic plan we describe this as Track A (see box on page 23).

Another way in which DPI is going to broaden its partnership base is by looking for partners in the entire polymer value chain, from raw material to end product. This will enable us to unlock a great deal of innovation potential. It also fits in with our desire to include more SMEs in our programme, since the polymer value chain includes many innovative SMEs.

Forming consortia

The experience that DPI has gained with consortia is increasingly proving itself in Europe. We are frequently asked to act as coordinator in forming European consortia. We are a recognised

Jacques Joosten
Managing Director

partner of the EU and are able to bring together all relevant parties, including partners in non-EU countries such as Russia. We have for example formed consortia on subjects such as nanocomposites and modelling under the seventh EU Framework Programme.

But outside the EU context, too, we are capable of bringing together relevant business and research partners to form consortia. We are engaged in various new topics, including electrospinning of fine fibres, in which there is interest from companies in the plastics sector and the agro food sector.

DPI's international profile has become much more prominent recently. As a result, we are often the first choice as an initiator of new public-private partnerships. We are going to build on this strength in the coming years with Track B in our strategic plan. This track focuses on collaborations along existing value chains. In these collaborations we will benefit from the experience that we have gained over the last year from our close involvement in the Knowledge Workers Scheme established by the Dutch government. The idea behind the scheme was to prevent the economic crisis leading to a reduction in the number of researchers in industry. The scheme enabled companies to retain their researchers by seconding them to a research institute, helped by a subsidy from the Dutch government. DPI helped 200 industrial researchers to keep their knowledge and expertise up to date. In this way, we helped prevent a 'lost generation'.

We have also chosen to employ a third track, Track C, in which we will address certain societal issues in our research agenda. We are aware that academia, industry and the government are not DPI's only stakeholders. Some societal issues lend themselves to a solution based on polymer science and technology. To give an example: we have for several years been involved in projects in the context of the Bottom of the Pyramid, in which we try to find solutions for the challenges facing developing countries, such as housing, health and nutrition. Another example concerns a major new international problem that has emerged in recent years, one that also affects our partner companies: the 'plastic soup' consisting of huge quantities of plastic waste that accumulate in oceans and seas and that constitute a threat to marine flora and fauna. We have decided to mobilise our knowledge to see whether we can help find a solution. We are putting together a consortium that will concentrate on the plastic waste in the North Sea and Wadden Sea.

In 2010 DPI intensified its cooperation with the DPI Value Centre. The DPI Value Centre plays a key role in identifying innovation opportunities because of its close ties with SMEs and its intimate knowledge of these companies' specific needs. At the DPI Annual Meeting in 2010 we took stock of a large number of these needs,

Martien Cohen Stuart
Scientific Director

for example in the construction sector, the packaging industry and the transport industry. By focusing on these concrete needs, DPI and DPI Value Centre ensure that their research remains immediately relevant for the market and that their polymer expertise leads to innovative products and solutions in the shortest possible time. All this is in line with the new Dutch government's objective of making SMEs benefit more from scientific research. DPI and DPI Value Centre already have a lot of experience in that regard.

Scientific excellence

DPI's ambition is to grow into an International Centre of Excellence for polymer science and technology. This means that we devote a lot of attention to the quality of our research output. The growing journal impact factor (4.43 in 2010) and high citation impact factor (2.19 in 2009) of our publications prove that we are moving in the right direction. To increase both the quality and the impact of our work even further, we have tightened up our protocols in consultation with our Scientific Reference Committee.

We are also taking steps to further improve the quality and use of our patents. We will start using the patents that are not assigned to our DPI partners to generate new business and expand existing business. It was for this purpose that we created an 'option scheme' with the DPI Value Centre. We will actively promote this scheme in the market to increase the effectiveness and efficiency of our patents.

All in all, 2010 was an exciting and eventful year. This annual report provides a good overview of the results we achieved. However, 2011 will be a crucial year for DPI. A lot will depend on the outcome of the discussions on the 'top sectors' in the Netherlands and the position DPI is able to secure in them.

DPI team – From left to right: Peter Nossin, Richard van den Hof, Christianne Bastiaens, Peter Kuppens, Martien Cohen Stuart, Jan Stamhuis, Johan Tiesnitsch, John van Haare, Renée Hoogers, Miranda Heuvelmans and Jacques Joosten. Second row: Thomas Manders, Annemarie van den Langenberg, Marc Ruis and Shila de Vries. Absent in this picture: Monique Bruining, Harold Gankema, Jeanne van Asperdt and Sherida Koenders.

Apart from that, we will also focus on new strategic targets for innovation. The aim of the strategy is to generate €33 million in revenues by 2014. We also want to become an international 'hub' for public-private partnerships in excellent polymer research in 2014. We believe that we can accomplish this, because time and time again we have shown ourselves to be capable of attracting leading international researchers, PhDs and post-docs who, like us, are committed to excellence. In this way we will continue to live up to our adage that today's science is tomorrow's business.

Jacques Joosten
Managing Director

Martien Cohen Stuart
Scientific Director

DPI Value Centre team – From left to right: Louis Jetten, Martin van Dord, Jos Lobée, Arie Brouwer, Femke Markhorst, Judith Tesser, Peter Nossin, Karin Molenveld, Johan Tiesnitsch and Lonneke de Graaff.

Contents

Organisation 2010

Supervisory Board

- Dr. H.M.H. van Wechem, *Chairman*
- Prof.dr. M. Dröscher
- 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. E. Drent, Leiden University, *Chairman*
- Prof.dr. L. Leibler, Ecole Supérieure Physique et Chimie Industrielles, Paris
- Prof.dr. H. Sirringhaus, 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*
- R.P.A. van den Hof MSc, *Performance Polymers (Engineering Plastics)*
- Prof.dr. J.W.M. Noordermeer, *Performance Polymers (Rubber Technology)*
- 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, *Emerging Technologies and 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. van den Langenberg, *Project Administration*
- S.K. de Vries MSc, *Intellectual Property and Legal*

DPI Value Centre

- A. Brouwer MSc, *Managing Director*
- Dr. L.A.M.J. Jetten, *Business Development*
- F.E. Markhorst MSc, *Project Leader New Business*
- L.C. de Ruijter- van Blommestein, *Secretariat*
- J.J.D. Tesser, *Programme and Communications Manager*

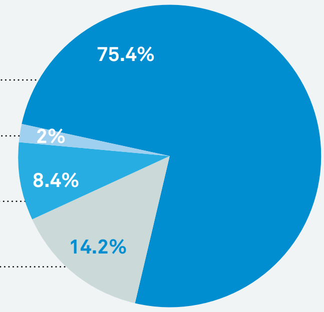
Summary of financial data 2010

Income	(x EUR million)	%
Contributions from industrial partners	4.31	17.4
In-kind contributions from industrial partners	3.31	13.4
Revenue Patents	0.06	0.2
Revenue DPI Value Centre	0.43	1.8
Contributions from knowledge institutes	4.26	17.2
Contributions from Ministry of EA&I	9.00	36.5
Knowledge Workers Scheme	3.33	13.5
Total income	**24.70**	**100**

Expenditure (x EUR million)

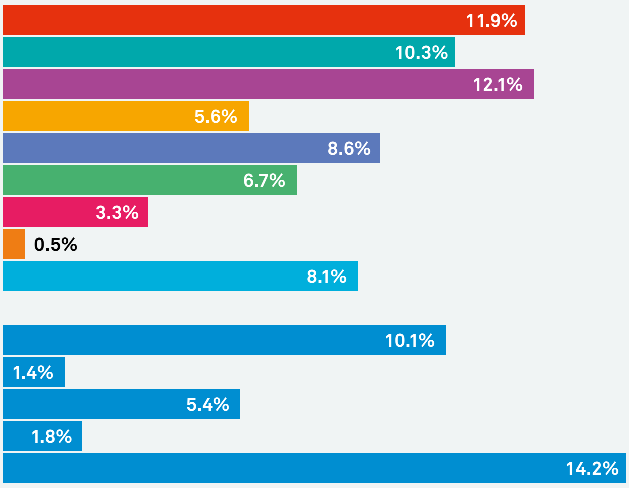
By nature

Personnel costs	18.33
Depreciation	0.49
Other costs	2.03
In-kind contribution	3.45
Total expenditure	**24.30**



By Programme Area

Polyolefins	2.89
Performance Polymers	2.51
Functional Polymer Systems	2.94
Coating Technology	1.37
High-Throughput Experimentation	2.09
Bio-Inspired Polymers	1.62
Large-Area Thin-Film Electronics	0.81
Emerging Technologies	0.12
Corporate Research	1.97
Knowledge Workers Scheme	2.45
Knowledge Transfer	0.33
Organisation and support	1.32
Support to DPI Value Centre	0.43
In-kind contribution	3.45
Total expenditure	**24.30**



Key Performance Indicators 2010

Number of industrial partners

2009	32
2010	34

European governmental funding (% of total funding)

2009	0%
2010	0%

Number of partner knowledge institutes
(universities, etc.)

2009	48
2010	49

Participation of foreign knowledge institutes
as % of total expenditure

2009	33%
2010	29%

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

End 2009	30%	EUR 4.602.674 cash + EUR 1.549.221 in kind
End 2010	31%	EUR 4.378.245 cash + EUR 3.307.655 in kind

Overhead costs
as % of total expenditure

2009	6.5%
2010	5.4%

Expenditure for knowledge transfer

2009	EUR 379,000
2010	EUR 334,229

Contribution Ministry of Economic Affairs
as % of total income

End 2009	44.5%
End 2010	36.5%

Number of patents filed by DPI

2009	10
2010	15

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

2009	6
2010	4

Interest shown by industrial partners	2
Interest shown by university partners	2
Interest shown by DPI Value Centre	16

Number of patents to be transferred **20**

Track record DPI researchers

Left in total	40
Employed by partner knowledge institute	21
Employed by non-partner knowledge institute	7
Employed by partner industrial company	3
Employed by non-partner industrial company or start-up	5
Returned to native or foreign country	0
Unknown	4

Research output

	2009	2010
Scientific publications	176	141
PhD theses	26	5

Partners 2010

Industry

AkzoNobel
BASF
Bayer
Borealis
Braskem
Celanese
Chemspeed Technologies
Dow Benelux
DSM
ECN
Evonik
ExxonMobil (new per 2010)
Food and Biobased Research Wageningen UR
Forschungsgesellschaft Kunststoffe
Freeslate
FrieslandCampina
Industrial Technology Research Institute Taiwan
LyondellBasell
Merck
Michelin
Microdrop Technologies (new per 2010)
Océ Technologies (left in 2010)
Philips
Petrobras (new per 2010)
Sabic Europe – Sabic Innovative Plastics

Saint-Gobain (new per 2010)
Shell
SKF
SNF Floerger (new per 2010)
Solvay (new per 2010)
Teijin Aramid
TNO
Waters Technologies Corporation

NL Agency
Ministry of Economic Affairs, Agriculture and Innovation

Knowledge institutes

- Delft University of Technology
- Deutsches Kunststoff Institut
- ECN
- Eindhoven University of Technology
- ESCPE Lyon
- ESPCI
- Food and Biobased Research Wageningen UR
- Forschungsinstitut für Pigmente und Lacke
- Friedrich-Schiller-University Jena
- Imperial College London
- Innovent
- Japan Advanced Institute of Science and Technology
- Leibniz-Institut für Polymerforschung Dresden
- Loughborough University
- Martin-Luther University of Halle-Wittenberg
- Max-Planck Institute fur Polymerforschung
- Nanoforce Technology
- National Technical University of Athens
- NWO
- Polymer Technology Group Eindhoven
- Queen Mary & Westfield College, University of London
- Queens University
- Radboud University Nijmegen
- Stellenbosch University
- TNO
- University Maastricht
- University of Algarve
- University of Amsterdam
- University of Bayreuth
- University of Cambridge
- University of Cologne
- University of Duisburg-Essen
- University of Glasgow (new per 2010)
- University of Groningen
- University of Haute-Alsace
- University of Leeds
- University of Leiden
- University of Liverpool
- University of Manitoba
- University of Münster
- University of Naples Federico II
- University of Ottawa
- University of Perugia
- University of Salerno
- University of Twente
- University of Ulm
- University of Wuppertal
- Utrecht University
- Wageningen University

Intellectual Property (IP)

Substantial output in 2010

In 2010 DPI filed fifteen patent applications on the basis of 23 reported inventions. These numbers are significantly higher than in previous years and provide solid evidence that companies are absorbing the results of the DPI research, since a patent application is only filed when a partner company is interested.

The technology areas High-Throughput Experimentation, Functional Polymer Systems and Coating Technology have traditionally generated a large number of inventions. Interestingly, the relatively young technology areas such as Bio-Inspired Polymers, Large-Area Thin-Film Electronics and Emerging Technologies are now also generating a number of inventions and patent applications.

To honour the researchers who came up with inventions that proved of interest for our partners, we again awarded a number of Certificates of Invention during our Annual Meeting in 2010. A total of 23 Certificates of Invention were presented to the researchers responsible for inventions that led to eight patent applications filed during the academic year 2009-2010.

Positive effects of IP policy change

It is apparent that the numbers for the second phase of the patenting process, i.e. the national filing and granting phase, are significantly lower. This is a direct result of DPI's IP policy of not maintaining a large patent portfolio. Patent applications are already transferred either to partners (companies and knowledge institutes) or to the DPI Value Centre during the first phase, before national filing takes place.

This ensures that the IP rights generated within the DPI programme are owned by the parties that can further develop the processes and products and that academic research is converted into business.

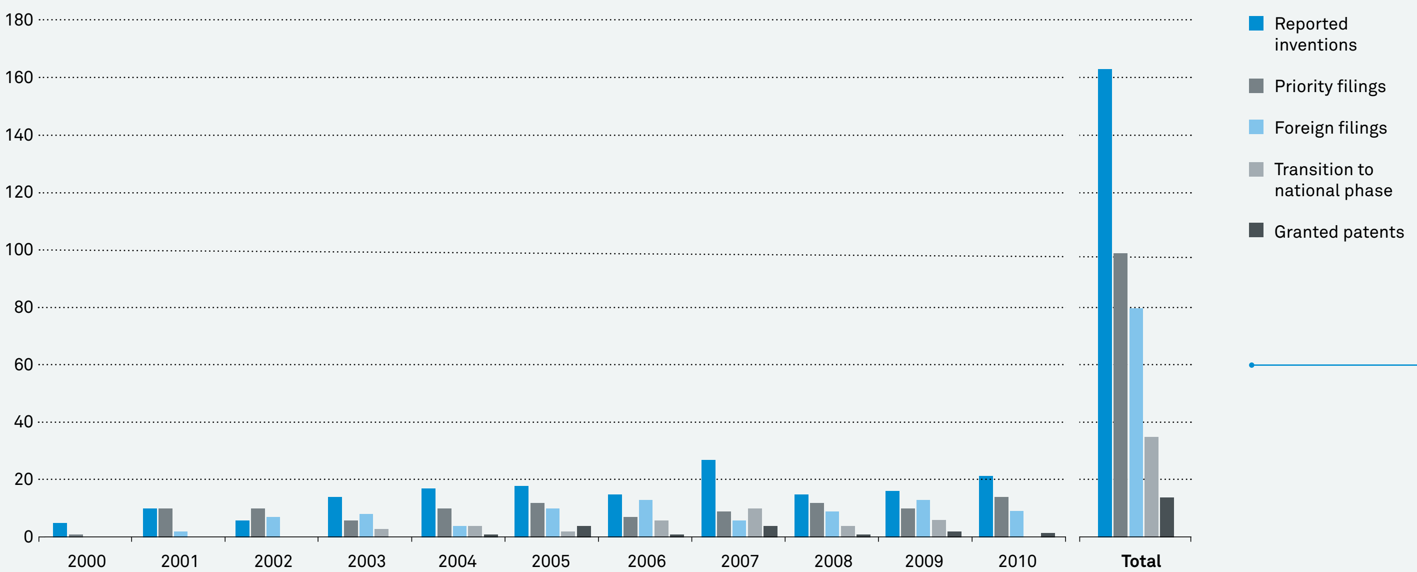
Valorisation is clearly taking shape

The cooperation with DPI Value Centre with regard to the patent portfolio has been formalised with the signing of the first Patent Purchase Agreement for three patent families between DPI and DPI Value Centre. The DPI Value Centre has strong business cases for these patent families and is making appropriate deals with third parties to apply the technologies developed within the DPI research programme in commercialisable products and processes.

In 2010, two of DPI's participating knowledge institutes also reported that they have business cases for two patent families generated by DPI. The negotiations on the transfer were finalised early in 2011. The universities have since made deals with both a start-up company and a multinational.

Last but not least, one of the partner companies acquired a license for a DPI patent family in early 2010. These positive developments are an incentive to enhance the potential value of the DPI research output.

DPI patents 2000-2010



KWR strengthens relationships between companies and research institutes

Approximately 200 R&D employees of companies and some twenty young researchers were involved in projects carried out under the Knowledge Workers Scheme (KWR*). The impact of the investment of €15 million by the former Ministry of Economic Affairs was greater than simply preserving the jobs of knowledge workers who would otherwise have become unemployed because of the economic crisis.

Under the scheme, companies worked with universities on strategic projects that were previously regarded as confidential by the companies concerned. The partnerships accelerated the pace of the projects. Companies were able to make use of the advanced equipment and knowledge available at universities, while university employees had the opportunity to share their ideas with experts from the companies.

The KWR implied a shift from pre-competitive to pre-commercial research in the regular DPI projects. Thanks to the close collaboration of DPI and DPI Value Centre it was easy to handle both types of projects. The feedback from the participating companies about the activities was positive, so more projects with a medium-term horizon are expected to be launched. Government support for these projects is uncertain, however.

Peter Nossin who manages the KWR project for DPI says: “We were able to make the switch quickly thanks to DPI’s existing formula, which is based on cooperation between companies and universities. For example, the KWR helped us to retain a relatively large number of knowledge workers. We have already started with the implementation of the projects. Officially, the knowledge workers are seconded from the companies to the universities. The universities are also formally responsible for their supervision. But of course they don’t suddenly have an additional 150 fume cupboards, so the knowledge workers remain where they are and we employ an exchange program. For every ten knowledge workers there is one young scientific researcher who is supervised by the professors concerned. People from the companies and the universities hold intensive consultations and visit each other regularly.”

Louis Jetten, project manager KWR at DPI Value Centre cites the evaluation that was conducted among the companies and universities involved: “The benefit of this type of cooperation is that the young scientists have far more direct contact with the knowledge workers from the companies, which gives them a better understanding of how companies perform R&D. The objectives of the different sub-projects correspond with the wider social objectives of developing products that are smaller, lighter and less energy-intensive.

Companies are pleased with the speed at which the projects are started and observe that there was less bureaucracy than with many other schemes. Another advantage was that they were able to limit the financial risks during this difficult economic period. The KWR is a temporary scheme. It would be great if we could continue with similar joint projects.”

DPI has incorporated the model of cooperation between one or more companies and knowledge institutes in production-oriented research in its strategy, alongside the existing model of pre-competitive research.

* The KWR was an initiative of the Ministry of Economic Affairs aimed at helping companies to maintain their research capacity during the ‘crisis’ period.

IP statistics per area 2010	PO	PP	FPS	CT	HTE	BIO	LATFE	EMT	Corp	Total
Reported inventions	2,5	0,5	5	5	5	2	2	1		**23**
Priority filings	1,5	2,5	1	2	6	2				**15**
Foreign filings		2	2	1	4					**9**
Transition to national phase	1									**1**
Patents granted										**0**

Valorisation in polymers works for companies

"Looking back, 2010 was a year that confirmed that our activities are highly valued by our clients, whether they are companies involved in projects, people joining networks, workshops and market days or entrepreneurs that we coach. We were able to help more companies with their innovation ambitions than we had planned, even in a time of economic crisis. Our formula works," says Arie Brouwer, Managing Director of DPI Value Centre.

"Key to the success is the combination of a qualified team, our independent position, the hands-on approach and the unique network of warm contacts within the polymer sector – ranging from small and large industry partners to knowledge institutes in the Netherlands and abroad ", adds Arie Brouwer in conversation with the DPI Value Centre team.

Innovative projects

Last year, twenty projects started involving more than fifty companies. Most of them were feasibility projects, designed to assess the technology or market feasibility, or larger innovation projects to develop new products or processes up to the prototype stage. Three consortia projects also started, each involving at least five companies. Jos Lobée: "Our independent position is important, as well as our experience and our working methods. We know our way around in our unique network, we believe we really understand entrepreneurs and are keen to focus on the added value of the consortium. It takes quite some time to shape and form such a collaborative effort. The companies involved greatly appreciate our efforts. Our role fills a gap in the Dutch innovation landscape." NL Agency recognises the importance of the role of DPI Value Centre and therefore supports its activities.

Sustainable chemical plant

Early in 2010, AkzoNobel, BECO, DPI Value Centre, DSM, Royal Cosun, Search and Witteveen+Bos challenged each other to join forces to design the Factory of the Future, a conceptual, yet typical, chemical plant. We have developed a conceptual production environment based on sustainable principles, in terms of people (equity), planet (ecology) and profit (economy), for the

Ioniqa – Magnetic smart materials

Dutch Design Week – Workshop 'Rethink'

entire value chain. The aim of the virtual facility is to close the biological and the technological cycles of a product and its related manufacturing as far as possible.

The critical factor in the development of the virtual Factory of the Future is a sustainable design, based as far as possible on Cradle to Cradle principles. The design of the facility strongly emphasises renewable energy, water management and active materials and transport management. Following the successful completion of the first phase, the results of which were presented at the Sustainability Congress in November 2010, the partners have decided to proceed with the second phase in 2011.

Sharing knowledge

A special type of project was launched with the aim of retaining highly qualified R&D personnel in times of economic crisis, under the so-called Knowledge Worker Scheme. Louis Jetten: "These projects have opened doors between companies and knowledge institutes. The companies involved are enthusiastic about the new cooperation and the good results. Both companies and knowledge institutes want to continue with this type of projects."

"The networking and the options for cooperation they provide is one of the strengths of DPI Value Centre" adds Lonneke de Graaff. "We also see this within the Cradle to Cradle network. Companies share knowledge, they bring knowledge and come to get knowledge. They get to know each other through the network, which consists of more than 100 companies. They share their experiences and also work together.'' As an independent organisation with knowledge of the subject, DPI Value Centre plays an essential role in discovering how to get initiatives started.

For the third time we participated at the Dutch Design Week with a workshop entitled 'Rethink', which focused on sustainable polymers. Industrial designers are keen to hear the latest developments in materials such as bio-polymers. "The bio-polymers workshops we have organised have brought suppliers and potential clients closer together" according to Karin Molenveld. The practical approach adopted for these workshops was greatly appreciated by all of the participants. The suppliers who attended now have a very good notion of the products they can work with and which materials will have potential for the future."

Industry needs chemical experts

Our network makes it possible to accelerate business development. This creates opportunities for new companies as well as existing companies. In 2010 a pilot was completed to boost new business in a medium-sized polymer-processing company. In the first phase various new product/market combinations were defined. The challenge now is to create new business. This can be accomplished within the company itself or as a spin-off activity. "In our sector, the technology is often the starting point for a new company. Knowledge of the market is needed to create success. Some fifty start-ups have already benefited from our expertise and our network. We offer tailor-made support. We know where the pitfalls are and we help companies to avoid them. Our support is greatly appreciated. Start-up companies in the Netherlands advise other start-ups to seek our support" says Femke Markhorst.

We encounter a lot of people who are considering starting a company. Young people who are still studying and people who already have some working experience with a company. Some have ideas but no facilities, while others are still hesitant because they do not yet have an clear idea. We can help both. With our expertise and our network, we offer a supplement to regular education. We work together with the incubator departments of universities. Judith Tesser: "The challenge is to find the potential starters among those working in the industry. The sector is faced with an increasing labour shortage. We aim to retain as many chemical specialists as we can – within companies or knowledge institutes or as entrepreneurs".

Opportunities for innovation

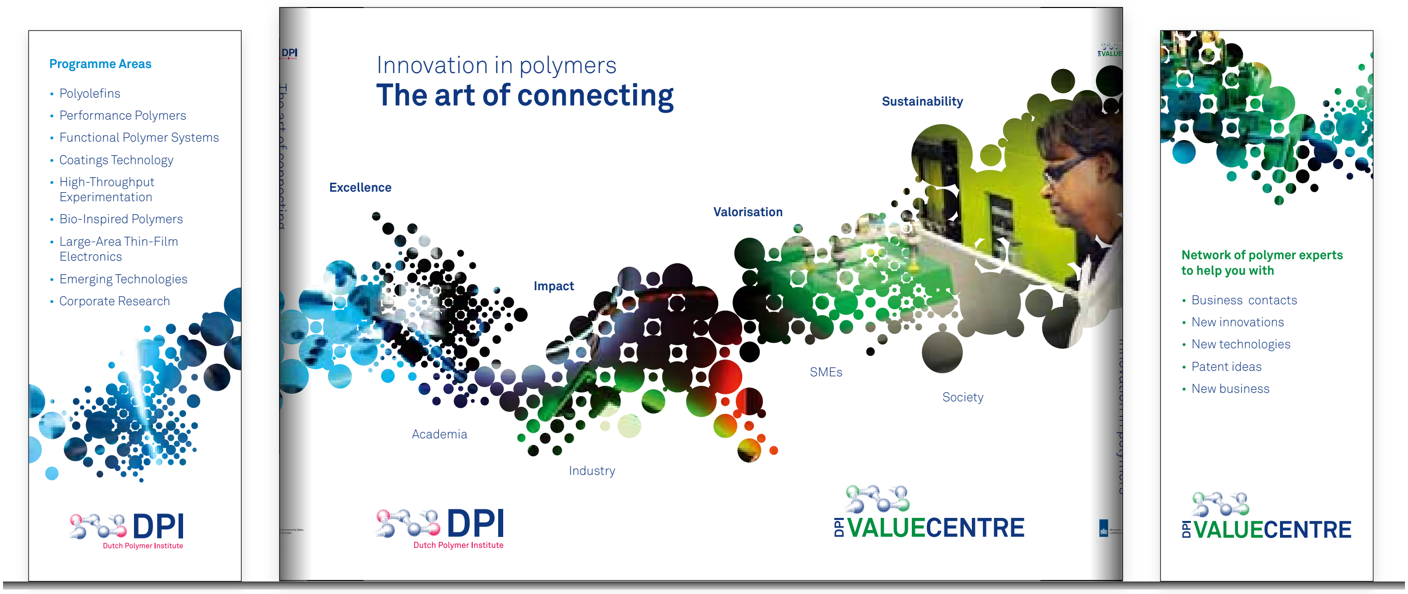
We have several promising technologies which need to be developed further. We have selected twenty promising ideas from the DPI patent portfolio in which the developer is being kept involved. In the meantime, four of these ideas are being exploited by companies, each in a different way. For the coming years there are many opportunities for innovation, for example in bio-based materials and applications. Building on our experiences, the good results, the satisfied clients and these opportunities, we plan to further enhance and strengthen our activities in 2012 and beyond.

Optimal forming solutions – The flexible mold

DPI VALUECENTRE

The strength of the network of DPI and DPI Value Centre

The strength of the partnership between DPI and DPI Value Centre lies in the combination of DPI's international network of leading companies and prominent universities active in the field of polymers and the network that DPI Value Centre has created among SMEs, start-ups, the Dutch Rubber and Plastics Federation (NRK) and other trade associations and consultants specialising in innovation over the last three years. Although concentrated mainly in the Netherlands for the moment, that network is increasingly expanding into Belgium, in association with the Vlaams Kunststoffen Centrum and Flanders Plastic Vision, and Germany, with Kunststoffland NRW (Nordrhein-Westfalen).



Our shared ambition is to promote innovation in the field of polymers, in particular by leveraging the strength of the network. For example, large companies often face specific problems that could be of interest to smaller companies. But which companies should they approach? On the other hand, companies in DPI Value Centre's network have questions that could be answered by employees of universities or one of the companies. "This interaction does not take place automatically" says Arie Brouwer, Managing Director of DPI Value Centre. "We know the actors personally, so there is trust between us. Our independent status also helps. Once they get to know us companies dare to take the next step and we can then help these companies to greatly increase their competitiveness."

Strong combination of flexibility and capital

During the Polymer Innovation Day, jointly organised by DPI and DPI Value Centre in November 2010, host Frank Kuijpers of Sabic expressed his company's desire to work more intensively with SMEs. Whereas large companies like Sabic have the money but are too large to change quickly, smaller companies can respond flexibly to new developments but do not have the venture capital. By working together, they can explore possibilities and innovate more quickly.

Open innovation formula leads to innovation

Well-known larger companies like BAM Bouw, FrieslandCampina, Océ and Assembléon laid bare the challenges their sectors face in the coming period, some of which can be met with advanced knowledge of materials. Senior researchers from companies like Nuplex, Lightweight Structures, Holst Centre and Sabic described promising new developments in the field of polymers. During the ensuing workshops, the participants had an opportunity to suggest solutions for the problems that were raised. Strength in numbers is one answer, and that is possible with open innovation and a good network. In the Netherlands we are willing to work with competitors, who then become 'colleague competitors'.

Supply of knowledge

Another benefit of the cooperation is that the knowledge generated by DPI can be transferred to DPI Value Centre in the form of patents, which can then be licensed to or acquired by other companies. DPI Value Centre investigates which parties might benefit from the new technologies. Johan Tiesnitsch, who is responsible for Intellectual Property at DPI and DPI Value Centre: "Take technologies in the fields of self-healing materials, biopolymers or conductive polymers, for example. We can see the potential of these technologies because of the possibilities for commercial applications. This is important and good for society as a whole. For example, with our new technologies we can make environmentally friendly products but also, for example, provide people with back problems with a new intervertebral disk. There is so much that can be done with polymers." At the end of 2010, DPI Value Centre's portfolio contained twenty patents from DPI. The first royalties have already been earned. Consequently, the knowledge created in the DPI programme but not acquired by its partners, does not slip through the gaps. The knowledge is actively used by companies in DPI Value Centre's network.

Start-ups

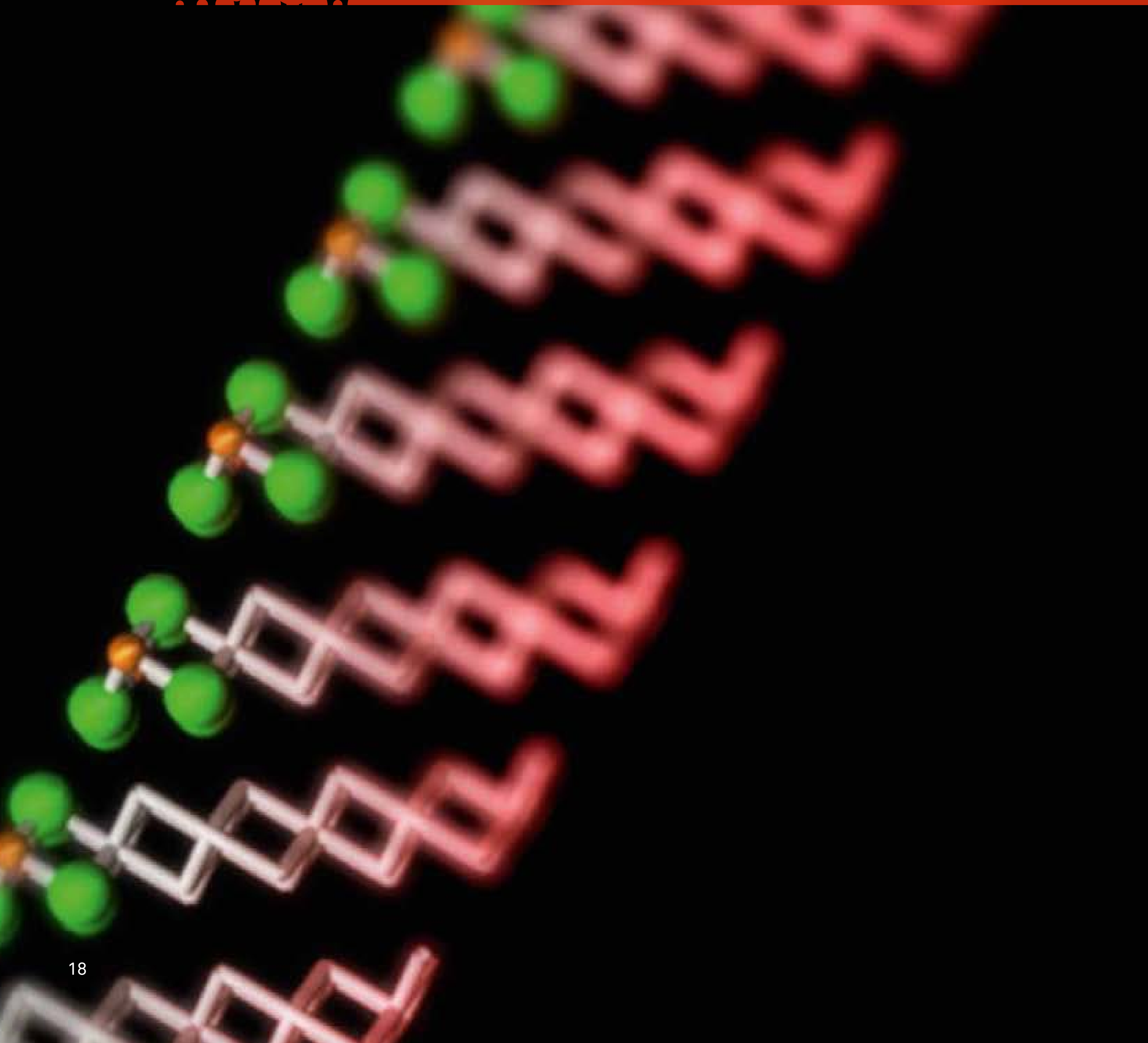
DPI research generates many promising new ideas. There is nothing strange in that when you recall that the research progammes are driven by companies. This research produces ideas that can generate new business activity. Some researchers are happy to start their own company to use the knowledge and technology they have developed in their research. DPI Value Centre offers tailored assistance for these start-up companies to increase their chance of success. DPI Value Centre has a lot of experience in advising start-ups that innovate with polymers. They have found that the network can be leveraged to promote the success of start-ups. They can also hire experts with business experience in this domain, which further increases the prospects of success. Most researchers engaged in DPI projects are employed by DPI partners after they finish their project. Some immediately take the step of starting their own business, while others wait until they have gained a few years of experience.

Continuity is essential

Promising ideas are often shelved because people are not given the opportunity to take them further, or fail to take it. "In other countries – outside Europe – opportunities are grasped more often", says Jacques Joosten, Managing Director DPI. "We must continue to stimulate new business activity in the Netherlands. In times of austerity, investment in innovation could provide precisely the leap forward we need. DPI and DPI Value Centre together form a Centre of Excellence in polymers, but without the official status. The Dutch government's role in promoting this is crucial, both now and in the future. That is impossible with only short-term research; you have to keep investing in long-term research. A growing number of companies realise this and are making a longer commitment to DPI. Now that Minister of Economic Affairs, Agriculture and Innovation Verhagen has said he wants to continue the leading sectors policy, we hope that our Polymers Innovation Programme can be expanded in the coming years."

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.



Mastering the process with the aid of computers

Curiosity about the process and the desire to optimise it are the twin driving forces behind the DPI project dedicated to gaining a better understanding of the process of producing polyolefins with Ziegler-Natta catalysts. Computers are proving a great help.

"The bulk of the polypropylene you encounter in daily life is produced using a process with a Ziegler-Natta catalyst. Karl Ziegler and Giulio Natta won the Nobel Prize for Chemistry for that process in 1963, so you would think the process must be thoroughly understood by now, but it isn't," Andrea Correa begins her explanation of the project. "The catalyst is a complicated heterogeneous system with several components, including magnesium chloride, titanium chloride and aluminum alkyls. Changes in the composition and in the preparation conditions result in end products with different properties, but the causal relationship is not clear. This lack of comprehension is certainly due to the peculiar nature of Ziegler-Natta catalytic systems, which raises several chemical and technical obstacles to attempts at their experimental characterisation. So we are trying to learn more by means of 'in silico' experiments, varying the different parameters step by step and identifying the consequences. We can then draw up guidelines to help industry optimise the process."

Feedback

By 'in silico' experiments Correa means computational chemistry, or the simulation of chemical processes on a computer. She has been working in this field since graduating, first for her PhD project and now as a post-doc on a DPI project at the University of Salerno in Italy.

Feedback from industry is obviously very important in this kind of work, and working on a DPI project facilitates that. But Correa also appreciates the fact that contacts with other universities are so much easier. "I did my PhD work in cooperation with LyondellBasell, and now, through DPI, I have access to even more industrial partners. They will help us to incorporate the relevant variables in our models. Even though computers are increasingly powerful, it is impossible to incorporate all the variables. We have to choose. It is a trade-off between the costs of computation and the number of variables that we want to calculate and their accuracy." One of the things Correa reported on at the most recent cluster meeting in the Polyolefins technology area was a benchmark investigation of the different models with the accompanying accuracies.

Confidence

Although the production process with Ziegler-Natta catalysts works well in many polymer-producing companies, a clearer understanding of the behavior of the active sites, where the polymerisation starts, would help to gear the process better towards the desired end result, which is to produce polyolefins with specific properties. It could also enhance the efficiency of the process, for instance by making it faster or less expensive. "You never know what the industrial consequences of your research will be," says Correa. She has published a few papers about the heterogeneous catalyst systems that are cited in the scientific literature "An advantage of doing this kind of work in a DPI project is that you have access to unpublished experimental data from industrial partners against which to check the results of your simulations. This is very important for being able to state with confidence that our models are valid."

Andrea Correa is a post-doc working at the University of Salerno, Italy, on DPI project 707, *Advanced static and dynamic modelling of heterogeneous Ziegler-Natta catalytic systems*.

The art of molecular modelling

In industrial research organisations, experimentalists usually outnumber the scientists engaged in modelling work. DPI can play a role in intensifying relations between members of the latter group to the benefit of all.

"At the end of the 1980s software companies were promising the moon to the chemical industry, but then failed to live up to the expectations," says Betty Coussens, Senior Scientist Molecular Modelling at DSM. Since that time she has been actively involved in computational chemistry. "Now, with the increased computing power, we are seeing some of those promises come true." Coussens is one of the few scientists in DSM working in the field of theoretical chemistry. The main reason for such work is that the results can be used to extract guidelines for experiments. In a sense it is a lonely job and Coussens is happy to have contacts with scientists doing similar work through DPI.

White box

One of the projects Coussens closely follows is the modelling of the Ziegler-Natta catalysis process. Indeed, since DSM sold its petrochemical activities to Sabic it is not as closely involved in the process as it used to be and Coussens has been seconded to Sabic for the project. She is very positive about the project: "The quality of that work is really very good and I am very hopeful that within a reasonable time, a few years at most, we will have a better insight into the effects of the different species in the process. In some respects, the project complements what I do for Sabic. For instance, I am looking for correlations between calculated properties of a whole series of ingredients in the Ziegler-Natta catalyst and the resulting properties of the polymers. We call this approach black-box modelling, since it does not require a detailed mechanistic understanding of the functioning of the catalyst. We will then link our results to those of Correa and others, which will give us that mechanistic understanding and which we call white-box modelling results. We hope this will give us a deeper insight into the process."

Benchmark

Apart from these direct results, Coussens feels the project has further advantages for her work and thus for DSM and Sabic. The benchmark investigation that Correa carried out is very helpful. "For people like me, who are working in a more practical environment, it is not always easy to choose between the available methods. Of course you perform a small-scale literature screening before you choose a method or perform your own small-scale validation study. However, the fact that some more or less standard methods produce such diverse results for chemical interactions of importance to Ziegler-Natta catalysis, one of the results of Correa's benchmark, was completely new to me. The benchmark investigation allows me to make a more deliberate choice of a method to describe Ziegler-Natta systems and gives me more confidence in my results. Yet another advantage is that when you know people in universities with alternative methods to yours at their disposal, you can ask them to do small calculations for you."

The Ziegler-Natta catalysis is not the only chemical process that is not yet fully understood and where modelling work can provide more insight. Coussens is also using software for high-throughput computations. Computing the same reaction steps for various conformations of a catalyst can be boring and uninspiring. The automated approach developed by the University of Manitoba should help a lot. "But there are also other projects going on in the field of computational chemistry that it would be useful to know about," says Coussens, who would obviously welcome a more structured approach to modelling issues in DPI.

Betty Coussens is senior scientist molecular modelling at DSM, the Netherlands, and is involved in DPI project 707.

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, with the aim of increasing 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).

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.

FACTS AND FIGURES

Partners from industry
- Borealis
- Braskem
- Dow Benelux
- DSM
- ExxonMobil
- Freeslate
- LyondellBasell
- Petrobras
- Sabic Europe
- Shell
- 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 2010 totalled € 2.89 million (budget: € 2.81 million). A total of € 116k was spent on equipment.
The total number of FTEs allocated at year-end 2010 was 29 (38 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 seven reviewed papers and one thesis; three inventions were reported and two patent applications were filed.

For details, see page 70.

DPI: International Centre of Excellence

The Dutch Polymer Institute is entering a new phase in its development. It wants to embark on a new growth curve and transform itself into an 'International Centre of Excellence' for polymers and plastics, one of the objectives being to broaden its financial base and so become less dependent on subsidies from the Dutch government.

DPI was one of the first generation of Leading Technological Institutes (LTIs) in the Netherlands. The idea behind LTIs was to enable knowledge institutes (universities and research institutes) and companies to conduct joint long-term-oriented research on industrially relevant topics. This was a response to an emerging trend in the Netherlands: large companies were steadily reducing their spending on long-term-oriented scientific research and were increasingly shifting their R&D focus to topics that were of direct relevance for their business results. At the same time, it was generally acknowledged that long-term-oriented explorative research is crucial for companies in strategic terms. This is particularly true for the polymer industry. The strong fibres Twaron® and Dyneema® are just two examples of highly successful products that owe their existence to such long-term-oriented explorative research.

To address the R&D gap that was threatening to emerge, the government, companies and knowledge institutes formed strategic public-private partnerships in the form of leading technological institutes (LTIs). These LTIs, including DPI, conducted what is known as pre-competitive research, the results of which were shared by the participating companies and knowledge institutes.

The former Dutch Minister of Economic Affairs, Hans Wijers, who is now CEO of AkzoNobel, considered it very important for the Netherlands to establish specialist institutes in carefully selected fields. The idea was that these institutes could eventually evolve into international centres of excellence in the chosen fields, one of which was polymers. The government initially contributed fifty percent of the costs, industry a quarter and the universities provided a quarter 'in kind'.

This formula proved a brilliant move because it allowed companies to leverage their R&D investments: for every euro they invested, the Dutch government contributed two and the knowledge institutes another one. The companies moreover shared the risk of the research, since the choice of topics was a joint one. The LTI concept has proved to be a way of carrying out high-quality scientific research on industrially relevant topics.

The skeptics who initially thought that research institutes would compromise their scientific integrity by carrying out research for industry now see that this is not the case. In fact, the scientific research performed by DPI researchers has turned out to be world-class in terms of quality and impact. The cooperation between companies and knowledge institutes is like the cooperation between the driver and the navigator of a rally car. To produce a top-class performance, both have to be excellent. In the LTIs the universities are in the driver's seat as far as the scientific standards and methods of the research are concerned, but the companies determine the direction of this research.

There is another interesting aspect to this successful cooperation. To perform cutting-edge scientific research, you need top researchers. DPI has not only been able to attract top researchers, but has trained them in subjects that are relevant for industry. This means that when these researchers join a company after completing their DPI assignment, they understand what industry is and what it is trying to do, and they are capable of performing research that helps their company to enhance its international competitive position.

After a few years, DPI opened up to companies and knowledge institutes in other countries as well, the idea being that this would lead to the international growth and improvement in quality it was striving for. Dozens of international companies and knowledge institutes are now participants in DPI and the expectations have been met.

There has been a lot of praise for the Dutch approach in Europe and beyond. It is still quite special for competing companies to form consortia and share the knowledge generated by their joint research, with each of the companies using that knowledge to develop its own new products and processes.

This model of public-private cooperation has existed since DPI was founded. But, to return to the metaphor of rally driving, the landscape is changing and the DPI 'vehicle' needs modification. The terrain is becoming more variable and the Dutch government, until now DPI's major sponsor, has other priorities. DPI is therefore compelled to revise its business model and alter its strategy.

DPI's ambition is to become an International Centre of Excellence for research into polymers, a hub that links companies and institutes worldwide. This will raise DPI's international profile, hopefully to the point where DPI becomes the place to go for industrially-relevant scientific research into polymers.

The principal opportunities for DPI lie in the BRIC countries (Brazil, Russia, India and China), where industrial demand for knowledge and expertise about polymers is growing strongly, where a productive partnership between companies and knowledge institutes is a challenge and where companies have a great need for well-trained young scientists whom they can immediately employ in their projects.

DPI wants to reduce its dependence on government subsidies, for example by raising more funds from industrial companies. True, these companies have become even more selective in how they spend their R&D budgets, but they are under growing pressure to innovate, and they lack the scientific concepts to achieve those innovations. DPI will therefore zoom in even more closely on topics that are relevant for these companies, since even in pre-competitive research there could be a sharper focus on subjects with a high innovative potential. Based on its long experience, DPI can quickly find topical research subjects and form consortia around those subjects. One such subject is the electrospinning of fine fibres, a subject that is relevant for the polymer industry as well as the food industry.

Besides the changes in industry and in the government landscape, DPI is also 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 can harm the eco-system. DPI has become increasingly aware in recent years that companies, knowledge institutes and the government are not its only stakeholders. In its new strategy DPI will also turn its attention to the social aspects of polymers, and this includes searching for possible solutions to the 'plastic soup' problem.

Having conducted a great many interviews with its stakeholders, DPI has drawn a number of conclusions regarding its future. The institute needs more funds, from new sponsors, in order to reduce its dependence on the Dutch government and so become less vulnerable to changes in government policy that could form an obstacle to DPI's ambitions for growth. DPI will also place greater emphasis on its unique selling point: its extensive experience with pre-competitive research, enabling it to add a great deal of value to industrial companies' innovation processes.

DPI intends to address medium-term developments in the polymer value chain, including the globalisation of markets, the future role of the BRIC countries and the changing demands of societal stakeholders.

DPI plans to intensify the international profile of its programme because there is a need for additional knowledge and expertise. This will lead to wider participation by academic institutes outside the Netherlands.

To meet all these challenges, DPI has adopted a strategy along the following tracks:

- pre-competitive research and training programmes according to the current model of the leading institutes but with a wider European/international scope.
- industrial pre-commercial research programmes with industrial partners and knowledge institutes and targeted at specific innovation and business objectives, with consortia in the value chain and in bilateral projects.

There will also be a third track: specific programmes and projects that follow from social challenges and that demand top-class polymer research and technology.

With this strategy, DPI will be ready for the next phase of its growth: the path to international excellence and a broader customer base.

Track A

pre-competitive research and training programmes

1. Current activity: continue to generate and share industrially relevant research
2. 'World Polymer Academy': educating and coaching of R&D employees
3. Organising and exploiting events and congresses
4. Projects focused on (exploratory) technology development in consortia (within Europe)
5. Georgraphical expansion of the current DPI programme
6. In-kind contribution of industrial participants

Track B

industrial pre-commercial programmes

7. Initiating programmes through existing value chains

Track C

specific programmes and objects driven by societal challenges

8. Solving societal themes and challenges

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.

A toolbox for making copolymers

Polymers are versatile materials. By changing the building blocks, their properties can be adapted to specific applications. But producing polymers from those buildings blocks is not always easy.

"While studying for my Master's I worked for a year at ICI Paints, which is now part of AkzoNobel. It was there that I realised I wanted to work with polymers, since they bring together different aspects of chemistry. Their synthesis is based on organic and catalytic chemistry, while in applications it is often physical chemistry that dominates their properties. I heard of this position in Eindhoven from a colleague. I wanted to go abroad for my PhD project, but being English and not speaking many languages, I hesitated. I now realise I needn't have worried since the working language in the lab here is English anyway," says Gemma Sanders when asked how she ended up working on the project with the acronym SMURF which, with a little stretch of the imagination, stands for 'Smart surface modifiers for engineering plastics'.

Domains

Sanders has been working on the project for two and a half years and has now built a toolbox of methods to synthesise block or graft copolymers that derive their properties from the different monomers they are composed of. She explains: "Monomers can impart different properties to a polymer. For instance, one might be hydrophilic, while another might interact with an engineering plastic, such as polyolefins or polyamides. With block or graft co-polymers of these different monomers, the polymers can arrange themselves in such a way as to produce domains with different properties. 'Painting' them on engineering plastic leaves you with a surface that has a desired property. However, such combinations of monomers are not often found in a single polymer since you cannot make them with a single synthesis technique, like radical polymerisation. All the polymerisation techniques that I have investigated involve a double bond which can serve as a macro-initiator or react directly with another polymer. As far as I am aware, I am the only person using this approach. My toolbox makes it possible to choose the desired properties for a polymer, based on the monomers and techniques I have available, for application on the engineering plastic you want to modify."

Modified surfaces

Sanders has now reached the point in her project where she can start looking into specific applications and testing whether her polymerisation techniques do indeed result in modified surfaces of engineering plastics. Changing side groups of building blocks of her polymers does not influence the polymerisation process but it can cause the desired changes in the surface properties. It is then possible to add anti-fogging or anti-static properties to engineering plastics. "I'm now working in collaboration with industry to make polymers that contain the specific combination of monomers required to obtain a material with specific properties; glasses that do not fog up, for example. Of course, we still have to test the materials, but the toolbox gives us a broad outline of the possibilities," says Sanders. Working on a DPI project, it should not be too difficult to find applications industry is interested in. A driving force in Sanders' work is her curiosity to find out how and why her approach works, but equally important is the knowledge that there will be a practical use for her work, even if it is only in the distant future. She likes this industrial aspect of her work and certainly wants to continue her career in an industry related to polymers. "I hope one day to see my materials actually being used in practice."

Gemma Sanders is a PhD student at Eindhoven University of Technology, the Netherlands, working on DPI project 651, *Smart surface modifiers for engineering plastics*.

Making good materials better

Materials suppliers want to improve the properties of their materials and add useful new properties to them, preferably without compromising the existing ones. Modifying the structure of polymers is a better way of achieving this than resorting to additives.

Theo Hoeks has been working in the field of new, innovative plastics and the technologies to make them for more than twenty years now, first at GE Plastics and then, after its take-over, at Sabic Innovative Plastics in Bergen op Zoom in the Netherlands. Naturally, he is interested in new methods of making materials with improved properties. "What Gemma Sanders is doing in her project, making new materials using a combination of different types of radical polymerisation techniques, is a new approach to us. It is a way of making well-defined structures. If we want polycarbonate, our main product, to have a certain property without endangering its present properties, such as its transparency, we can mix it with a block copolymer with a well-defined structure, in which one block represents that property and the other block guarantees the solubility in polycarbonate," says Hoeks. "We can, for instance, prevent algae growing on our polycarbonate or prevent graffiti remaining permanently."

Non-fogging

Hoeks is a visiting scientist at the polymer department of the Eindhoven University of Technology, where Sanders works. He had read the project proposal before the start of the project, but was not involved in it from the start. "I had not realised the impact this method could have on our materials, but when I saw the initial results I was immediately convinced. With the toolbox of methods that Sanders is developing we can adapt our materials to better serve our needs. It is never just one property that you are striving to improve; it is always a whole range of properties. You want your material to retain all of its original properties but then improve it in one respect, and that is exactly what these block copolymers can do for us," says Hoeks, explaining his later involvement in the project. Hoeks gives the example of car lamps to illustrate the usefulness of the method. "LEDs that are used in the future will not generate as much heat as the current halogen lamps. It will be necessary to prevent water vapor from condensing on the envelope of polycarbonate. It would be nice for my company to have such a polycarbonate, not only for car lamps also for non-fogging transparent doors of freezers in supermarkets, but it will not be easy."

Open innovation

For scientists at Sabic Innovative Plastics, without the large research organisation of GE Plastics to fall back on, contacts with other researchers in the field of polymers are extremely important. DPI plays a major role in that respect, not only because of the projects that Sabic participates in. "Sabic is a relatively unknown company in the Netherlands and Europe. Graduates looking for a job do not have the company's name imprinted on their minds, but through DPI we can establish a reputation as an interesting employer. That was one of the reasons we hosted the Annual Meeting in 2010," explains Hoeks. But the company's reputation was not the only factor. Hoeks is also very pleased that DPI invites its partners to workshops and brainstorming sessions to discuss new trends. "I gather a lot of information in a very short time, without having to search for and read the relevant literature myself," says Hoeks. "A few years ago we had such a session about self-healing polymers that was really useful for me. This pre-competitive research in DPI, and of course also the concept of Open Innovation, is a blessing to us."

Theo Hoeks is principal scientist at Sabic Innovative Plastics in Bergen op Zoom, the Netherlands, and is involved in DPI project 651.

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.

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 visco-elastic materials.

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

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 life-cycle. Studies of self-healing in polymeric materials as paradigm shift to realise improved fit-for-purpose lifetimes.

FACTS AND FIGURES

Partners from industry
- BASF
- Bayer
- Dow
- DSM
- Evonik
- Sabic Innovative Plastics
- 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 2010 totalled € 2.51 million (budget: € 2.41 million). A total of € 26k was spent on equipment. The total number of FTEs allocated at year-end 2010 was 28.2 (35 researchers). Richard van den Hof MSc and Prof.dr. Jacques Noordermeer acted as Scientific Chairmen and Dr. Jan Stamhuis as Programme Area Coordinator of the Performance Polymers programme.

Publications and inventions
This Technology Area generated a total of 22 reviewed papers and one thesis; one invention was reported and three patent applications were filed.

For details, see page 71.

Annual Meeting 2010

The Annual Meeting, held on 16 and 17 November in Bergen op Zoom, was a great success. Around 220 members of the DPI community attended the first day of the meeting and almost 300 people attended the second day, which was organised jointly by DPI and DPI Value Centre. Sabic hosted the entire event, which was devoted to the theme of 'Creating Value'.

The proceedings on the first day focused on the value that the members of the DPI community can provide for each other, both in terms of knowledge transfer and the capacity to translate knowledge into product and process innovation. Throughout the day a series of speakers shared their vision on that theme.

The first speaker of the day, Vice President Technology of Sabic Innovative Plastics Tom Stanley, gave a very illuminating presentation on the current activities of Sabic IP. Among the topics he discussed were the LEXAN product range (transparent polycarbonate with applications in glazing, doming, protection and more) and company's sustainability-driven solutions.

DPI's Managing Director, Jacques Joosten, gave the audience an update of DPI's activities in 2010. Some of the highlights were the expansion of the organisation with five new industrial partners last year, the appointment of Katja Loos as the second DPI Fellow and the start of the implementation of DPI's updated strategy.

The second DPI Fellow Katja Loos believes that Enzymatic Polymerisations offer possibilities for new polymer systems. In her presentation she explained how to create value with fundamental research in this field.

Brigitte Voit, who heads the Macromolecular Chemistry department at the Leibnitz Institute for Polymer Research in Dresden, Germany, addressed the theme of the meeting by giving the audience more insight into the use of dendritic glycopolymers in biomedicine and nanotechnology.

For her PhD project at the University of Maastricht, Inge van der Meulen focused on developing a biodegradable material with the ability to restore damaged peripheral nerves. Together with Ron Deumens, a neurobiologist at Maastricht University, she presented the results of their successful efforts to produce this new and innovative material.

There were three speakers during the afternoon session, when Carlos Härtel from GE, Jonq-Min Liu from ITRI Taiwan and Jacques Joosten from DPI gave the audience their views on the theme 'From fundamental knowledge to product and process innovation'. Their brief lectures were followed by a discussion of the topic with the audience.

During the day, the poster jury faced the difficult task of awarding the prizes for the best scientific posters. The jury announced its decision during the dinner on the evening of 16 November. The third prize was awarded to Jing Wu, Nicole Franssen came second and the prize for the best poster went to Abhijit Saha. DPI was also delighted to present 23 Certificates of Invention to fifteen researchers, who had filed patent applications during the academic year 2009-2010. In view of the very small number of theses submitted in the previous year, DPI decided not to present the Golden Thesis Award at this time.

The second day of the meeting, Polymer Innovation Day, was dedicated to a discussion of market demands and the technologies on offer in the field of polymers. After the plenary session, during which presentations were given by DPI, DPI Value Centre and Sabic, the participants broke up into groups for separate sessions with presentations on market demand and the technological possibilities, respectively. During the meet-and-match session in the afternoon, the participants had an opportunity to discuss the findings of the group sessions. The debate generated a lot of valuable solutions for existing problems.

Annual Meeting 2010 - Sabic, Bergen op Zoom




Meeting



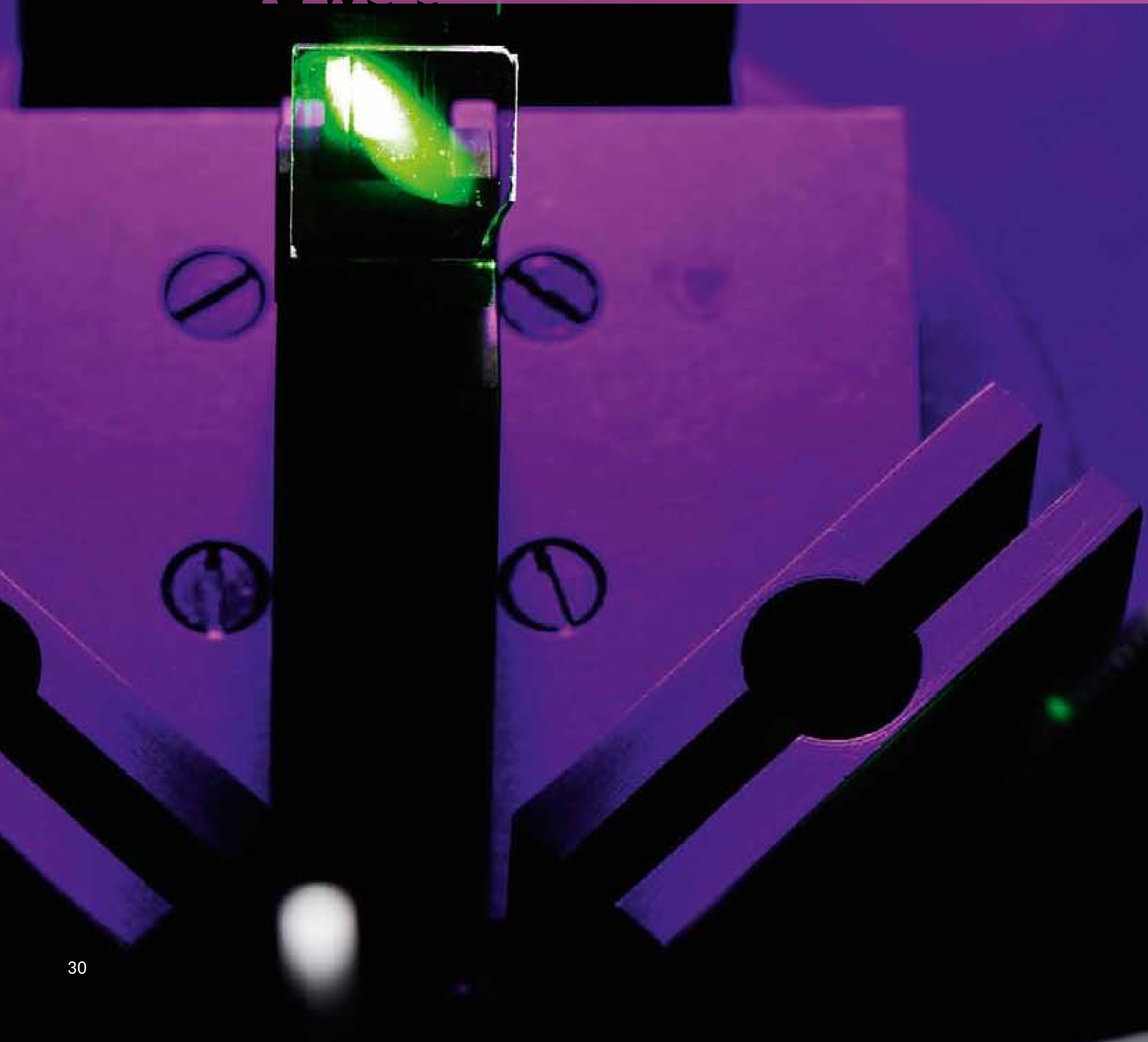






FUNCTIONAL POLYMER SYSTEMS

The Functional Polymer Systems (FPS) Technology Area performs research on the 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.



Getting to the core of the problem

Organic photovoltaic cells may be less efficient than inorganic cells, but for a large area their production costs are, in principle, lower. Understanding the charge generation, its relationship with materials and their processing is a prerequisite.

"After graduating in physics in Milan, Italy, I knew I wanted to work in the field of organic photovoltaics. I started sending e-mails to prospective employers and secured a position in René Janssen's *Molecular materials and nanosystems* group, a group that is renowned in the field. I grasped the opportunity with both hands. My project happened to be funded by DPI," Daniele Di Nuzzo replies, when asked what brought him to DPI. He is now studying a fundamental aspect of photovoltaics: what really happens when a material absorbs a photon, how charges are created. In particular, he wants to quantify the unwanted process of recombination of holes and electrons before they are transported to the electrodes.

Neutral

The technique he uses is optical spectroscopy. "This method allows me to see what happens if a photon is absorbed; whether I am creating charges and, if so, how many. Unfortunately, in organic photovoltaic cells many of these charges recombine before reaching the electrodes and, therefore, reducing the amount of electricity generated. The recombination can already occur when the electron and hole are created, before they start traveling to the electrodes. This detracts from the efficiency of an organic solar cell," explains Di Nuzzo. More insight into this mechanism and how it relates to the materials and the way they are processed will help to optimise organic photovoltaic cells. The active layer in organic photovoltaic devices is a more complex system than in inorganic devices, so it is more difficult to manage this materials-processing relationship.

"It has been found that processing the layers in a particular way can increase efficiency, so it will be rewarding to understand this relationship," adds Di Nuzzo, who is now midway through his project. "We have already found that the morphology of the blend of donor and acceptor molecules plays an important role. There appears to be an optimal size for the domains of donor and acceptor molecules. They should not be too big, but also not too small for the charges to separate at the interfaces and to be efficiently transported. The optimal size for acceptor domains is in the order of 50 to 100 nm. But apart from the size, the crystallinity is also a factor. We used atomic force microscopy and transmission electron microscopy to verify that."

Solar bag

The efficiency of organic photovoltaic cells has reached 8.3% in lab-scale samples, but even as much as 4 or 5% on larger scales. Di Nuzzo believes that practical applications are within reach. In fact, there are some already, such as Konarka's Solar bag. Although these efficiencies are, and will continue to be, lower than those of traditional inorganic cells, naturally the major advantage of organic cells is the possibility of producing them at relatively low cost by printing the materials on a large area in a roll-to-roll process. This would allow them to be incorporated in all kinds of products. "To succeed in that, we need to fully understand the interaction between the materials and the production process of the cells. The morphology plays an important role and depends on the way you process the polymers. The first step is to find the optimal morphology, before considering the details of production."

Daniele Di Nuzzo is a PhD student at Eindhoven University of Technology, the Netherlands working on DPI project 631, *Triplet recombination in polymer solar cells*.

Negative result, positive impact

It is important for the supplier of materials for solar cells to keep up to date with the latest insights into the generation of electricity in solar cells, even when they do not concern their own specific materials. DPI provides an excellent platform for sharing this knowledge.

Steven Tierney is a senior scientist with Merck in the United Kingdom and is involved, among other things, with Merck's efforts to develop new semiconducting materials for organic solar cells. "A recent trend in organic photovoltaic cells has been to use low-bandgap polymers in conjunction with fullerenes, C_{60}-derivatives, as the photoactive layer. As a materials supplier, it is very important for my company to understand the compatibility of these two types of materials, since it appears that the wide discrepancies in the efficiency of solar cells are connected with the precise type of fullerene that is used. However, the combination of fullerenes and low-bandgap polymers has not lived up to expectations in terms of yielding greater efficiency. It seems that this may be due to the mechanism that Di Nuzzo proposed in his DPI project," says Tierney, coming straight to the point.

Jumps

The combination of low-bandgap polymers and novel fullerenes looked promising on paper. It was expected to yield an appreciable efficiency increase compared with established material combinations using PCBM[60] as the fullerene. The reality proved otherwise. "Apparently the driving force for electron transfer from the polymer to the fullerene is no longer sufficient," says Tierney. The outcome may have been disappointing and not what people hoped for in terms of improvements in efficiency, nevertheless the findings may help Merck to avoid exploring poor material combinations and allow it to steer its work towards types of fullerene that can best be combined with newly-developed low-bandgap polymers to achieve leaps in efficiency. "The result may have been negative, but it has still had a positive impact," says Tierney. Even though Merck's work does not involve the precise combination of materials that Di Nuzzo used in his project, his explanation will help to steer Merck and its partners in the right direction when considering material choices for this application.

Sensitive

Di Nuzzo's project is not the only one in the Functional Polymer Systems technology area that Tierney is involved in. He is also responsible for the projects relating to organic field effect transistors. "I have to follow numerous projects, so it is difficult to really keep as up to date with all of them as I'd like. It is, of course, only one aspect of my job. But working with DPI brings us into contact with the leading experts in the (Dutch) chemical community and allows us to discuss new ideas with them. And they are perhaps a bit more open about their work in the context of a DPI project than if we were to approach them on a one-to-one basis," says Tierney, when asked for his opinion about the association with DPI. "But there are limits to what we can do together with DPI. What I mean is, as researchers we would love to give our materials to lots of academic partners for them to study and find out more about them and then give us feedback on their findings. But academics have to publish and give presentations on aspects of the work, which is not always in the best interests of Merck's commercial goals. So it's a delicate balance, deciding how much we can give away and how much we can get back in return." Merck hosted one of the cluster meetings in the United Kingdom last year at which it presented a survey of its activities. "It is definitely a positive thing, this cooperation with DPI, but it is sometimes very difficult to assess at this time what the value will be in the years to come," Tierney adds.

Steven Tierney is a senior scientist with Merck Chemicals based in Southampton, UK and is involved in DPI project 631.

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); responsive materials, (bio)sensors and actuators.

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
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 sensoring of gases and bio-fluids as well as the actuating principles of rubber-like materials and corresponding devices.

FACTS AND FIGURES

Partners from industry
- BASF
- DSM
- ECN
- Industrial Technology Research Institute (ITRI), Taiwan
- Merck
- Océ Technologies
- Philips
- 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 2010 totalled € 2.94 million (budget: € 2.41 million). A total of € 135k was spent on equipment. The total number of FTEs allocated at year-end 2010 was 29.6 (42 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 33 reviewed papers, five inventions were reported and one patent application was filed.

For details, see page 72.

New partners in 2010

Six new participants joined the DPI network in 2010. DPI is naturally delighted at the large number of new participants, which shows that more and more companies are learning about DPI and the added value of the institute. It also demonstrates that companies are again willing to invest in pre-competitive research after the dip following the economic crisis in 2008.

Companies participate in DPI for a minimum period of four years. They pay an annual fee for each participation in a technology area. For each participation, a company is entitled to one vote in the Programme Committee of the technology area, so the more participations in an area the more votes a company has to influence the programme content. Five companies chose the option of a 'full participation' in 2010.

SOLVAY

Solvay took one participation in Functional Polymer Systems and one participation in Large-Area Thin-Film Electronics. The company offers a broad range of products and solutions that contribute to improving the quality of life. Solvay is a global leader in specialty polymers, vinyls, essential chemicals like soda ash, caustic soda, hydrogen peroxide and special chemicals like fluorinated products and high-purity grades. It is Solvay's goal to become a major player in sustainable chemistry, developing and producing products and processes that meet the challenges of today's world with a reduced energy footprint.

ExxonMobil

ExxonMobil took two participations in Polyolefins. The company is the world's largest publicly traded international oil and gas company. They hold an industry-leading inventory of global oil and gas resources. ExxonMobil is the world's largest refiner and marketer of petroleum products, and the chemical company ranks among the world's largest. They are also a technology company, applying science and innovation to find better, safer and cleaner ways to deliver the energy the world needs.

BR PETROBRAS

Petrobras took one participation in Polyolefins and one participation in Bio-Inspired Polymers. It is an integrated energy company with operations in oil and gas exploration, production, refining, petrochemical, marketing and transportation, in Brazil and other countries. Petrobras is the largest company in Latin America. It controls significant oil and energy assets in more than twenty countries. The company also has activities in renewable energies, especially in bio-fuels and bio-products.

In the last few years DPI has observed that more and more SMEs showed an interest in participating in DPI's worldwide network. DPI therefore introduced two possibilities for participation by SMEs. The two new methods of participation are called 'basic participation' and 'group participation', in addition to the regular 'full participation'. A single SME can participate through a basic participation. This form of participation gives the company observer status and access to the network, projects and intellectual property but no voting rights. A number of SMEs can also participate as a group. Two or three SMEs participate as a group in the same way as a larger company does. The two or three companies have access to the network, projects, intellectual property and also have one vote in the Programme Committee of the Technology Area they participate in.

SNF FLOERGER

SNF Floerger is involved in Emerging Technologies with one participation. SNF is the leading producer of acrylamide-based polymers. The company's production capacity is the largest in the industry, accounting for 40% of global capacity. SNF has 30 years of experience in Enhanced Oil Recovery (EOR) and was one of the pioneers in the technology in the USA. SNF is continuously improving its EOR polymer technology through close working relationships with research teams from oil companies

microdrop
TECHNOLOGIES

Microdrop took one 'basic participation' in High-Throughput Experimentation. The company, established in 2005, is the leading provider of equipment, software and services for advanced microdispensing and inkjet printing applications. Microdrop's technology is a versatile tool for liquid handling and material deposition. The company's team of skilled engineers and technicians guarantees the best solution for applications in Microtechnology, Nanotechnology, Material Science, biochemistry and medicine as well as Plastic Electronics.

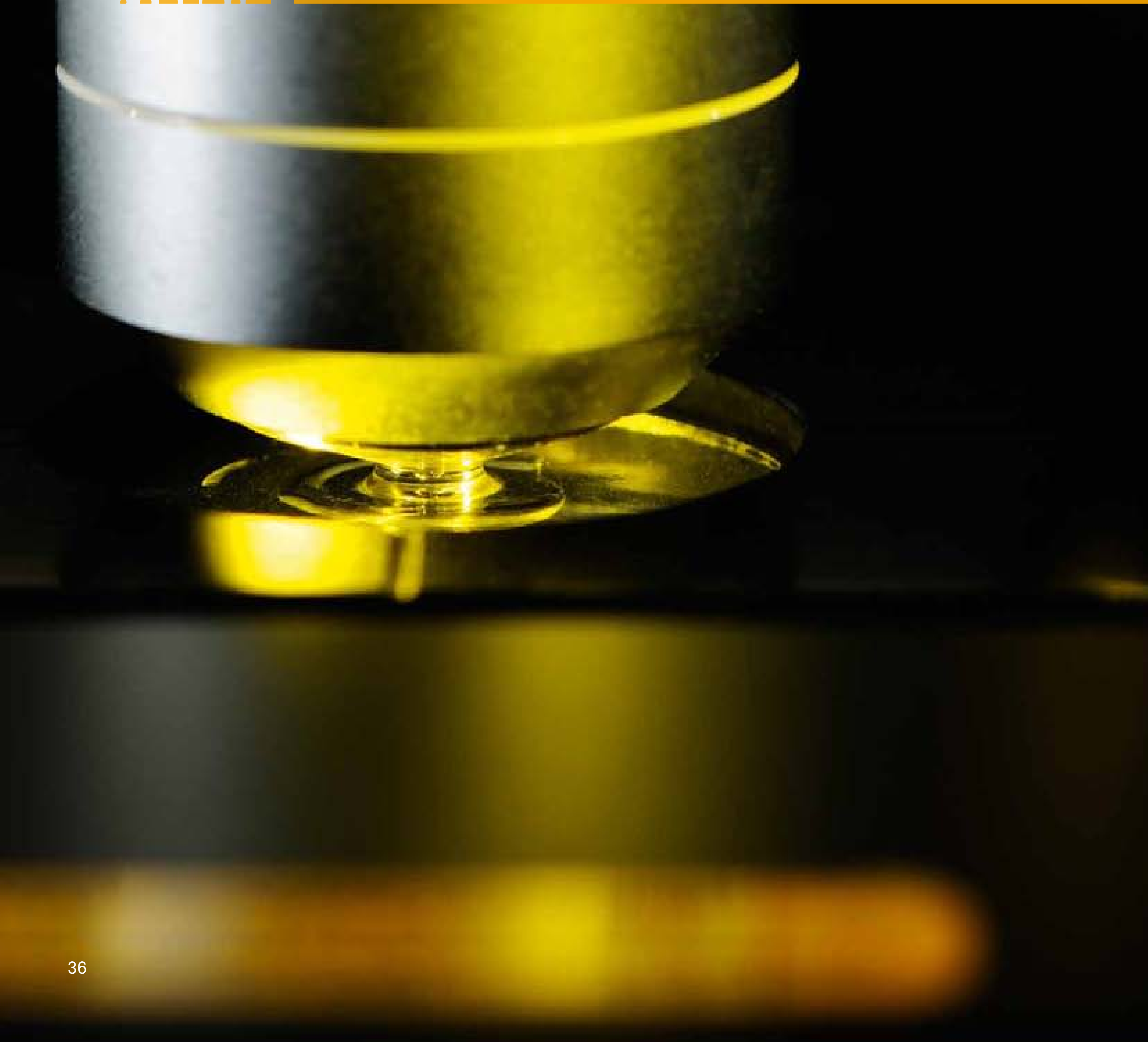
SAINT-GOBAIN

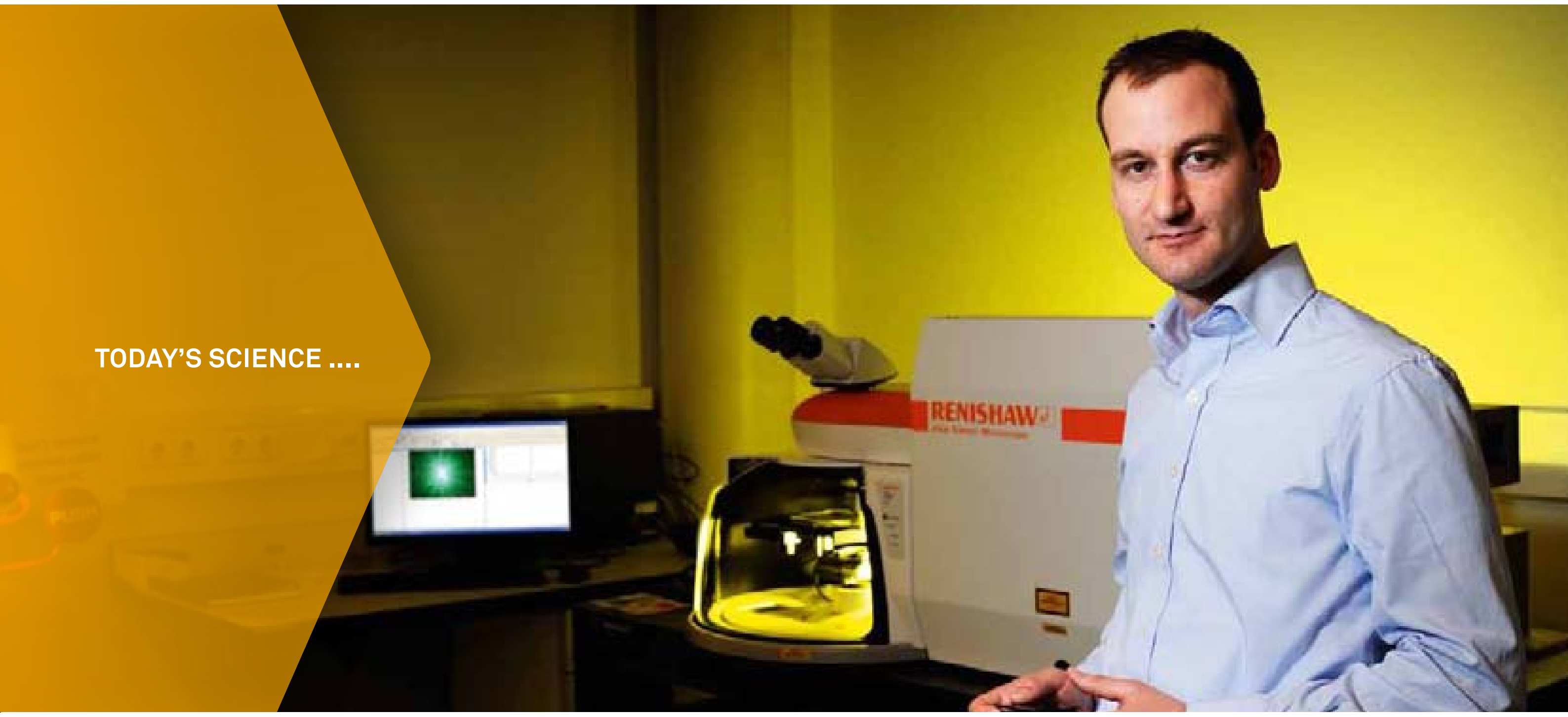
Saint-Gobain took one participation in Coatings Technologies. The company is the global leader in the habitat and construction markets. Saint-Gobain has more than 190,000 employees in 64 countries. The group designs, manufactures and distributes building materials, providing innovative solutions to meet the key challenges of growth, energy efficiency and environmental protection. Innovation is at the heart of the Saint-Gobain strategy. This notably involves working closely with young companies.

DPI aims to expand interaction with (potential) partners in 2011 with a view to building an even stronger international network in polymer science. The institute is targeting emerging economies such as Brazil and China. These countries have a significantly lower *per capita* use of plastic and are highly focused on innovation in R&D. Collaborations between industrial partners from these countries and the current DPI industrial partners will be a win-win situation.

COATINGS TECHNOLOGY

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.





Curing of organic coatings in daylight conditions

Photopolymerisation transforms a liquid formulation into a solid film. UV light is normally used, but for various reasons it would be better to use daylight. This 'green' coating technology is now close to introduction in industrial applications.

"During my year-long internship at GE Plastics, now Sabic, in the Netherlands I realised how much I would like to work in the research & development department of a large chemical company. I was a student of the National Chemistry School in Mulhouse at the time, and my colleagues told me I would need a PhD in chemistry to achieve that goal. So I did a Master in polymer chemistry at the University of Haute Alsace. I worked in the Department of Photochemistry at ICI Paints, now AkzoNobel. When I was asked to continue working there for a PhD project funded by DPI, I eagerly accepted, especially because it would involve working with other companies," says François Courtecuisse, explaining his present activities.

Scavengers

His project concerns the curing of coatings by polymerisation under the influence of light. That process has advantages compared to the conventional thermal process: no emissions of volatile organic compounds, less energy is required, the reaction takes place at room temperature, and it is fast. A coating can be cured in less than ten seconds. UV light is generally used in industrial applications. "We use photo initiators that work in daylight generated by LEDs. UV lamps still use a fair amount of energy and lose most of it in the form of heat. They generate UVC light that damages the skin and creates ozone that can irritate the eyes, nose and throat. The main problem with light curing is that oxygen inhibits all three steps of the polymerisation: initiation, propagation and termination. Particularly when daylight is used, the deleterious effect of oxygen is enhanced. So we are trying to find combinations of new photo initiating systems with additives which can scavenge oxygen to prevent that," says Courtecuisse. He is now in the final year of his project and has found two kinds of molecules that serve as an oxygen scavenger. "I follow that process in real time with Fourier transform infrared spectroscopy and subsequently characterise the applied coating with confocal Raman microscopy. Such expensive equipment is not always readily available at universities and I am very grateful that DPI has made it possible for me to use it", adds Courtecuisse.

Prospects

The structure-property relationships of the photopolymer film and the influence of the oxygen scavengers is another of Courtecuisse's interests. With atomic-force microscope experiments he tries to correlate the local hardness of the surface to the thermodynamic properties of the bulk. He also hopes to discover the relationship with end user properties, such as scratch resistance or hardness, as measured with standard industrial tests. "My results can easily be applied in industry. Not many additives are needed. It would only be necessary to replace the heaters or UV lights with powerful LEDs." Asked what he would like to accomplish with his work, Courtecuisse says, "What I hope is that in one way or another people will some day use my findings for their everyday painting jobs."
Courtecuisse appreciates having to write reports every three months. His reports are very detailed and can run to twenty pages. But they serve an important purpose. Courtecuisse: "It will be easier to write my PhD thesis since I already have everything on paper. The reports help me to organise my ideas." Courtecuisse will probably have no difficulty in finding a job in industry. He has already been approached by several potential employers.

François Courtecuisse works at the University of Haute-Alsace in Mulhouse, France, on DPI project 416, *UV to daylight curing of organic coatings*.

Open innovation in a pragmatic way

Changing from UV-light curing to visible-light curing of industrial coatings has advantages but must not be at the expense of the coatings' performance. Understanding the mechanisms, in particular the inhibiting role of oxygen, is of crucial importance.

Thomas Rölle is currently head of the Chemistry & Photoactives department in Bayer MaterialScience after working for twelve years in research and innovation management. As an industrial researcher, he is very interested in what is going on in DPI's Coatings Technology Area. Bayer, known mainly for its activities in the health care and crop science sectors, also has a materials division where, amongst other things, raw materials for coatings are investigated and produced. "Bayer is involved in radiation-cured coatings. By changing the additives you can alter the properties of the coatings. Of course we are always interested in new chemistry leading to new coating systems with a low viscosity that can be applied easily and, for example, become hard and scratch-resistant in a very short time. In industrial coatings the short time is particularly important. The standard in industry is now to use UV light for this radiation-curing step but with the ongoing penetration of LED light into our daily life and its obvious advantages in all kinds of applications, using less energy and having less damaging side effects, it is only natural to look at their use in radiation-induced photo-polymerisation as well," says Rölle, explaining his interest in François Courtecuisse's project.

Oxygen

Visible light can be used for curing purposes. However, the inhibiting role oxygen plays in the radical polymerisation process must be understood and managed. Understanding the mechanism behind this process and inventing additives that prevent oxygen from playing a deteriorating role are important to further develop this system for certain applications. "There is certainly an industrial relevance," says Rölle. "UV lamps are expensive, so if you want to use visible light sources you have to find a solution for the oxygen sensitivity. But not only in industry, in repair jobs too the benefit of not having to handle UV lamps in all kinds of circumstances with all the accompanying disadvantages, offers opportunities. But this is still looking into the bright future.
If you want to replace UV curing systems with visible-light curing systems, the performance must at least be at the same level. You therefore have to understand what is going on. You have to understand the role oxygen plays. Many attempts have been made in the literature over the last few decades, but the problem is still unsolved."

Clear rules

In Rölle's opinion DPI is very well positioned for these kinds of investigations of a pre-competitive nature. When something happens, for instance an invention is made, there are clear rules to follow. Rölle: "Yesterday we had a project meeting, which was also attended by people from M2i, the Materials Innovation Institute, a similar organisation to DPI in the field of metals.
The idea of open innovation really works here in a pragmatic way. You can find books and a lot of literature about open innovation but here I saw it work in practice." He also appreciates the continuity in the activities of DPI, the benefit of not having to form consortia for every new project but participating in an ongoing program by buying a participation for four years. And what he welcomes in particular is that DPI is a European venture, which in his opinion could also be expanded to the Far East or the United States. "If a company stands still while others develop, it loses ground, and that is also true for a research organisation like DPI."

Thomas Rölle is Head Chemistry and Photoactives in Bayer MaterialScience AG, in Leverkusen, Germany and is interested in DPI project 416.

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.

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 water-borne polyurethane dispersions, as well as starch-based performance coating materials. The results are promising in that coatings have already been obtained which match and/or improve on the properties of purely synthetic coatings.

Functional (smart) coatings
'Smart coatings' are capable of responding to an external stimulus, such as light, temperature, pressure, pH, odors 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 industry's 'Materials to Innovate' (M2i) programme in the study of anti-corrosion coatings.

FACTS AND FIGURES

Partners from industry
- AkzoNobel
- Bayer
- Dow
- DSM
- Evonik
- Océ Technologies
- 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 2010 totalled € 1.37 million (budget: € 1.41 million). A total of € 15k was spent on equipment. The total number of FTEs allocated at year-end 2010 was 13.7 (19 researchers). Prof.dr. 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, five inventions were reported and two patent applications were filed.

For details, see page 74.

DPI Fellow Katja Loos
Polymers go green

Enzymatic polymerisation is environmentally friendly and safe and is an efficient alternative for traditional polymerisation methods. It can lead to higher product yields, fewer undesirable by-products and even, in some cases, to unique or improved products.

"I want to find ways to produce plastic material in an environmentally friendly manner," says Katja Loos, associate professor at the Zernike Institute for Advanced Materials at the University of Groningen. Loos (39) is an expert in the field of enzymatic polymerisation: "Enzymatic polymerisations are environmentally friendly and safe, and form an efficient alternative to traditional polymerisation methods. They can also lead to higher product yields, fewer undesirable by-products and sometimes even to improved and/or unique products. For instance, part of my research group is working on the synthesis of polysaccharides. Well-defined polysaccharides are difficult to synthesise. The problem is the complex stereochemistry of the monosaccharide building blocks and the enormous number of possible glycosidic combinations. In traditional organic chemical reactions you always need to work with a series of protecting groups, but with enzymes you can polymerise well-defined polysaccharides reasonably easily. Here, the advantage of enzymatic polymerisations manifests itself immediately. Polysaccharides are an abundant source of raw materials that are interesting due to their bio-degradable, bio-compatible and renewable character. They are important bio-based materials with applications spanning the entire spectrum from inexpensive commodity plastics to advanced medical applications. The major constraint on the use of polysaccharides in these applications is the difficulty of producing large quantities of well-defined molecules efficiently. Saccharides are expected to play a steadily greater role as raw material and are expected to replace petrol-based materials in the future. Polysaccharides are already used in many disparate fields of industry. Of course, we're also working on enzymatic polymerisations of 'normal polymers', such as polyester, polyamides, etcetera." Katja Loos was appointed DPI Fellow in 2010.

Complex

As a DPI Fellow, Loos has received a grant of one million euro from DPI for her research. She will spend this money on the synthesis and characterisation of (highly) branched polysaccharides in order to clarify the structure-property relationship of branched polymers. Saccharide synthesis *in vivo* is a very complex process that is not regulated by universally conserved codes, and has not been automated *in vitro* yet. Ultimately, a combination of chemical and enzymatic techniques will be necessary to produce useful quantities of materials. "My ultimate objective is to translate the newly-gained knowledge on polysaccharides, as a model system, to other polymeric materials. I will appoint one PhD student to create extremely well-defined branched polysaccharides and another to characterise these polymers. They will be working very closely together. We know exactly what the branched polymers we produce ourselves look like. We can use these model systems to test methods and equipment for unknown polymers," says Loos.

The first project started in January 2011 and the necessary equipment has already been purchased and/or partially installed. The well-defined branched polysaccharides will be synthesised via cascade enzymatic polymerisation using two enzymes. In nature, the bio-synthesis of starch involves a cascade of enzyme catalysed reactions. When selecting the appropriate enzymes and reaction circumstances, reactions with multiple enzymes can be performed *in vitro*. Synthetic glycogen can be synthesised *in vitro*, for instance, through the cooperative action of phosphorylase and branching enzyme. In this reaction phosphorylase catalyses the polymerisation of glucose-1-phosphate in order to obtain linear polysaccharide chains with α-(1→4) glycosidic linkages; the branching enzyme is able to transfer short, α-(1→4) linked, oligosaccharides from the non-reducing end of starch to an α-(1→6) position. By combining the branching enzyme with phosphorylase it becomes possible to synthesise branched structures via a one-pot synthesis as phosphorylase will polymerise linear amylose and the glycogen branching enzyme will introduce the branching points which are again extended by phosphorylase. "With our method we can tune variables such as molecular weight, polydispersity and the presence and degree of branching in the synthesised polysaccharides relatively easy. We will use the synthesised polymers as model systems for the establishment of new characterisation protocols for branched polymers using size separation techniques with multiple detectors," says Loos.

Bio-catalysis

At present four of the six enzyme classes are known to induce or catalyse polymerisations. The enzymes Loos uses for polymerisations have been designed or isolated in-house. She prefers to use enzymes that are available commercially, but that is not always possible. The first step in Loos' research is to synthesise existing macromolecules in an environmentally friendly manner. She continues: "But the fun part is, of course, creating entirely new polymers through bio-catalysis. Scaling up to an industrial level must, in principle, be possible, but has not yet been done. At present, pharmaceutical products are produced commercially by means of bio-catalysis. However, for the time being, the industry only uses bio-catalysis for large-scale production of monomers"

The industrial sector is already showing interest in Loos' project. Loos: "LyondellBasell, BASF and DSM, among others, are interested in improved characterisation methods for highly branched polymers. And when I purchase equipment, I will certainly seek cooperation with partners of DPI. That is the good thing about DPI: the vast network of people involved in polymers, not only in research institutes but also in industries active in chemistry and methodology. This helps newcomers such as me to find their way around very easily and makes me feel at home right away."

Loos completed her studies in Germany and has worked in Brazil and the United States. She has been awarded prestigious prizes and awards at every stage of her career, including a Feodor-Lynen Research fellowship from the Alexander von Humboldt Foundation and a fellowship from the Spanish Ministry of Education as a visiting professor at the Technical University of Catalonia in Barcelona, Spain. She specialised in Organic Chemistry and Polymer Chemistry during her university studies. As a research fellow, she moved into the field of bio-catalysis in polymer science. She is interested in the different aspects of enzymatic polymerisations, bio-catalytic modifications of polymers and polysaccharides. In addition, part of her work has also focused on other controlled/living polymerisation techniques including anionic and controlled radical polymerisations. When asked why she opted for the Netherlands, she says: "I was offered several positions, but Groningen came out best. During the interview, there was an immediate click with the people there. Furthermore, polymer science in Groningen enjoys a truly excellent worldwide reputation." Last year, Loos received a VIDI research grant from the Netherlands Organisation for Scientific Research (NWO). "It's wonderful to have received funding from one source for basic research and from another for applied research within a four-month time span. Bridging the gap between the two worlds is precisely my research philosophy."

DPI Fellows are ambassadors of the polymer science community. According to Loos, excellent research, interesting publications and making active contributions to DPI-related conferences are the main aspects of the position. "I want to speak to a lot of people; from small children to industry representatives and academics. My message is: 'polymers are good and DPI is better.' Naturally, I am delighted to see that more and more German companies are becoming affiliated with DPI."

Katja Loos – associate professor at the Zernike Institute for Advanced Materials at the University of Groningen

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 by systematic variation of composition. Detailed characterisation of such libraries will help to develop an in-depth understanding of structure-property relationships.

A library to choose from

Robots can be used in automated experimental set-ups to synthesise a large number of different polymers with desired properties. It is more complicated, however, when highly reactive compounds are involved.

"Polyethylene oxides are very useful in a wide range of applications," Jürgen Vitz begins his explanation of his current DPI project, which is his fourth position as a post-doc and his second DPI project since he earned his PhD in 2004. At the University of Jena he is now investigating how to make libraries of well-defined polyethylene oxides that can be used as drug delivery agents or catalyst carriers for personal care products and food packaging, but also as soft segments in polyurethane products. Vitz: "The fact that polyethylene oxides are soluble in water and non-toxic makes them very attractive. Moreover, because we use a 'living' polymerisation technique we can make them with very narrow mass distributions and we can end them with all kinds of different groups and so tailor them to specific applications."

Controlled

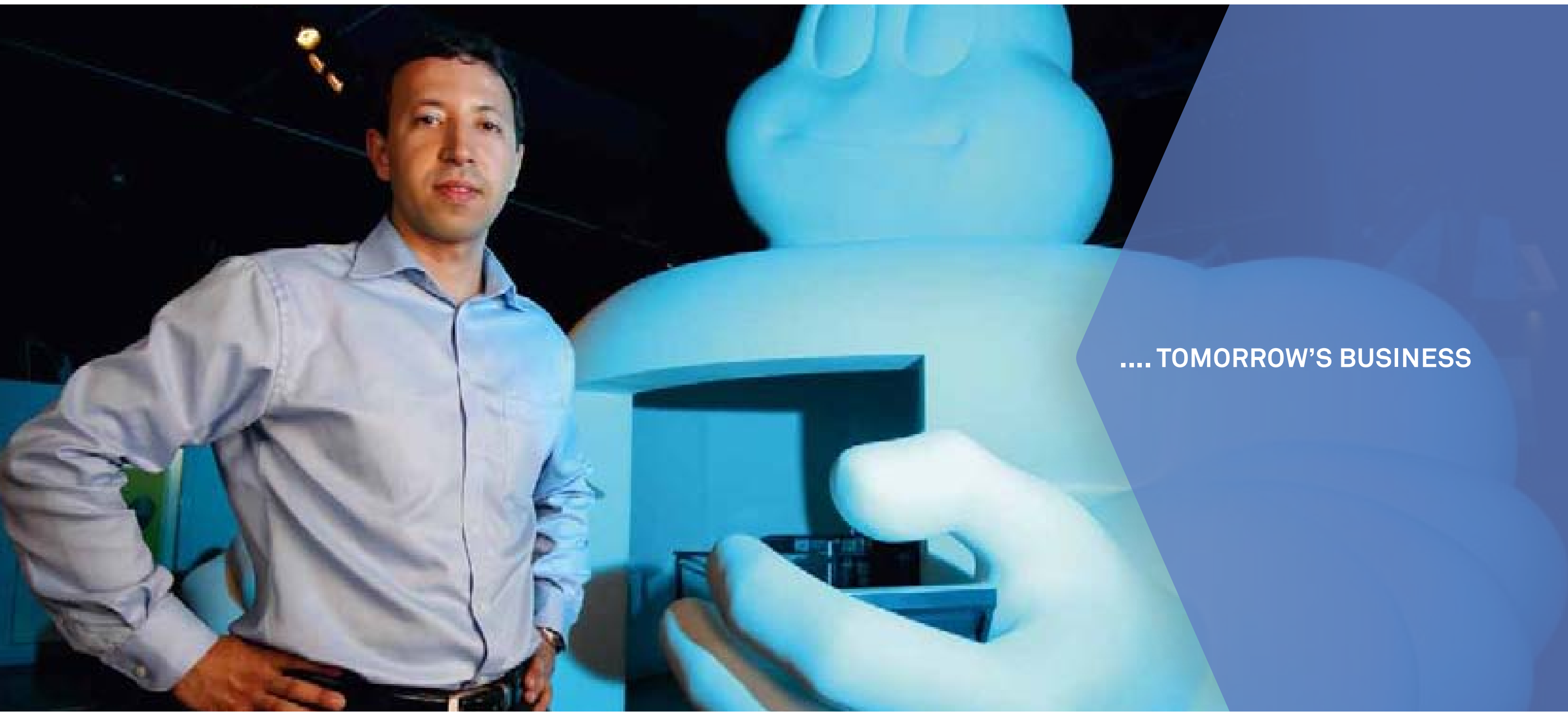
'Living' polymerisation in fact means controlled polymerisation. In such reactions polymer chains continue to grow at a constant rate, so that when the reaction is stopped the length of all the molecules is more or less the same. This is important for drug delivery applications, for instance, in which chains that are too short can be trapped in unwanted reactions and chains that are too long can agglomerate somewhere in the body. A controlled and reliable method of making a library of polyethylene oxides to choose from for the different applications would be very useful. That is the idea behind the project and of course this library will be produced using high-throughput experimentation techniques.

Vitz started his project by installing the necessary equipment, manually operated reactors for purification of the monomers and the subsequent polymerisation. It took a while because a lot of safety precautions have to be taken before it is possible to work with the reactive ethylene oxide. "We were able to successfully polymerise some polymers, such as polyisopropene and polystyrene, as well as polyethylene oxide. Now we want to continue with simple block copolymers and modify the polymers with end groups for click reactions. We want to combine them with dyes, for instance, so that they can be monitored in applications such as drug delivery. The next step will be to synthesise libraries of these polymers and to look for structure-property relationships. We will start using the Chemspeed robot for the automated synthesis of different types of copolymers," says Vitz when asked where the project stands now. Because of the necessary safety precautions, the high-throughput experimentation workflow was not straightforward and had never been performed before.

Useful

If such libraries are found to contain polymers that industry can use for different applications, the next step will be to produce them in useful quantities. The maximum size of a batch in the lab is twenty or thirty grams. "The polymerisation is quite difficult because you need very pure solvents and you have to work in the right conditions. I think industry can handle this, but it will take some time," says Vitz when asked about the prospects for industry.

Jürgen Vitz is a post-doc working at the University of Jena, Germany, on the DPI project 690, *Libraries of polyethylene oxide via parallel living anionic polymerisation*.



Making coherent materials

Improving materials consisting of many components, like polymer-additive mixtures for tires, is a time-consuming business. Compatibility maps could help in this kind of research and the hope is that they can be drawn up using high-throughput experimentation.

"I was introduced to DPI by one of my colleagues and I was already given some original and useful suggestions for our research at the kick-off meeting for this project. These contacts are certainly useful for me," says Rachid Matmour, a chemist working in the research department of Michelin in Clermont-Ferrand at the start of our conversation. Matmour is involved in the development of new tires at Michelin. Together with physical chemists, physicists and the people who prepare the formulations, he develops materials for new tires for cars, trucks and motorcycles. "When one of my colleagues comes and asks for a polymer that will improve a tire's performance (rolling resistance, grip, endurance and wear, etc.), we have to think of new polymers that could be used in combination with the approximately 200 other components in a tire, such as silica, carbon black, metals and textiles." The polymer accounts for more than half of the weight of a tire. A new polymer, or an existing polymer with a modified structure, has to be compatible with all the other components, including other polymers and additives. Consequently, testing its suitability involves many time-consuming experiments. And all too often that time is no longer available. Matmour's interest in High-Throughput Experimentation is evident.

"As soon as it became clear that Vitz's experimental set-up in Jena was operational and the sequence of the tests he would perform had been decided, we sent him four of the polymers we had previously used to see if he could characterise them. Naturally, however, our ultimate goal is to produce so-called compatibility maps that show whether polymers can be mixed with each other and with the other components," says Matmour, explaining the current phase of the project. He expects to be able to say more about the results and the prospects of the method in a few months' time.

Opportunity

Matmour is generally positive about his involvement in DPI's activities, but also has a few suggestions for improvements. "The Annual Meeting is very interesting for me. Listening to the presentations and having discussions during the poster sessions keeps me up to date with what is going on in DPI, including technology areas other than my own. It is also a good opportunity to meet PhD and post-doc students with a view to recruiting good new researchers to work in our company. It might prove even more useful for us if the present circle of good university groups, which is now concentrated in the Netherlands and Germany, were to be expanded with groups from other European countries."

The poster sessions in particular offer a good opportunity to meet with students and Matmour would like to see more time devoted to them. Furthermore, he thinks that both the industrial partners and DPI itself could be more critical with respect to the students' presentations, which he feels could be more to the point and concentrate more on answering any questions that the industrial partners in particular might have. Another challenge lying ahead for DPI, Matmour feels, is to make its procedures and its modus operandi more transparent. "It would help me to sell a DPI project within our company if I had more statistical data about the results of the projects at my disposal and knew more about the timetable for a project. In this project, for example, for a long time it was unclear when our experiments were scheduled," says Matmour.

Rachid Matmour is a research scientist with Michelin in Clermont-Ferrand in France and is involved in DPI project 690.

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.

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 methodologies. 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.

FACTS AND FIGURES

Partners from industry
- Chemspeed Technologies
- Dow
- 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 Cambridge
- University of Liverpool

Budget and organisation
Expenditure in 2010 totalled € 2.09 million (budget: € 1.81 million). A total of € 75k was spent on equipment. The total number of FTEs allocated at year-end 2010 was 21.7 (39 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 fifty reviewed papers and one thesis; five inventions were reported and six patent applications were filed.

For details, see page 75.

Workshop on hybrid materials
Maintaining Europe’s competitive edge in materials manufacturing

New materials make a vital contribution to improving the quality of life. Often, these are hybrid materials with polymers as one of their components. DPI helped to organise a workshop on hybrid materials to catalyse the process of innovation.

On Wednesday 3 and Thursday 4 March 2010 the European Technology Platform for Sustainable Chemistry (SusChem) organised, in close collaboration with DPI, the ‘Hybrid Materials Workshop’ in Luxembourg. In five parallel sessions, about 100 participants from fourteen different countries discussed the prospects for the development of new materials over the next ten years in the following industrial sectors: automotive, solar energy, solid-state lighting, civil engineering and aviation and aerospace. With the growing demand for raw materials and energy as the world population grows, the materials and processes used must have a smaller ecological footprint than those currently used without compromising on the desired properties of the materials.

Europe has many materials manufacturers, giving it a competitive edge over Asia and the USA. Innovation is a key driver in maintaining Europe’s competitiveness. Preserving the strength of materials research will promote sustainability and help the European economy by creating job opportunities. Stakeholders throughout the value chain in different industrial sectors need to work together to maintain European technology leadership. The EU initiates and facilitates research programmes intended to raise the level of materials performance. SusChem organised the workshop to lay the groundwork and set the research agenda in this field for the next ten years. Since polymers play an important role in material innovation, DPI was a logical partner for the event.

List of topics

During the five workshops, presentations were given by speakers from end users, materials suppliers and academia. After the presentations, the participants and the speakers held a panel discussion about the research topics that need to be addressed to achieve major breakthroughs in the development of materials for the relevant sector. A list of priorities in the research topics to be addressed was produced for each of the five application areas. Despite the wide variety of applications of the materials, the five workshops arrived at some common conclusions with respect to new polymer composite materials.

Main conclusions:

- New materials should be considered in relation to the industrial-scale processes needed to produce them in light of overall costs, industrial safety and environmental requirements. Naturally, the lowest costs and the lowest environmental impact will be achieved if existing material flows and renewable resources are used.
- On the one hand, there is a need for multi-scale models to predict the properties of proposed new materials. At the same time, validation tools, standard characterisation methods and high-throughput tools are required to shorten the evaluation times when current materials are being replaced by other (hybrid) materials.
- New materials should preferably be recyclable or degradable. Recyclable products should, in view of the difficulty of separating different plastics, preferably comprise a single polymer. The disassembly and recycling process should be considered in connection with the production process. Life cycle analysis is important in order to determine when to recycle or disassemble. New business models which treat the materials less as a product and more as a service will play a role in some sectors in the future. This will make recycling more centralised and thus a more standardised activity, which can then be performed as efficiently as possible.
- The aim in every area of application should be to use light-weight materials without making concessions on mechanical properties. Lighter-weight materials need less energy to move and thus reduce emissions.
- To reduce maintenance costs, materials should be 'smart', meaning that they can clean or heal themselves or in some way sense when intervention or replacement is necessary.
- Materials should combine functions such as corrosion prevention, reduction of water penetration, flame retardation, resistance to wear and UV light and should have the capacity to store energy.
- Insight into fundamental aspects such as compatibility and interface properties between different hybrid materials and the influence of molecular structure on the properties of materials is evidently needed to meet all of the above requirements for new hybrid materials.

Stakeholders

R&D needs to cover the spectrum from fundamental research to applied development, which will call for an intensive partnership between public funding bodies and industry. Fundamental studies should be funded from public sources, while applied materials development and modifications should be the sole responsibility of industry. Between these extremes, pre-competitive R&D on new hybrid materials and coatings, monitoring methods and applied modelling tools should be jointly financed with public and private funding. It is important for stakeholders in the entire value chain to be involved in this process. The European Commission and DPI both have an important role to play in bringing stakeholders together to correctly identify the R&D that is required.

The open atmosphere encouraged the participants to build value chains between end users, materials suppliers and academic leaders. The conclusions of the workshop were collected in an advisory report, which was sent to national governments and the European Commission. The document has also been published on the websites of SusChem and DPI. The report was enthusiastically received by the European Commission and the communities of SusChem and DPI. The output from the workshop will definitely lead to a more detailed investigation, which will serve as input for the European research agenda.

Knowledge transfer

DPI's entire management team attended the meeting. Since DPI and DPI Value Centre collaborate closely in creating knowledge (DPI) and translating knowledge into new processes and products (DPI Value Centre), the name of the game is to close the value chain from the polymer producer to the end user. For DPI and its partners, the main benefit of the workshop on hybrid materials was that it brought together polymer producers, who are DPI's predominant partners, and the end users of innovative new materials, who often define the necessary specifications for new materials. Because hybrid materials offer considerable potential for new process and product innovations, in terms of closing the value chain DPI and DPI Value Centre were particularly interested in the specifications and demands of end users with regard to new materials. That information will enable DPI to match the demands of the end users with those of the polymer producers in each technology area in the definition of future calls for proposals.

The outcome of the workshop is that DPI now has a clearer impression of the specifications that new materials will have to meet to generate the new innovations the market needs to address the 'grand challenges' facing the EU in the areas of mobility, energy saving, health, climate change and water shortages, in the five markets (automotive, solar energy, solid-state lighting, civil engineering and aviation and aerospace). At the same time, there is a better understanding of progress in the development of hybrid material solutions for specific markets as presented by polymer producers and academic experts. This information provides useful input for defining DPI's future research agenda, its updated strategy and the innovative activities of the DPI Value Centre.

The event in Luxembourg was organised with the support of the European Commission.

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.

Improving on nature

Biological polymers inspire polymer scientists to synthesise polymers with useful properties, but synthetic emulsifiers with enhanced performance can also provide inspiration for trying to create biological emulsifiers.

"The prospect of constantly finding new applications was one of the reasons I chose to study food technology at Wageningen University. After earning my Master's degree, I gladly seized the opportunity to continue working with the same group for my PhD project," says Silvia van Kempen, who has been working on the project for two and a half years now. Her work involves synthesising and testing new emulsifiers that could be used in food. An emulsifier is a molecule consisting of water-loving and oil-loving blocks, which allows water and oil to mix and form stable food products such as desserts and sauces. Inspired by synthetic emulsifiers that perform better than the bio-materials that are currently used (such as proteins, fatty acids and sucrose esters), Van Kempen tries to create similar molecules from food-grade ingredients. "We have combined hydrophilic oligofructose and a hydrophobic fatty acid to create a molecule that bears a closer resemblance to the synthetic emulsifier. Sucrose esters based on sucrose and fatty acids are already commercially available. The difference between those products and ours is the size of the hydrophilic group. We use an oligosaccharide instead of the dissaccharide sucrose. We are among the few in the world to do that," says Van Kempen, when asked about the essence of her approach.

Obesity

Improved emulsifiers could help in the production of healthy food with a low caloric value and hence in solving the ever-growing problem of obesity. But these polymers can also be used as foam agents, where water and air have to be mixed to form a stable substance. The applications of the polymers are clear enough. Van Kempen is now testing the molecules she has synthesised in model systems, consisting of water and fat or water and air. "The next step will be to test them in real food products with a different pH and in the presence of other ingredients. In particular, we have to test them in the presence of proteins that also serve as emulsifiers. Our polymers have to replace these proteins at the interfaces between the water and fat phases. We do not yet know whether our polymers will display the same efficient emulsifying behavior with and without these proteins present," says Van Kempen. But she is confident that they will and has enough time to perform all the necessary experiments before her project ends. There will also be time to test whether these polymers could prove useful in encapsulation applications for the pharmaceutical industry.

Challenge

Van Kempen is assisted in her work by Bachelor's and Master's students engaged in their research projects. "The challenge lies in trying to steer them in the right direction without telling them what to do," she says of this aspect of her project. Presenting her work at the DPI cluster meetings certainly has advantages, according to Van Kempen: "I am often given useful suggestions, and once I received an offer to use special equipment that we do not have in our lab. I will certainly take up that offer when the time is right." The questions asked by the industrial partners during these meetings often relate directly to potential applications and are sometimes impossible to answer yet. Even so, Van Kempen realises the importance of keeping in mind the application aspect and the advantages of alternatives. The current generation of emulsifiers works, but if better ones could be used in smaller quantities, for instance, it might be possible to reduce the costs.

Silvia van Kempen works at Wageningen University, the Netherlands, on DPI project 687, *BioAmphiphiles: functionality of novel amphiphylic biomaterials synthesised by enzymatic linking of polysaccharides, food proteins and fatty acids*.

Linking micro-structure to texture

Food products such as cheese can be investigated with the same methods as other materials. The challenge is to link the parameters of a material's microstructure to texture and, eventually, to the consumer's taste.

"My company is naturally interested in making emulsifiers from biological materials that are as good as synthetic emulsifiers. And if this project leads to an application, we already have all the ingredients in-house," says Timo Faber, who plays a dual role in DPI's Bio-Inspired Polymers technology area. He is a PhD student in the Polymer Technology Group at Eindhoven University of Technology as well as the industrial contact person from FrieslandCampina for Van Kempen's project. After graduating in Chemical Engineering in 2004, Faber joined Campina, which later merged with Friesland Foods, as a process developer. He initially worked on the applications side of the business, but five years later he decided to start a research project. For the duration of his project he is seconded to Han Meijer's Polymer Technology Group, where he is investigating the relationship between the micro-structure of cheese and its texture. His hope is that the texture of cheese can be directly related to measurable rheological parameters.

Contradictory

Models play a large role in this study. Cheese can be regarded as a matrix of water and proteins sprinkled with fat particles. It is not only the amount of fat, but also its position in the matrix, that determines the structure and the texture of the cheese. Emulsifiers play a role in the relative position of fat and water and accordingly they are of interest, not only for cheese but also for foamed milk for cappuccino coffee and whipped cream, for example. "Essentially, we have to reconcile two contradictory requirements in such food products," says Faber. "On the one hand, we want them to remain stable from the moment they are produced until they are consumed, but at the same time they must disintegrate in the desired way. Surfactants and emulsifiers play an important role in that process, but also, for example, in terms of the possibility of adding just enough fat to a food product to give it the correct taste but not too many calories." This fits in with the FrieslandCampina's innovation strategy, which is focused on health & wellness and functionality. The company is the largest dairy cooperative and one of the three largest dairy companies in the world.

Fundamental

"I am embedded in the university world now, but I also have first-hand experience of a company's needs. I have to translate fairly fundamental knowledge into applications. I like that aspect, but the work is also of benefit for FrieslandCampina, since it has access to potentially interesting new knowledge. One of my Master's students, for instance, will do part of her project at FrieslandCampina's research facility in Deventer. To give another example, last summer I invited one of my colleagues from Eindhoven to give a presentation in Deventer on 'soft matter', a subject that I thought would be of interest to the company. That contact generated a new project proposal," says Faber to illustrate the strong links between DPI and FrieslandCampina. In general, he is very satisfied with the effectiveness of knowledge transfer from DPI to its partners, not only in specific technology areas but also across the boundaries. He is particularly pleased with the recent attention devoted to multi-scale models.

Timo Faber is working in research at FrieslandCampina and has been seconded to the Polymer Technology group of the Eindhoven University of Technology, the Netherlands, for the duration of his own PhD project. He is also involved in DPI project 687.

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.

Bio-Inspired Polymers can be produced from renewable or fossil resources through either chemo-catalysis 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.

FACTS AND FIGURES

Partners from industry

- DSM
- Evonik
- Food and Biobased Research, Wageningen UR
- FrieslandCampina
- Océ Technologies
- 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 2010 totalled € 1.62 million (budget: € 1.81 million). A total of € 31k was spent on equipment. The total number of FTEs allocated at year-end 2010 was 14.7 (23 researchers). Prof.dr. Gerrit Eggink acted as Scientific Chairman and Dr. Peter Nossin as Programme Area Coordinator of the Bio-Inspired Polymers Technology Area.

Publications and inventions

The research programme in this Technology Area generated a total of seven reviewed papers and one theses; two inventions were reported and two patent applications were filed.

For details, see page 77.

Workshop on nanocomposites

Exploiting the increased interface surface to enhance the properties

On 27 May 2010 over thirty people attended a DPI workshop on nanocomposites to discuss the science and technology of these fascinating materials. After an inspiring lecture by Professor Costantino Creton, PhD students and other scientists discussed their research work and shared their experiences and ideas with the aim of learning from each other and promoting research in the field of nanocomposites.

"Why are nanocomposites so interesting for materials research and applications?" That was the main question raised by Costantino Creton, who studies the mechanical properties of polymers at interfaces at the French ESPCI ParisTech research institute. He focused on the mechanical aspects of nanocomposites, which are – especially the polymeric ones – interesting due to a combination of properties. The large interfacial surface area between the polymer and the relatively small fraction of nano-sized filler material can change the properties of the material in a positive way. Because the particles are so small, transparent materials with improved mechanical properties can be manufactured. Furthermore, the size of the filler nanoparticles is comparable to, or even smaller than, the radius of gyration for polymer chains, so nanoparticles are able to influence polymer chain configurations and structure formation through self-assembly.

Killer application

Although nanocomposites are hot in the academic world, no 'killer' industrial applications of nanocomposites have been found yet. There are two reasons for that. First, it is not yet clear how the processing variables of an industrial-scale process influence the nanocomposite structure. Second, the relationship between the nanocomposite structure and the macroscopic properties of products made from them is largely uncertain. The path to industrial application will open up once there is a suitable model for 'translating nano to macro'. To make such a model successful, we also need to look at the microscopic scale, so it is necessary to understand the processes taking place at the length-scale in between nano and macro.

According to Creton, polymer nanocomposites are especially useful when more than one property of 'standard' polymers has to be improved. Take elastomers, thermoplasts or thermosets, for example, which need to be tougher but still have to be transparent. Or polymers that have to be electrically conductive and transparent. Nanocellulose is interesting as filler material when mechanical properties have to be improved, whereas carbon nanotubes improve electrical properties.

Other applications were mentioned, such as the use of nanocomposites in water-borne transparent coatings. The exchange of knowledge between coating and engineering applications is well organised within DPI.

Preparation

Problems arising in relation to preparation mainly concern the dispersion of nanoparticles into the polymeric matrix. Several routes are being investigated to disperse nanoparticles made of, for instance, calcium carbonate, silica, titanium, carbon (nanotubes or graphene sheets) or nanoclay: melt compounding, solution and evaporation or precipitation, in-situ preparation of the particles during synthesis of the polymer itself. And would it even be possible to develop hierarchic composites (with an ordered structure on very different length scales) by reactive self-organisation?

It seems to be difficult to control the state of dispersion and the quantity of nanoparticles within the dispersion during these processing steps. And what is the right dispersion technique for a given morphology? It is already a challenge to develop well-defined 'model' materials for understanding nanocomposite features. At this nanoscale, a method needs to be found to properly 'measure dispersion' - beyond the images that show dispersion.

Characterisation

There is a wide variety of characterisation methods for nanocomposites, for both surface and bulk. Besides 'conventional techniques' such as Transmitting Electron Microscopy, Scanning Electron Microscopy, Scanning Transmitting Electron Microscopy, etc. to show materials structures and morphology, it is possible to obtain chemical information via techniques like Tip Enhanced Raman Spectroscopy (TERS) and Enhanced Ellipsometry. Specific techniques are available to measure mechanical properties at nanoscale (stress/strain, local), and it is possible to use conductive AFM for measuring electrical properties.

To find your way through this 'labyrinth' of characterisation techniques, it is essential to carefully define what you would like to know and to work in close collaboration with a characterisation expert. More than one characterisation technique is often required to find answers at the nano, macro and micro-scale. And how do you characterise a mechanical interface at a nanometer scale? For nanocomposites, knowledge from both sides, organic polymer and inorganic filler, is necessary. Apart from this experimental approach, reliable predictive models – including models for non-linear properties that can be validated by the experiments – are needed.

Qualitative interpretation of nanoscaled structures already presents many challenges, but the necessary quantification to connect the nanoscale effects to the macroscopic properties is even more difficult to achieve.

Insights

A lot of questions remained unanswered at this workshop, or raised new questions. But new insights were also gained. For example, take the filler as the starting point instead of the polymer matrix. If we know how to organise the particles, we can perhaps make the polymers afterwards. Self-healing aspects are also challenging. And, can we go supramolecular?

As a general conclusion, this workshop showed that it is necessary to bring our knowledge of what is going on at the different length scales together – atoms, intermediate scales and 'the real world'. Nanocomposites are still quite difficult to understand and going straight from nano-fillers and polymers to car bumpers or solar panels (to name just two of the many possible applications) requires a giant leap. To make that leap, we need at least an understanding of the intermediate length scales.

The ins and outs of polymer nanocomposites

Engineering plastics can be improved – for example, made mechanically stronger or electrically conducting – by incorporating filler materials. Traditional fillers such as microscopically small talc, glass or carbon black particles have to be added to the polymeric 'matrix' in amounts of at least fifteen to twenty volume percent to obtain a noticeable result. Unfortunately, this relatively large fraction will impair the 'looks' of the original material (make it less smooth, less transparent) or make it more brittle or denser. It would be wiser to put smaller – nanoscale – fillers into the polymer matrix. Et voila, a polymeric nanocomposite has been born.

A nanocomposite can be defined as a solid material, consisting of more than one phase: matrix and nanoparticles with typical dimensions of less than 100 nanometer. These nanoparticles are, for example, carbon nanotubes with a diameter of a few nanometers and a length of micrometers or exfoliated clay platelets with a thickness of a few nanometers and a much larger diameter. Especially these non-spherical nanoparticles can form a continuous network (conducting when using a conductive filler) at lower volume fractions – less than one volume percent – than their traditional counterparts.

Due to the very high surface-to-volume ratio of the nanoparticles, mechanical, electrical and other properties of nanocomposites will differ from 'normal' composites. Thinner and smaller nanotubes or platelets result in more surface area for interaction with the polymer. Material properties of the polymer will differ considerably in the vicinity of these nanoparticles. Even a small fraction of nanoparticles will have a large influence. For an optimal effect, the nanoparticles have to be dispersed into the polymer matrix during processing. There are still many challenges to overcome in this regard.

Besides mechanical improvement of polymers, nanoparticles with a high aspect ratio that are homogeneously dispersed in polymers will act as a barrier for oxygen transport through plastic sheets (cling films), or as a flame-retarding material by forming barriers between air and fuel.

LARGE-AREA THIN-FILM ELECTRONICS

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

Multilayer doped devices by solution processing

The major advantage of polymer light-emitting diodes (PLEDs) is that they can be processed on large areas from solutions. But the light generation has to be thoroughly understood before the influence of process conditions can be assessed.

The advantage of PLEDs is that, in principle, they can be fabricated on a large surface using roll-to-roll processing. However, a larger area means that there is a greater chance of short circuits. To avoid that problem, the light-emitting layer can be made thicker, but unfortunately the efficiency of the PLED then declines. Mingtao Lu is trying to remedy that by making the light-emitting process more efficient. "One way to overcome these issues is by fabricating multilayer PLEDs. With this method electrons and holes are conducted via the charge transport layers, recombine in the emission layer and generate light. To increase the efficiency we have to dope the transport layers. For multilayer LEDs based on small organic molecules, doping can be accomplished by simultaneous thermal co-evaporation of the dopant and the host. That is not the case with PLEDs, since polymers cannot sustain high temperatures. So we have to blend the dopant and the host materials in solution. At the same time, we have to deal with the issue of solubility. The deposition from the subsequent layer must not dissolve the existing layers, so we also have to consider the solvent system in combination with the doping," says Lu to explain the challenge he is facing. With n-type doping, reactive metals, such as barium or calcium, can be replaced by non-reactive metals, such as aluminum or silver, as the cathode, and the lifetime of the device can be greatly extended without sacrificing on its efficiency."

Dopant

Making a dual-layer PLED with a doped hole transport layer (HTL) is a fairly new method that has not been employed by many researchers up to now. The polymer for the HTL can be spin-coated from a chloroform solution. However, blending the dopant solution in the polymer solution may destroy the solubility and the ensuing aggregates may ruin the spin-coating process, so a delicate balance has to be found. Lu is trying to discover a method of suppressing the aggregation. The emission layer can subsequently be spin-coated from a toluene solution without dissolving the p-doped HTL. "We are now working on the third layer. We have already found a very efficient air-stable n-type dopant for that layer and we plan to dissolve both the dopant and the polymer in ethanol," says Lu when asked about the status of his work.

Mystery

"People at DPI are more interested in the performance of a device, such as its lifetime or efficiency," says Lu, "while we always focus on the mechanisms of the charge transport and light generation. A better insight into those mechanisms can help us to understand the behavior of the device and give us guidance on how we can improve its performance. Some of the solvents we use will certainly not be used in an industrial process because they are toxic. But by designing energy-efficient devices we can contribute to the future of large-area lighting. Finding solutions that can be used in an industrial environment is the next issue to be addressed."

It is apparent that Lu wants to get to the bottom of this mystery, but he also realises the importance of being guided by the possible applications of his work. "DPI forms a useful bridge between universities and companies. The three-monthly reports help me to organise my research and systematically arrange the work I have done."

Mingtao Lu is a PhD student at the University of Groningen working on DPI project 618, *Polymer light-emitting diodes with doped charge transport layers*.

Towards efficient and versatile light

The advantages of organic light-emitting diodes are clear. They are efficient and can, in principle, be designed to fit any surface, provided that the processing methods for large surfaces live up to expectations.

Vincent Thulliez is a materials scientist with Solvay. For the last ten years he has been involved in new business development, an important activity now that Solvay has sold its pharmaceuticals division and will in future concentrate on polymers and chemicals. After formerly devoting his time to subjects such as lithium batteries and electrodialysis membranes, since 2006 Thulliez has been engaged in organic electronics. "When organic electronics was identified by internal and external advisers as a field in specialty polymers and chemicals that was worth exploring, we started conducting some basic research in this new field. In 2006 we started cooperating with Georgia Tech and in 2008 we set up our own laboratory. For the last year Solvay has been a partner of DPI in the Large-Area Thin-Film Electronics technology area," Thulliez says to explain his association with DPI. One of the subjects in organic electronics is organic light-emitting diodes for lighting.

Trade-off

Organic LEDs have an emission layer consisting of either small organic molecules or polymers. The existing products, displays in mobile phones, are mainly based on small molecules, but it has long been believed that the best prospects for large lighting surfaces lie with polymers. "There is always a trade-off between the cost of production and efficiency," says Thulliez. "Polymers are less efficient but can be solution-processed, while small molecules have a higher efficiency but are more complicated to process. That situation is changing now. At Solvay, as in other companies, we are investigating small molecules that can also be solution-processed. But that does not mean that Lu's work is not useful," Thulliez hastens to add. "The dopants and the solvents systems he is working on can also play a role in small-molecule OLEDs. I also expect that hybrid systems based on combinations of vacuum processing and solution processing will play a role in some of the envisaged products."
In terms of general lighting, Thulliez believes that applications such as luminous tiles could become reality in about five years from now, while the larger surfaces of luminous wallpaper will probably take longer. "For the tiles a combination of solution and vacuum processing is feasible and even advantageous. If you deposit the hole transportation layer from a solution this layer acts as a planarisation layer for the other layers." Lu's work will provide insight into the compatibility of the materials and the processing technologies.

Less risky

As a relative newcomer to a field that has existed since the 1980s, the connection with DPI is very valuable for Solvay. "Through DPI we have access to some of the top scientists in the world in this field. Their research may not be directly connected with what we are doing today, but it could open up opportunities for us. The dopants, for instance, are something we are interested in. Device modelling, in which DPI's academic partners excel, might seem to be of less direct relevance for a raw materials supplier like Solvay, but the results of this work have consequences for the materials as well. The fact that we share the costs of this pre-competitive research with other companies makes it less risky and gives us access to results that would be too off-topic to conduct the research ourselves." The fact that most meetings take place in Eindhoven, only one and a half hours from Brussels, where Thulliez works, is another advantage.

Vincent Thulliez is technical marketing manager for organic electronics at Solvay, Brussels, Belgium, and is involved in DPI project 618.

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.

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 the device performance (efficacy, homogeneity of light output).

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 2010 totalled € 0.81 million (budget: € 1.21 million). There was no money spent on equipment. The total number of FTEs allocated at year-end 2010 was 10.6 (12 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 five reviewed papers and two inventions were reported.

For details, see page 78.

Workshop on bio-polymers
Still a few missing links

The market wants partially or completely green plastics. The bio-polymer process industry and its customers – such as the packaging industry, the automotive industry and building contractors – are in the starting blocks.

Plastics manufacturers and research institutes such as DPI are often approached for advice and ideas about new bio-materials and associated processing methods. Bio-polymers are in demand because consumers want a 'greener' lifestyle. We want environmentally friendly packaging for the products we use, and green plastics in our homes and cars. The market is crying out for green products, but the manufacturers and process industries are lagging behind. At an academic level and on a small scale it is all possible, but the supply of suitable green plastic cannot yet meet the demand. There are still quite a few missing links, particularly towards the end of the value chain.

DPI brought together parties in the demand and supply chain for green plastics for the first time on 12 October 2010. During this workshop it became apparent how far apart the two sides still are. Representatives from the various industries were given the stage and they were eager to present their demands, proving how topical this subject is. The presentations provided clear evidence that large chemical companies in a position to supply green plastics to meet the demand do not exist yet. Nobody had any real answers to the questions, and where there were answers they could not be used to build on.

Everybody agreed that it was a very interesting meeting, even if the only result was to determine the position of bio-polymers. Perhaps it is a typically Dutch approach: the academic research world is running at top speed in many different directions, exploring countless golden promises, but the hype has run away with itself. Only a few kilograms, or at best a few tonnes, of the most promising bio-plastics are currently being produced. There are still too few test plants and pilot production projects for the liking of the next links in the chain, the manufacturers and processors of biomaterials. There is not enough material to perform experiments or to conduct research into ways of adapting it to the processes and machinery. For example, for the bio-polymers that have been suggested for use in certain applications it is not yet clear how the material crystallises and how it behaves in the mould. We need to discover more about the manufacturing process. It is now time to determine how to take the next steps towards large-scale production.

Who and how?

The largest manufacturer of bio-polymers in the world, Cargill's subsidiary NatureWorks, currently produces 140,000 tonnes of polylactide in the United States. It is the only manufacturing plant of a reasonable size in the world. Of course, there are many initiatives to make existing products greener. The Japanese company Teijin, which produces aramid fibres in a process acquired from AkzoNobel, recently announced that together with the Amsterdam-based research company Avantium, it was going to make its strong fibres greener, employing furandicarboxylic acid developed from carbohydrates by Avantium. Even Coca-Cola, which is heavily involved in packaging, is planning to make its PET bottle greener. One of the ingredients for PET can already be produced organically, which makes the famous bottle 20% greener. Replacing the other ingredient, terephthalic acid (TPA), with furans would make the famous carbonated drinks bottle completely organic. But from the choice of words, 'would make', it is apparent that this is not imminent. The global production of terephthalic acid is approximately 50 million tonnes, a third of which is required for the packaging of soft drinks alone. The first test plants for the production of its replacement, (bio)furans, which will produce several tonnes, have been announced. This example clearly demonstrates that apart from missing links in the supply chain, production still needs to be scaled up.

Cost

Consumers want green products and green packaging. They want green cars, not only in terms of fuel consumption, but also in the materials used. Those materials are increasingly polymers, and more specifically bio-polymers. The manufacturers not only want the materials to be green but preferably also to have better properties than existing materials. Some green nylons, for instance, have better resistance to salt and could be used for a base plate. But most of the materials still need to be assessed to judge whether they are better or worse than the fossil polymers currently in use. The bio-polymer industry has now reached that point. To sum up, there is certainly a demand for bio-polymers, but industry cannot meet it and cannot provide the answers to all the questions about properties of the materials.

The industry finds itself in a vicious circle, in which, according to various representatives of the end users, one aspect plays a dominant role: cost. Scaling up production and testing materials are very expensive activities. Useful bio-materials will remain very expensive as long as they are only manufactured in small quantities. The price first needs to come down, but this is only possible if production is higher. The day is approaching when we will break out of this vicious circle, and if the green trend continues it will arrive soon. The Netherlands will have to pay attention. It is not enough to just deliver one academic tour de force after another, the country must also clearly demonstrate in practice that the new bio-materials can fulfil a role.

Tremendous interest

It was interesting to note how many end users were almost begging for new materials. Representatives from the automotive industry, the packaging industry, the construction industry, and even the head of research at a large manufacturer of personal care products, had questions about new materials. These questions related not only to the green image of bio-polymers and how they could use it to cater to consumer demands, but also more specific questions concerning material properties.

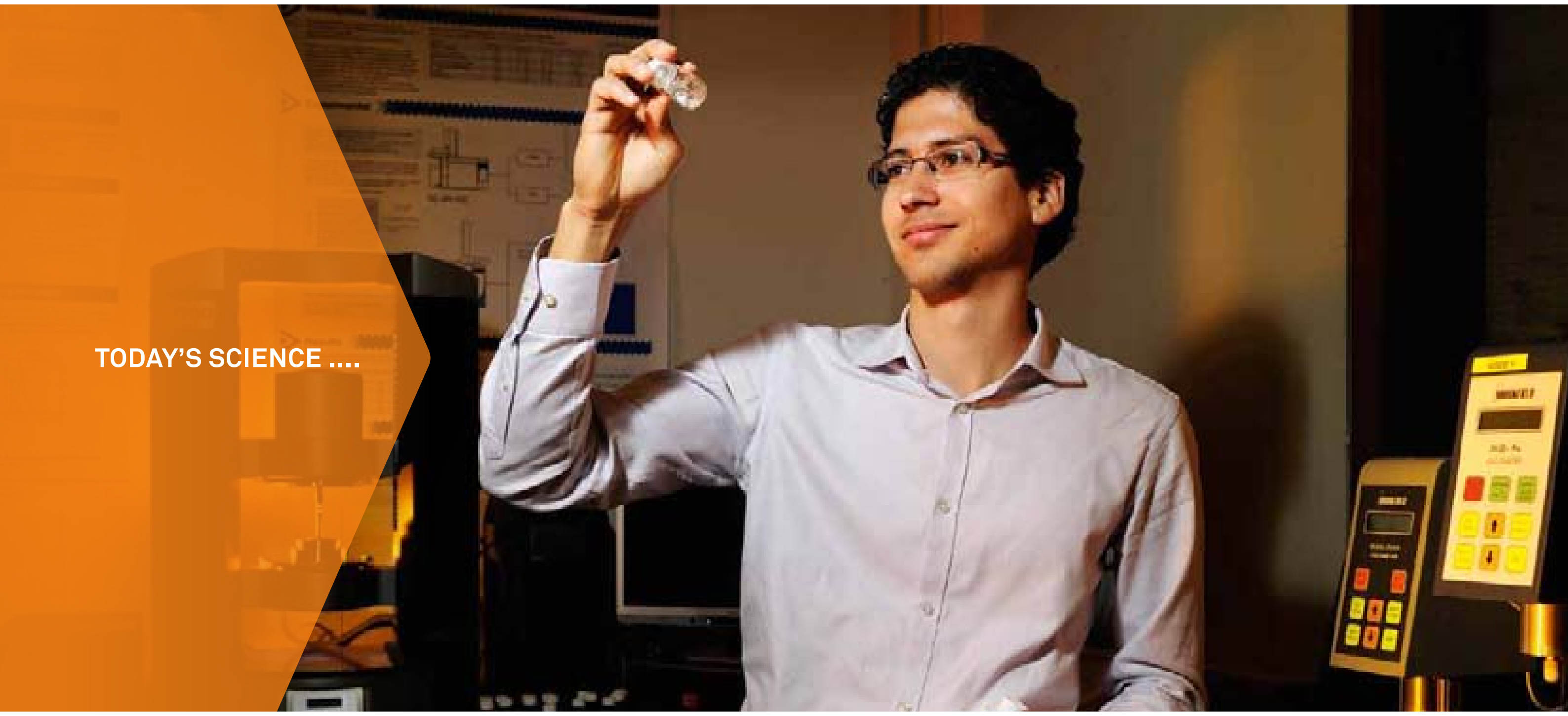
The building industry, for instance, is wrestling with the problem of what to do when the economic life of a building ends and it has to be demolished. For them, the ideal situation would be if the materials could simply be recycled or are naturally degradable.

Perhaps it is a good thing that the academic world, focused as it is on new materials and new processes in which fermentation and other forms of (bio)catalysis play a role, is also asking itself how to apply these materials in industrial practice. DPI is planning to send out a call for proposals in 2012 as a basis for a bio-based programme as part of the technology areas Coatings Technology, Performance Polymers and Bio-Inspired Polymers.

Some examples of bio-plastics

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.



Polymers for transport

Newly synthesised polymers with special properties could help to increase the volume of oil recovered from existing oil fields, but may also improve the transport of drugs in the human body and facilitate the incorporation of additives into cosmetics.

Diego Wever commenced his DPI project eighteen months ago. Enthusiastically, he explains what it is all about. "In a light oil field, about 20% to 25% of the oil automatically comes to the surface once a well is drilled. Another 30%, on average, can be extracted by injecting water in the oil-bearing rock and forcing the mixture of water and oil to the surface. By heating the water or using steam, about 10% more oil can be recovered, but that obviously uses energy. An alternative way of extracting more oil is to add an extra ingredient to the water to make it thicker, so that more oil will be dragged along. Oil and water do not mix readily, but the oil can be mobilised more efficiently with special water-soluble polymers."

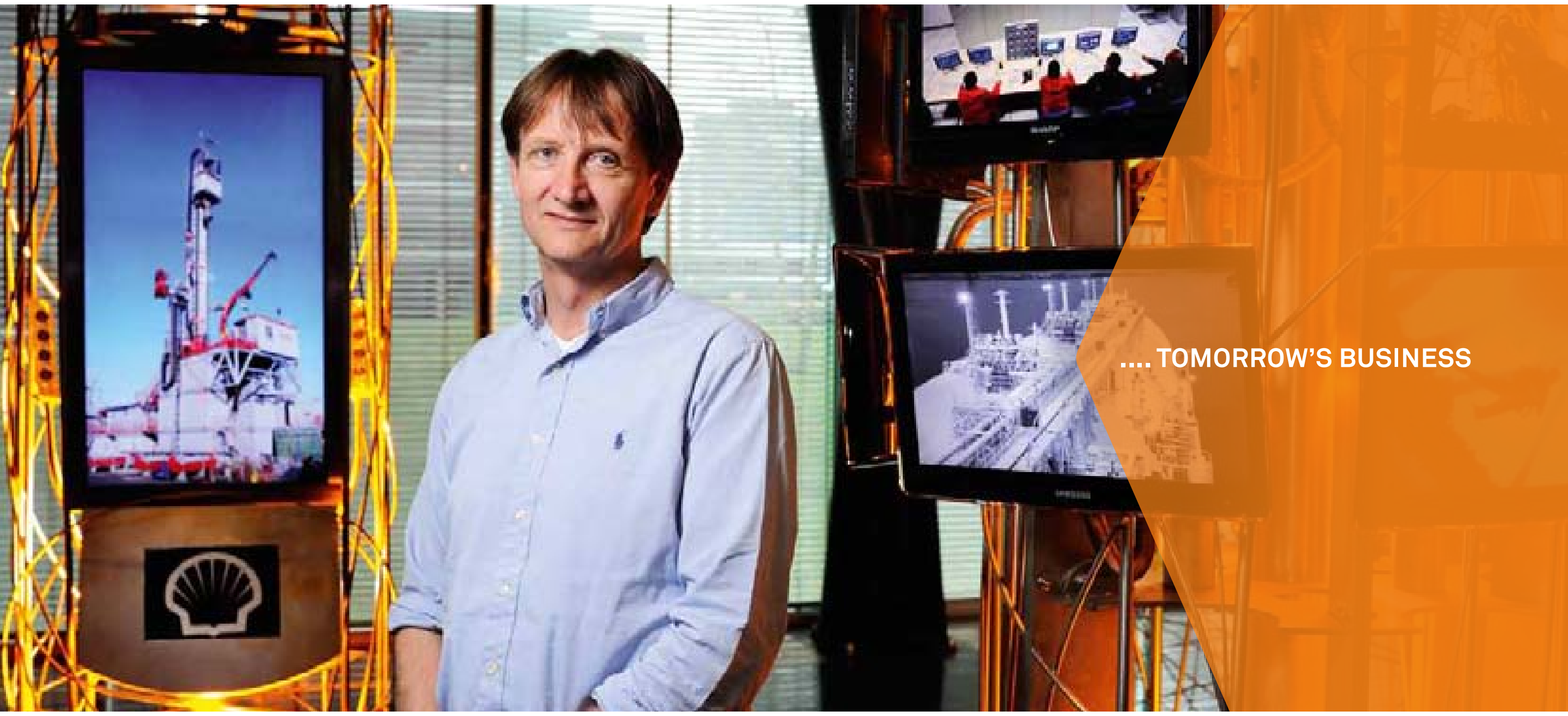
Water-soluble

This method of producing oil is already applied in some countries, for example in China, where oil fields are easily accessible. However, there is a lot of trial and error involved in choosing the right polymer. An understanding of why some polymers have the desired effect and others do not would be helpful. Wever started by making an inventory of the properties that suitable polymers must possess. Some of them are self-evident. They must, of course, be water-soluble. They must also be resistant to high temperatures and biodegrade in a controlled and sustainable fashion. They should not be too small to drag the oil along, but also not so big that they get caught in the pores of the rock. Finally, they should not cross-link. Naturally, the polymer should not be toxic because, even though it can be reclaimed for reuse, small concentrations may still end up in the environment. Particularly in the North Sea oil fields, the regulations are very strict. Wever's analysis resulted in an article that was accepted for publication in Progress in Polymer Science.

Patent

From the list of properties Wever deduced the ideal structure and properties of the polymers. He is now trying to synthesise them. "I am sorry, but I cannot say much about that, since we are currently applying for a patent," he says apologetically. No mean achievement for a PhD student eighteen months into his project: a publication already accepted and a patent application underway. "The project is going really well," Wever concedes. "Once we have produced the polymer we can test it in an experimental set-up. We have small samples of rock with pores similar to oil-bearing rock and can measure the mixture flow and the oil concentrations before and after the rock. We will be able to evaluate the influence of parameters such as temperature and pressure and the effect of adding certain chemicals, such as salts. The process can be scaled up later, but for now the important thing is to gain a clear understanding of why the system works. Of course, the polymer we design should not be too expensive. The solution must be economically viable."
Although the current focus of the research is on Enhanced Oil Recovery, the polymers concerned could also be used for applications where components have to be transported in a flow, such as drugs transport, or as additives in cosmetics. "Water-soluble polymers have many advantages, and since most DPI research is concerned with polymers in a melt they could represent a rewarding new technology area," says Wevers. In the course of 2011 Wever will be joined by a post-doc student, who will investigate how the use of polymeric-surfactants could improve the performance of chemical Enhanced Oil Recovery.

Diego Wever is a PhD student at the University of Groningen, the Netherlands, working on DPI project 716, *Design of new chemical products (polymers and amphiphilics) for Enhanced Oil Recovery*.



Practice challenges science

When speed is of the essence, there is often a tendency to resort to proven methods without necessarily fully understanding how they work. The role of polymers in the field of oil recovery is a case in point. When their role is better understood, they can be applied more widely and effectively.

Diederik Boersma returned to the Netherlands eighteen months ago and is now working in Shell's Upstream division, its research organisation for oil recovery. For the previous six and a half years he had been working in the oil fields of Oman, where he returned to the subject of his PhD at Delft University of Technology, Enhanced Oil Recovery. "Oman has oil, but it is less accessible than the oil in the other countries of the Middle East. The oil there is either very deep beneath the surface, has a high viscosity, is very heavy or the oil-bearing rock has a low permeability. It is therefore not surprising that the largest polymer injection project outside China is in that country," says Boersma. By injecting water with polymers to make its viscosity similar to that of oil, more oil can be brought to the surface. When he mentions that 100,000 barrels of water with polymers are used in that process every day, Shell's interest in making the polymers perform more efficiently becomes very evident. Another reason to look for alternative polymers is that the current generation can only be used at temperatures below 70 degrees Centigrade and with water that is not too saline. There are plenty of oil reservoirs around the globe where polymer flooding would be an efficient oil recovery method if only the polymer was more stable and more resistant to higher temperatures and salinities.

Simple

"But," says Boersma, "we are not in the business of making polymers. Our business is recovering oil, so obviously we have to cooperate with others. The polymers that are used now are simple and not too expensive, but like so many things in the oil industry, they are chosen more or less arbitrarily. There has never really been any structural investigation of what we want the polymers to do and how they could do it. And that is what Wever is doing in Groningen at the moment, very enthusiastically. It is very creative and innovative work, which may produce better results than the more experience-based approach that prevails in the oil industry. The results of current field experience are better than expected. Wever's work might explain why."

After the project had already started, the French polymer company SNF came on board. SNF is particularly interested in the technology to modify the existing polymers and make them more efficient or capable of being used beyond the current limitations. It is not only the viscosity that determines the yield; polymers with special properties can 'scrape' the rocks cleaner so that more oil is brought to the surface. And the viscosity of some solutions can change as they flow faster. Again, it would be nice to understand such relationships. "With DPI taking care of the meetings, the minutes and other organisational aspects, we can concentrate on the project itself and that is very agreeable", adds Boersma.

Less expensive

When SNF joined, there was more money for the project and the research could be extended. Boersma is pleased about that. "The more, the better", he says. "Speed is of the essence in oil recovery and with more companies involved in the production of polymers, there will be more innovation. That will improve the polymer efficiency and reduce the unit cost of producing a barrel of oil. This is particularly important, because although polymers can be reused in the lab, they cannot yet be recovered for reuse in the oil fields."

Diederik Boersma is R&D Manager Enhanced Oil Recovery at Shell in Rijswijk, the Netherlands, and is involved in DPI project 716.

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 2010 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.

SUB-PROGRAMMES

There was one active project in this technology area in 2010, involving water-soluble polymers to be used for enhanced oil recovery. The project is designed to investigate structure-performance relationships and new polymer structures to improve oil recovery from new and existing reservoirs. This project, which is being carried out at the University of Groningen, was initiated by Shell. Another company (SNF) joined the programme in 2010, and with effect from 2011 this project will be the first in a new technology area, Polymers for EOR. More projects and partners are envisaged for this technology area.

FACTS AND FIGURES

Partners from industry
- Shell
- SNF

Partners from the research world
- University of Groningen

Budget and organisation
Expenditure in 2010 totalled € 0.12 million (budget: € 0.60 million). A total of € 24k was spent on equipment. The total number of FTEs allocated at year-end 2010 was one (one researcher). Prof.dr. Martien Cohen Stuart acted as Scientific Chairman and Dr. Jan Stamhuis as Programme Area Coordinator of the Emerging Technologies programme.

Publications and inventions
This Technology Area has no publications yet, some have been submitted for review and one invention was reported.

For details, see page 79.

Plastic marine litter

No time to lose

DPI has committed itself to contributing to finding a solution for the ever-increasing problem of plastic in the oceans and seas. DPI's approach to the problem will address every relevant aspect – technical innovation, collecting, recycling and reusing plastic, education of the public. The intention is to produce an action plan before the end of 2011.

Plastic, versatile and useful as it is, is also a problem when it is no longer used. Like all other garbage it should be disposed of in the correct manner. Unfortunately, that does not always happen and because of its relatively light weight and long life it ends up in all sorts of places where it can cause harm, like the oceans. The normal lifetime of plastic is estimated to be hundreds or thousands of years, but in deep seas it is probably longer. Plastic has been with us for only about sixty years, and we do not yet know what its effects on the environment will be, in the short term or in the long term.

Stomachs

The plastic soup in the oceans and seas consists of plastic objects, parts and packaging, sometimes broken down into smaller particles. Those smaller particles cause particular problems. They end up in the stomachs of sea animals and birds. Sometimes the plastic is comprised of small particles, in which case it is actually impossible to stop them from ending up in the oceans and seas. An example is the plastic micro-beads in cosmetic products, such as scrubbers and toothpaste, which find their way straight into the oceans and seas because they are not intercepted in waste water treatment systems. And then there are the, often toxic, additives such as pigments, softening agents, anti-statics and flame retardants, which also end up in the oceans. Moreover, toxic materials like DDT and PCBs tend to adsorb to plastic and thus may also wind up in the stomachs of sea animals.

Eighty percent of the plastic found in the oceans and seas originates from land, having been carried out to sea by the wind, streams and rivers. The remaining twenty percent is plastic waste from the fishing and shipping industries. Under the influence of ocean currents, the plastic waste assembles in so-called gyres, places with rotating sea currents. There are two in the Pacific, two in the Atlantic and one in the Indian Ocean. The concentration of plastic is increasing, not only in the gyres but also closer to home in the North Sea. As the use of plastic will increase with the growth of the world's population, and since the processing of plastic waste and education about its harmful effects will not increase commensurately, unless we act now the problem will soon become insurmountable.

Stakeholders

The 'we' in that last sentence is the world population: it is a global problem that needs a global solution. All of us are guilty. We all use plastic, don't we? So we are all responsible for the solution. But that is a problem in itself: if everybody is responsible, nobody is. Still, over the last two decades several initiatives have been taken by the different stakeholders. These are researchers, authorities, NGOs, industries, media, consumers, the fishing and shipping industries and people involved in public relations and education. But a review of the literature in this field, as well as reports and publications, suggests that, at least for now, they are more concerned with assessing and investigating the problem than with solving it.

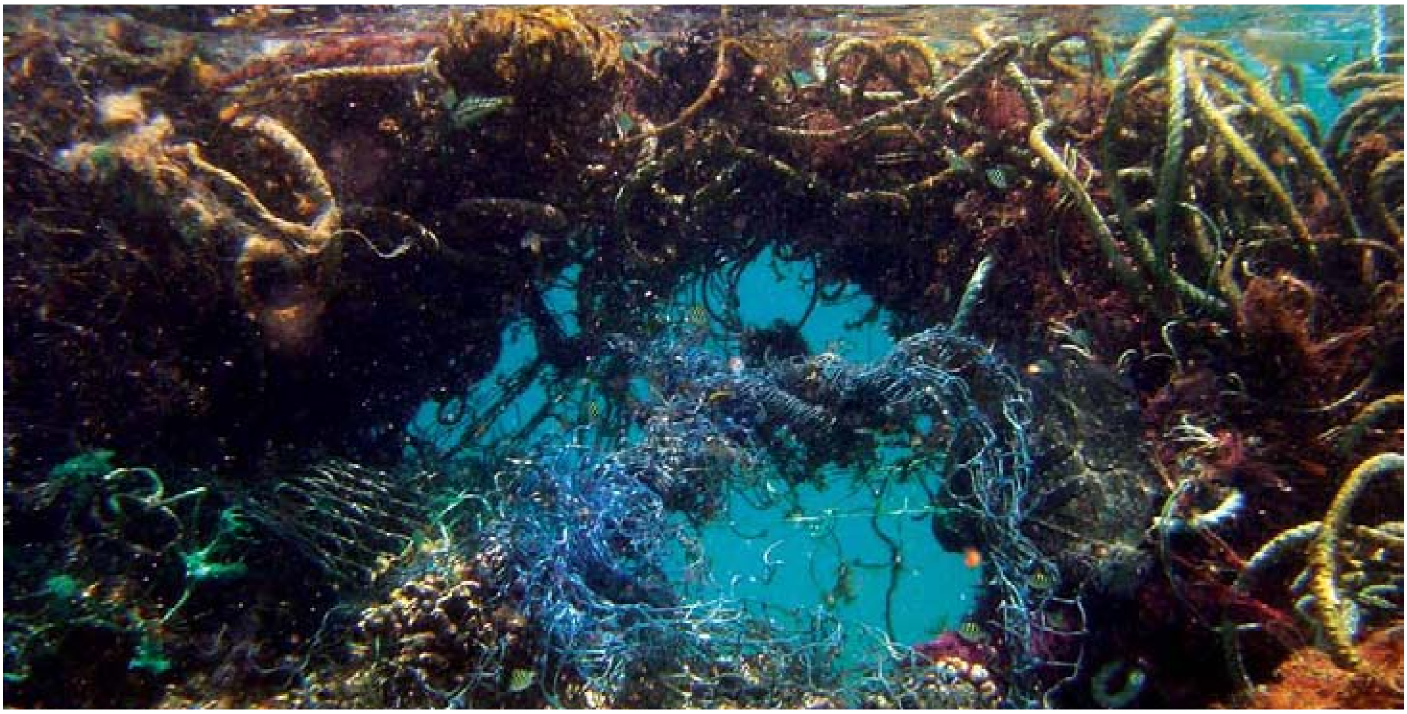
The likely reason is that it is a difficult problem to solve. Large objects can of course be fished out of the sea and there are many initiatives to promote that, one example being 'Fishing for litter' in the Netherlands. As for the smaller and more widespread plastic particles, cleaning the oceans is a hopeless task, not only because of the vastness of the oceans and the high cost to benefit ratio, but also because filtering the small plastic particles out of the sea will disrupt the marine ecosystem through the bycatch of sea organisms.

The most effective approach therefore seems to be to prevent more plastic from ending up in the oceans. Educating the general public about the negative effects of plastic litter is the first step. Interesting examples are the Plastiki, a fully seaworthy boat built from plastic litter collected from the oceans, and vacuum cleaners that in their transparent shell contain a harvest of plastic parts fished out of the sea.

Limiting the use of plastic is one way to go: encourage consumers to refuse to accept plastic shopping bags, retailers to refrain from handing them out, industries to look for alternatives to plastic packaging and authorities to collect plastic waste. All these measures will help to reduce the volume of plastic litter. Reusing plastic shopping bags would already help. A project in the Netherlands provides an example. 'De Tassenbol' is a transparent sphere in which people who no longer need their plastic bags can deposit them and customers who need a bag can take one. Recycling or reusing the plastic after it has served its initial purpose is a second step. Reuse is only viable if the price and the purity compare well with the price and purity of virgin material. If plastic cannot be separated and refined for reuse, the energy content can be used.

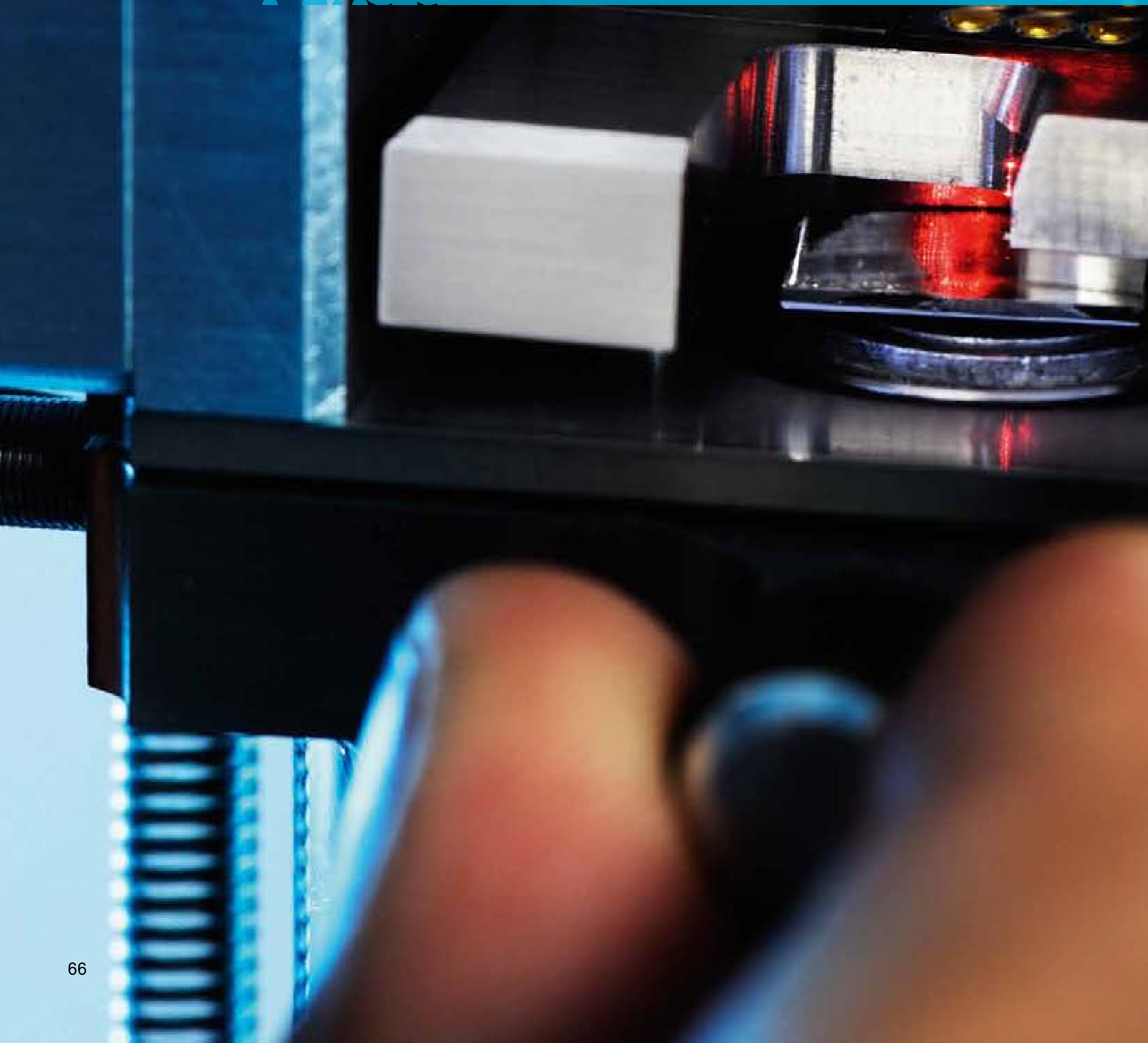
Action plan

There are many initiatives in the US and the EU to tackle the problem of plastic waste. Polymer producers accept their responsibility and participate in these activities. DPI and DPI Value Centre have taken the initiative to contribute to a more sustainable society by looking for solutions that encompass the whole value chain, from raw materials suppliers and producers of plastic products to end users and recyclers. These could be solutions for plastic at the end of its life, for the recycling of plastic, but equally for plastic at the beginning of its life. There is a lot to be gained by producing plastic in such a way that it can be processed in a sustainable manner at the end of its life. Technical system improvements are a natural activity of DPI but, together with other societal and industrial partners in the Netherlands, DPI has also committed itself to finding a way of dealing with the plastic litter problem. Its efforts will be targeted primarily at the North Sea and the Wadden Sea and will comprise clean-up actions and/or measures to prevent more litter ending up in those waters. Another element could involve the creation of a centre of expertise to answer questions from the general public, retailers, raw materials producers, recyclers and any other interested parties. The intention is to finalise the plans and put them into action before the end of 2011.



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.



Enlisting the help of nature

Many complex polymers can be found in nature. By studying them, we can learn from nature while also borrowing nature's production mechanisms to produce our own useful polymers.

Armando Hernandez Garcia started his university education with a Bachelor's degree in chemistry at the National Autonomous University of Mexico. He wanted to go to Europe for his Master's degree because, as he puts it, "it is always useful to see how science is practiced in other countries". Although the Netherlands was his first choice, he ended up taking a Master's degree in bio-technology in Sweden. He is now combining the two disciplines for his PhD project at Wageningen University.
"We are trying to define some polypeptides and produce bio-materials from them that can help to protect DNA against biotic attacks and degradation. A polypeptide consists of a sequence of building blocks that determines its function. Basically, there is a core, a tail and a head, and by altering them we can change the properties. We customise them, for instance, to serve as a vehicle to transport molecules into a living cell. The molecules would otherwise not be stable enough to get there on their own," says Hernandez Garcia, explaining his project.

Hijacking

He designs the molecules on paper or on the computer, but produces them with genetic engineering. Microorganisms, when correctly stimulated, can produce the required sequences of amino acids. Hernandez Garcia describes the process as 'hijacking' the production system of the cells of the microorganism. He has already shown that the method works for one specific poly-peptide, which binds single DNA molecules to form nanoparticles with enough stability to suggest that they could be inserted into a cell. The next step he wants to make is to incorporate self-assembly properties in the polypeptides, which would help the particles to organise themselves around the DNA in the cell that needs protection. Hernandez Garcia: "This self-assembly results in a configuration that resembles the shape and size of natural viruses. It also induces a property called cooperativity, which means that once one protein binds to the DNA the rest will follow, so we will coat the whole DNA."

That sounds like magic, being able to make a cell do what you want it to do. But of course it is not as simple as that. There is a good reason why the project is part of the Corporate Research technology area. "The research is risky," Hernandez Garcia explains. "It is like a new adventure. And, naturally, there are pitfalls. Cells are complicated systems. You cannot really predict what they will do. Sometimes we want them to produce a certain sequence but are unable to, perhaps because they are toxic or for some other reason we have not yet identified." However, the results after eighteen months are encouraging. He is now testing the polypeptides *in vitro* in cells. His hope is that in due course his work will lead to a better and more specific way of administering medicine to patients, for instance.

Game

Working in a DPI project is very stimulating, according to Hernandez Garcia. He likes the open atmosphere and the discussions about science. He has a little game he likes to play at DPI meetings and in his daily contacts with colleagues. "I always try to make a connection between what someone else says about his or her work and my own. How can it help me? What problem can we solve together? Questions like that sometimes generate promising ideas and it is challenging and fun." Not surprisingly, he wants to continue to work in fundamental research after his PhD, possibly in Mexico, but he may also first try to gain more experience in yet another country.

Armando Hernandez Garcia works at Wageningen University on DPI project 698, *Designer polypeptides for self-assembled delivery vehicles*.

Well-trained proteins

A dairy company like FrieslandCampina is always interested in exploring new routes for using proteins. Part of the strategy is to look beyond the immediate future.

FrieslandCampina, one of the three largest dairy companies in the world, has been participating in DPI since the Bio-Inspired Polymers technology area was established about five years ago. Gerard Robijn, Manager Food Structuring at FrieslandCampina Research, follows the projects in that area very closely, but also attends project meetings in the Corporate Research area from time to time. "If you want to innovate you have to broaden your outlook to disciplines other than your own. Food consists to a large extent of polymers. True, they are bio-polymers, but why should we not try to translate the new insights from other polymer fields to bio-polymers and food?" he says, explaining his interest in the Corporate Research projects in general. His interest in the project at hand is obvious.

Protect

"If you consider what Hernandez Garcia is investigating from a meta-level, it is the function a protein can have. How do polypeptides aggregate to form functional entities and how can you get them to do it? His example of building a protective layer through the self-organisation of and cooperativity between polypeptides is not only of interest for transporting molecules into a living cell, it could also play a role in food. An example would be food ingredients that are meant to produce their positive effects only when they arrive in the intestines, such as pre-biotics and pro-biotics. If these ingredients are unstable, and would be damaged during processing in the factory or by the low pH in the stomach, it is naturally very helpful if you can envelop them with polypeptides to protect them," says Robijn.

Milk contains many proteins which, if they are 'well trained', can serve numerous purposes. That is a field in which dairy companies traditionally excel: cheese and yogurt are in fact different structures of the same building blocks found in milk, in different proportions or produced by making minor modifications or by slightly changing the circumstances in which they are processed. The interest in finding even more uses for proteins is evident. "Fortunately, normal food-grade methods provide a lot of opportunities to make structures of proteins with specific properties, to influence the stability and texture, or even to save on costs by giving proteins more functions so that a lower protein content suffices," adds Robijn.

Spheres

One of the key drivers for research at FrieslandCampina is Health & Wellness. The company devotes a lot of effort to making food healthier without affecting the taste. "Low-fat cheese, for instance, can be made by substituting some of the fat with other ingredients. One way of doing this is with protein spheres with a thin skin of fat. However, you can also influence the proteins in the bulk protein matrix in such a way that the structure produces the same texture. When explaining our interest in DPI, and polymer innovation in general, I often use two electronmicroscopic pictures. One shows latex spheres in epoxy resin and looks very similar to the second picture, which shows fat spheres in the water and protein matrix of Gouda cheese. The spheres have the same function: they make an inherently brittle material, epoxy resin or cheese, more elastic," Robijn says. FrieslandCampina is therefore involved in studying food with techniques and models currently used in non-food polymer research (see also page 50 of this annual report). The DPI network has been crucial in getting that project started.

Gerard Robijn is Manager Food Structuring at FrieslandCampina Research in Deventer, the Netherlands, and is involved in DPI project 698.

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.

SUB-PROGRAMMES

Enabling Science

- Polymer characterisation (surfaces and interfaces, applying mainly microscopic techniques) and 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 bio-materials 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.

FACTS AND FIGURES

Partners from industry

- All DPI partners take part in Corporate Research

Partners from the research world

- 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
- Polymer Technology Group, Eindhoven
- 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 2010 totalled € 1.97 million (budget: € 2.20 million). There was no money spent on equipment. The total number of FTEs allocated at year-end 2010 was 18.1 (25 researchers). Prof.dr. Martien Cohen Stuart acted as Scientific Chairman and Dr. Monique Bruining as Programme Area Coordinator of the Corporate Research programme.

Publications and inventions

This research programme generated a total of fourteen reviewed papers and one thesis.

For details, see page 78.

Output per area 2010

Polyolefins

Projects

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

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

#634: Characterization of the specific density of semi-crystalline polymers

#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 behaviour of polyolefins

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

#639: Quantity and quality of active sites in immobilized and solid olefin Polymerization catalysts systems

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

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

#643: Development of High-Temperature 2-Dimensional Liquid Chromatograhpy 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 Modelling

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

#707: Advanced Static and Dynamics Modelling 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 MgCl2-supported Ziegler-Natta catalysis: an integrated experimental and computational approach

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

Thesis

E. Novarino
Reactivity and immobilization of group IV single-center olefin polymerization catalysts

Scientific publications

G. A. Shamov, G. Schreckenbach, 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
Journal of Chemical Theory and Computation 6 (11), 3442-3455

G. Ciancaleoni, N. Fraldi, P. H. M. Budzelaar, V. Busico, R. Cipullo, A. Macchioni
Structure-Activity Relationship in Olefin Polymerization Catalysis: Is Entropy the Key?
Journal of the American Chemical Society 132 (39), 13651-13653

L. Raka, G. Bogoeva-Gaceva, J. Loos
Characterization of polypropylene/layered silicate nanocomposites prepared by single-step method
Journal of Thermal Analysis and Calorimetry 100 (2), 629-639

N. C. Deen, G. Willem, G. Sander, J. A. M. Kuipers
Numerical Analysis of Solids Mixing in Pressurized Fluidized Beds
Industrial & Engineering Chemistry Research 49 (11), 5246-5253

N. Patil, L. Balzano, G. Portale, S. Rastogi
Influence of shear in the crystallization of polyethylene in the presence of SWCNTs
Carbon 48 (14), 4116-4128

N. Patil, L. Balzano, G. Portale, S. Rastogi
Influence of Nanoparticles on the Rheological Behaviour and Initial Stages of Crystal Growth in Linear Polyethylene
Macromolecular Chemistry and Physics 210 (24), 2174-2187

N. Patil, L. Balzano, G. Portale, S. Rastogi
A Study on the Chain-Particle Interaction and Aspect Ratio of Nanoparticles on Structure Development of a Linear Polymer
Macromolecules 43 (16), 6749-6759

Filed patent applications

#646/647: N.M.G. Franssen, B. de Bruin
New functionalized materials by Rh and Pd catalysts

#706: S. Licciulli, S. Gambarotta, R. Duchateau
Catalyst immobilization techniques on activity and selectivity

Reported inventions

#637: Y.D.M. Champouret, A.V. Pandey, S. Rastogi
Role of entanglements on the flow behavior of polyolefins

#646/647: N.M.G. Franssen, B. de Bruin
New functionalized materials by Rh and Pd catalysts

#706: S. Licciulli, S. Gambarotta, R. Duchateau
Catalyst immobilization techniques on activity and selectivity

Performance Polymers

Projects

#580: Modification/ Crosslinking of saturated elastomers using functio-nalised azides

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

#623: Fundamental aspects of Nanocomposites

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

#648: Graphene-based nano-composites- A study on the potential of graphene 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 thermo-plastic polymers based on in-situ solvent deployment

#697: Creating multiple distributed healing in fibre composites using compart-mented liquid filled fibres

Thesis

S.D. Mookhoek
Novel routes to liquid-based self-healing polymer systems

Scientific publications

A. Arun, K. Dullaert, R. J. Gaymans
The Melt Rheological Behavior of AB, ABA, BAB, and (AB)(n) Block Copolymers With Monodisperse Aramide Segments
Polymer Engineering and Science 50 (4), 756-761

A. Arun, K. K. J. Baack, R. J. Gaymans
Polyurethane Tri-block Copolymers-Synthesis, Mechanical, Elastic, and Rheological Properties
Polymer Engineering and Science 50 (4), 747-755

A. Arun, R. J. Gaymans
Hydrophilic poly(ethylene oxide)-aramide segmented block copolymers
European Polymer Journal 45 (10), 2858-2866

A. C. Ijzer, A. Arun, S. R. Reijerkerk, K. Nijmeijer, M. W essling, R. J. Gaymans
Synthesis and Properties of Hydrophilic Segmented Block Copolymers Based on Poly(ethylene oxide)-ran-poly(propylene oxide)
Journal of Applied Polymer Science 117 (3), 1394-1404

A. R. C. Baljon, S. Williams, N. K. Balabaev, F. Paans, D. Hudzinskyy, A. V. Lyulin
Simulated Glass Transition in Free-Standing Thin Polystyrene Films
Journal of Polymer Science Part B-Polymer Physics 48 (11), 1160-1167

G. J. E. Biemond, R. J. Gaymans
Elastic properties of thermo-plastic elastomers based on poly(tetramethylene oxide) and monodisperse amide segments
Journal of Materials Science 45 (1), 158-167

H. M. Zhang, R. N. Datta, A. G. Talma, J. W. M. Noordermeer
Modification of EPDM with Alkylphenol Polysulfide for Use in Tire Sidewalls, 1-Mechanical Properties
Macromolecular Materials and Engineering 295 (1), 67-75

H. M. Zhang, R. N. Datta, A. G. Talma, K. B. Lu, J. Loos, J. W. M. Noordermeer
Modification of EPDM with Alkylphenol Polysulfide for Use in Tire Sidewalls, 2-Mechanistic and Morphological Characteri-zations
Macromolecular Materials and Engineering 295 (1), 76-83

H. Zhang, R. N. Datta, A. G. Talma, J. W. M. Noordermeer
Maleic-anhydride grafted EPM as compatibilising agent in NR/ BR/EPDM blends
European Polymer Journal 46 (4), 754-766

M. Diepens, P. Gijsman
Photostabilizing of bisphenol A polycarbonate by using UV-absorbers and self protective block copolymers based on resorcinol polyarylate blocks
Polymer Degradation and Stability 94 (10), 1808-1813

M. Diepens, P. Gijsman
Photodegradation of bisphenol A polycarbonate with different types of stabilizers
Polymer Degradation and Stability 95 (5), 811-817

N. Grossiord, M. E. L. Wouters, H. E. Miltner, K. B. Lu, J. Loos, B. Van Mele, C. E. Koning
Isotactic polypropylene/carbon nanotube composites prepared by latex technology: Electrical conductivity study
European Polymer Journal 46 (9), 1833-1843

P. G. Malchev, G. de Vos, S. J. Picken, A. D. Gotsis
Mechanical and fracture properties of ternary PE/PA6/GF composites
Composites Science and Technology 70 (5), 734-742

R. L'Abee, M. Van Duin, H. Goossens
Crystallization Kinetics and Crystalline Morphology of Poly(epsilon-caprolactone) in Blends with Grafted Rubber Particles
Journal of Polymer Science Part B-Polymer Physics 48 (13), 1438-1448

R. L'Abee, M. Verbruggen, M. van Duin, A. Spoelstra, H. Goossens
Submicrometer Thermoplastic Vulcanizates Obtained by Reaction-Induced Phase Separation of Miscible Poly(Epsilon-Caprolactone)/ Dimethacrylate Systems
Rubber Chemistry and Technology 83 (2), 160-180

R. l'Abee, R. Sablong, H. Goossens, M. van Duin, A. Spoelstra, R. Duchateau
Thermoplastic Vulcanizates Based on Highly Compatible Blends of Isotactic Poly(propylene) and Copolymers of Atactic Poly(propylene) and 5-Ethylidene-2-norbornene
Macromolecular Chemistry and Physics 211 (3), 334-344

R. M. A. l'Abee, M. van Duin, A. B. Spoelstra, J. G. P. Goossens
The rubber particle size to control the properties-processing balance of thermo-plastic/cross-linked elastomer blends
Soft Matter 6 (8), 1758-1768

S. D. Mookhoek, S. C. Mayo, A. E. Hughes, S. A. Furman, H. R. Fischer, S. van der Zwaag
Applying SEM-Based X-ray Microtomography to Observe Self-Healing in Solvent Encapsulated Thermoplastic Materials
Advanced Engineering Materials 12 (3), 228-234

S. H. Chikkali, R. Bellini, G. Berthon-Gelloz, J. I. van der Vlugt, B. Bruin, J. N. H. Reek
Highly enantioselective hydro-formylation of dihydrofurans catalyzed by hybrid phosphine-phosphonite rhodium complexes
Chemical Communications 46 (8), 1244-1246

S. R. Reijerkerk, A. Arun, R. J. Gaymans, K. Nijmeijer, M. Wessling
Tuning of mass transport properties of multi-block copolymers for CO2 capture applications
Journal of Membrane Science 359 (1-2), 54-63

S. R. Reijerkerk, A. C. Ijzer, K. Nijmeijer, A. Arun, R. J. Gaymans, M. Wessling
Subambient Temperature CO2 and Light Gas Permeation Through Segmented Block Copolymers with Tailored Soft Phase
Acs Applied Materials & Interfaces 2 (2), 551-560

W. F. Dong, P. Gijsman
Influence of temperature on the thermo-oxidative degradation of polyamide 6 films
Polymer Degradation and Stability 95 (6), 1054-1062

Y. J. Choi, M. A. Hulsen, H. E. H. Meijer
An extended finite element method for the simulation of particulate viscoelastic flows
Journal of Non-Newtonian Fluid Mechanics 165 (11-12), 607-624

Filed patent applications

#656: J. Wu, D.S. van Es, J. van Haveren
Biobased building blocks for engineering plastics

#648: E.E. Tkalya, S. van Berkel, C.E. Koning
Graphene-polymer nanocom-posites

#646/647: N.M.G. Franssen, B. de Bruin
New functionalized materials by Rh and Pd catalysts

Reported invention

#646/647: N.M.G. Franssen, B. de Bruin
New functionalized materials by Rh and Pd catalysts

Functional Polymer Systems

Projects

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

#522: Towards a Push-and-Pull Muscle Fibre: An Electro-active Polymer Composite

#524: Polymer-fullerene solar cells and low band-gap donor materials for photovoltaics (combined #524 and #527)

#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 manage-ment

#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 hyperbrached polymers in solar cells

#677: Understanding inter-actions 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

Scientific publications

A. M. Andringa, M. J. Spijkman, E. C. P. Smits, S. G. J. Mathijssen, P. A. van Hal, S. Setayesh, N. P. Willard, O. V. Borshchev, S. A. Ponomarenko, P. W. M. Blom, D. M. de Leeuw
Gas sensing with self-assembled monolayer field-effect transistors
Organic Electronics 11 (5), 895-898

A. P. Zoombelt, S. G. J. Mathijssen, M. G. R. Turbiez, M. M. Wienk, R. A. J. Janssen
Small band gap polymers based on diketopyrrolopyrrole
Journal of Materials Chemistry 20 (11), 2240-2246

B. P. Karsten, R. K. M. Bouwer, J. C. Hummelen, R. M. Williams, R. A. J. Janssen
Charge Separation and Recombination in Small Band Gap Oligomer-Fullerene Triads
Journal of Physical Chemistry B 114 (45), 14149-14156

B. P. Karsten, R. K. M. Bouwer, J. C. Hummelen, R. M. Williams, R. A. J. Janssen
Charge separation and (triplet) recombination in diketopyrrolopyrrole-fullerene triads
Photochemical & Photobiological Sciences 9 (7), 1055-1065

D. Di Nuzzo, A. Aguirre, M. Shahid, V. S. Gevaerts, S. C. J. Meskers, R. A. J. Janssen
Improved Film Morphology Reduces Charge Carrier Recombination into the Triplet Excited State in a Small Bandgap Polymer-Fullerene Photovoltaic Cell
Advanced Materials 22 (38), 4321-+

D. J. D. Moet, P. de Bruyn, J. D. Kotlarski, P. W. M. Blom
Enhanced efficiency in double junction polymer:fullerene solar cells
Organic Electronics 11 (11), 1821-1827

D. J. D. Moet, P. de Bruyn, P. W. M. Blom
High work function transparent middle electrode for organic tandem solar cells
Applied Physics Letters 96 (15), -

F. Gholamrezaie, S. G. J. Mathijssen, E. C. P. Smits, T. C. T. Geuns, P. A. van Hal, S. A. Ponomarenko, H. G. Flesch, R. Resel, E. Cantatore, P. W. M. Blom, D. M. de Leeuw
Ordered Semiconducting Self-Assembled Monolayers on Polymeric Surfaces Utilized in Organic Integrated Circuits
Nano Letters 10 (6), 1998-2002

H. N. An, S. J. Picken, E. Mendes
Enhanced hardening of soft self-assembled copolymer gels under homogeneous magnetic fields
Soft Matter 6 (18), 4497-4503

J. C. Bijleveld, M. Fonrodona, M. M. Wienk, R. A. J. Janssen
Controlling morphology and photovoltaic properties by chemical structure in copoly-mers of cyclopentadithiophene and thiophene segments
Solar Energy Materials and Solar Cells 94 (12), 2218-2222

J. C. Bijleveld, V. S. Gevaerts, D. Di Nuzzo, M. Turbiez, S. G. J. Mathijssen, D. M. de Leeuw, M. M. Wienk, R. A. J. Janssen
Efficient Solar Cells Based on an Easily Accessible Diketopyrrolopyrrole Polymer
Advanced Materials 22 (35), E242-+

J. Cottaar, R. Coehoorn, P. A. Bobbert
Field-induced detrapping in disordered organic semi-conducting host-guest systems
Physical Review B 82 (20), -

J. Loos
Volume morphology of printable solar cells
Materials Today 13 (10), 14-20

M. C. Hermant, P. van der Schoot, B. Klumperman, C. E. Koning
Probing the Cooperative Nature of the Conductive Components in Polystyrene/Poly (3,4-ethylenedioxythiophene): Poly(styrene sulfonate)-Single-Walled Carbon Nanotube Composites
Acs Nano 4 (4), 2242-2248

M. J. Spijkman, J. J. Brondijk, T. C. T. Geuns, E. C. P. Smits, T. Cramer, F. Zerbetto, P. Stoliar, F. Biscarini, P. W. M. Blom, D. M. de Leeuw
Dual-Gate Organic Field-Effect Transistors as Potentiometric Sensors in Aqueous Solution
Advanced Functional Materials 20 (6), 898-905

M. Spijkman, S. G. J. Mathijssen, E. C. P. Smits, M. Kemerink, P. W. M. Blom, D. M. de Leeuw
Monolayer dual gate transistors with a single charge transport layer
Applied Physics Letters 96 (14), -

M. Yuan, J. Brokken-Zijp, G. de With
Permanent antistatic phthalocyanine/epoxy nano-composites - Influence of crosslinking agent, solvent and processing temperature
European Polymer Journal 46 (5), 869-880

N. Tian, D. Lenkeit, S. Pelz, L. H. Fischer, D. Escudero, R. Schiewek, D. Klink, O. J. Schmitz, L. Gonzalez, M. Schaferling, E. Holder
Structure-Property Relationship of Red- and Green-Emitting Iridium(III) Complexes with Respect to Their Temperature and Oxygen Sensitivity
European Journal of Inorganic Chemistry (30), 4875-4885

N. Tian, Y. V. Aulin, D. Lenkeit, S. Pelz, O. V. Mikhnenko, P. W. M. Blom, M. A. Loi, E. Holder
Cyclometalated red iridium(III) complexes containing carbazolyl-acetylacetonate ligands: efficiency enhance-ment in polymer LED devices
Dalton Transactions 39 (37), 8613-8615

P. de Bruyn, D. J. D. Moet, P. W. M. Blom
A facile route to inverted polymer solar cells using a precursor based zinc oxide electron transport layer
Organic Electronics 11 (8), 1419-1422

R. J. de Vries, S. L. M. van Mensfoort, R. A. J. Janssen, R. Coehoorn
Relation between the built-in voltage in organic light-emitting diodes and the zero-field voltage as measured by electroabsorption
Physical Review B 81 (12), -

R. K. M. Bouwer, J. C. Hummelen
The Use of Tethered Addends to Decrease the Number of Isomers of Bisadduct Analogues of PCBM
Chemistry-a European Journal 16 (37), 11250-11253

R. S. Ashraf, J. Gilot, R. A. J. Janssen
Fused ring thiophene-based poly(heteroarylene ethynylene) s for organic solar cells
Solar Energy Materials and Solar Cells 94 (10), 1759-1766

S. Harkema, R. A. H. J. Kicken, B. M. W. Langeveld-Voss, S. L. M. van Mensfoort, M. M. de Kok, R. Coehoorn
Tuning the voltage dependence of the efficiency of blue organic light-emitting diodes based on fluorene-amine copolymers
Organic Electronics 11 (5), 755-766

S. L. M. van Mensfoort, M. Carvelli, M. Megens, D. Wehenkel, M. Bartyzel, H. Greiner, R. A. J. Janssen, R. Coehoorn
Measuring the light emission profile in organic light-emitting diodes with nanometre spatial resolution
Nature Photonics 4 (5), 329-335

S. L. M. van Mensfoort, R. J. de Vries, V. Shabro, H. P. Loebl, R. A. J. Janssen, R. Coehoorn
Electron transport in the organic small-molecule material BAlq - the role of correlated disorder and traps
Organic Electronics 11 (8), 1408-1413

S. L. M. van Mensfoort, V. Shabro, R. J. de Vries, R. A. J. Janssen, R. Coehoorn
Hole transport in the organic small molecule material alpha-NPD: evidence for the presence of correlated disorder
Journal of Applied Physics 107 (11), -

S. S. van Bavel, J. Loos
Volume Organization of Polymer and Hybrid Solar Cells as Revealed by Electron Tomography
Advanced Functional Materials 20 (19), 3217-3234

S. S. van Bavel, M. Barenklau, G. de With, H. Hoppe, J. Loos
P3HT/PCBM Bulk Heterojunction Solar Cells: Impact of Blend Composition and 3D Morphology on Device Performance
Advanced Functional Materials 20 (9), 1458-1463

S. van Bavel, S. Veenstra, J. Loos
On the Importance of Morphology Control in Polymer Solar Cells
Macromolecular Rapid Communications 31 (21), 1835-1845

W. M. Zhang, J. Smith, S. E. Watkins, R. Gysel, M. McGehee, A. Salleo, J. Kirkpatrick, S. Ashraf, T. Anthopoulos, M. Heeney, I. McCullocht
Indacenodithiophene Semiconducting Polymers for High-Performance, Air-Stable Transistors
Journal of the American Chemical Society 132 (33), 11437-11439

Y. Han, K. Pacheco, C. W. M. Bastiaansen, D. J. Broer, R. P. Sijbesma
Optical Monitoring of Gases with Cholesteric Liquid Crystals
Journal of the American Chemical Society 132 (9), 2961-2967

J. C. Kuhlmann, P. de Bruyn, R. K. M. Bouwer, A. Meetsma, P. W. M. Blom, J. C. Hummelen
Improving the compatibility of fullerene acceptors with fluorene-containing donor-polymers in organic photovoltaic devices
Chemical Communications 46 (38), 7232-7234

Filed patent application

#679: O.T. Picot, C.W.M. Bastiaansen, T. Reynolds, A.A. Peijs
Smart textiles with new visual effects

Reported inventions

#679: O.T. Picot, C.W.M. Bastiaansen, T. Reynolds, A.A. Peijs
Smart textiles with new visual effects

#630: T. de Jong, D.K.G. de Boer, C.W.M. Bastiaansen
Nano- and micro-optics based polymer for solid state lighting management

#625: A. Saha, K. Pacheco, R.P. Sijbesma, D.J. Broer, C.W.M. Bastiaansen
Polymer sensors in smart packaging – water sensors

#625: A. Saha, Y. Han, R.P. Sijbesma, D.J. Broer, C.W.M. Bastiaansen
Polymer sensors in smart packaging – formaldehyde sensor

#625: A. Saha, Y. Han, R.P. Sijbesma, D.J. Broer, C.W.M. Bastiaansen
Polymer sensors in smart packaging – aceton and keton sensor

Coatings Technology

Projects

#565: Thiol-ene based 2-pack-in-1-pot waterborne coating

#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 modelling of weathering of polyester-urethane coatings

Scientific publications

D. Senatore, J. Laven, R. A. T. M. van Benthem, D. La Camera, G. de With
Microencapsulation of Epoxidized Linseed Oil Liquid Cross-Linker in Poly(N-vinyl-pyrrolidone): Optimization by a Design-of-Experiments Approach
Industrial & Engineering Chemistry Research 49 (8), 3642-3653

E. Spruijt, J. Sprakel, M. Lemmers, M. A. C. Stuart, J. van der Gucht
Relaxation Dynamics at Different Time Scales in Electrostatic Complexes: Time-Salt Superposition
Physical Review Letters 105 (20), -

M. Lemmers, J. Sprakel, I. K. Voets, J. van der Gucht, M. A. C. Stuart
Multiresponsive Reversible Gels Based on Charge-Driven Assembly
Angewandte Chemie-International Edition 49 (4), 708-711

T. N. Raja, A. M. Brouwer, K. Biemans, T. Nabuurs, R. Tennebroek
Detection of coalescing agents in water borne latex emulsions using an environment sensitive fluorescent probe
Photochem. Photobiol. Sci. (9) 975-984

Filed patent applications

#658: Y. Li, R.A.T.M. van Benthem, J. van Haveren, C.E. Koning
Polyurethane dispersions

#617: R.A.T.M.van Benthem, G. de With, L.G.J. van der Ven, A. Foyet, J. Wu
Corrosion protection of aluminium by electrical conductive coatings

Reported inventions

#673: J.R. Konieczny
Starch based performance coating materials

#565: M.S. Ottink, L. Klumperman, R. Janssen
Thiol-ene based waterborne coatings

#699: S.K. Namdeo, S.N. Khaderi, J.M.J. den Toonder, P.R. Onck
Partially Magnetized Elastica; an autonomous micro-swimmer

#653/#658: D.S. van Es, L. Gootjes, S. Thiyagarajan, J.H. van Haveren
New route towards diamine isohexides; green monomers

#617: R.A.T.M. van Benthem, G. de With, L.G.J. van der Ven, A. Foyet, J. Wu
Corrosion protection of aluminium by electrically conductive coatings

High-Throughput Experimentation

Projects

#449: Technical support and upgrade synthesizers/standard characterization

#500: Development of integrated knowledge capture systems for combinatorial materials and polymer research: a uniform platform approach for the HTE/CMR cluster

#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) behaviour

#613: Optimization of Acrylonitrile/Butadiene/Styrene (ABS) and Polycarbonate (PC)/ABS additive recipes by combinatorial compounding for UV stabilization

#619: Developing Polymer Ontologies

#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 H2 Storage

#670: Mechanical screening method a films for combinatorial compounding

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

Thesis

J.T. Delaney
Reactive inkjet printing & functional materials: a versatile route to new programmed materials

Scientific publications

A. Baumgaertel, E. Altuntas, K. Kempe, A. Crecelius, U. S. Schubert
Characterization of Different Poly(2-oxazoline) Block Copolymers by MALDI-TOF MS/MS and ESI-Q-TOF MS/MS
Journal of Polymer Science Part a-Polymer Chemistry 48 (23), 5533-5540

A. C. Crecelius, C. R. Becer, K. Knop, U. S. Schubert
Block Length Determination of the Block Copolymer mPEG-b-PS Using MALDI-TOF MS/MS
Journal of Polymer Science Part a-Polymer Chemistry 48 (20), 4375-4384

A. Can, E. Altuntas, R. Hoogenboom, U. S. Schubert
Synthesis and MALDI-TOF-MS of PS-PMA and PMA-PS block copolymers
European Polymer Journal 46 (9), 1932-1939

A. Wild, C. Friebe, A. Winter, M. D. Hager, U. W. Grummt, U. S. Schubert
pi-Conjugated 2,2 ':6 ',2 ''-Bis(terpyridines): Systematical Tuning of the Optical Properties by Variation of the Linkage between the Terpyridines and the pi-Conjugated System
European Journal of Organic Chemistry (10), 1859-1868

A. Wild, F. Schlutter, G. M. Pavlov, C. Friebe, G. Festag, A. Winter, M. D. Hager, V. Cimrova, U. S. Schubert
pi-Conjugated Donor and Donor Acceptor Metallo-Polymers
Macromolecular Rapid Communications 31 (9-10), 868-874

A. Wild, S. Hornig, F. Schlutter, J. Vitz, C. Friebe, M. D. Hager, A. Winter, U. S. Schubert
Complexation of Terpyridine-Containing Dextrans: Toward Water-Soluble Supramolecular Structures
Macromolecular Rapid Communications 31 (9-10), 921-927

B. Beyer, C. Ulbricht, A. Winter, M. D. Hager, R. Hoogenboom, N. Herzer, S. O. Baumann, G. Kickelbick, H. Gorls, U. S. Schubert
Unexpected metal-mediated oxidation of hydroxymethyl groups to coordinated carboxylate groups by bis-cyclometalated iridium(III) centers
New Journal of Chemistry 34 (11), 2622-2633

B. Happ, D. Escudero, M. D. Hager, C. Friebe, A. Winter, H. Gorls, E. Altuntas, L. Gonzalez, U. S. Schubert
N-Heterocyclic Donor- and Acceptor-Type Ligands Based on 2-(1H-[1,2,3]Triazol-4-yl) pyridines and Their Ruthenium(II) Complexes
Journal of Organic Chemistry 75 (12), 4025-4038

C. A. Fustin, H. M. L. Thijs-Lambermont, S. Hoeppener, R. Hoogenboom, U. S. Schubert, J. F. Gohy
Multiple Mice liar Morphologies from Tri- and Tetrablock Copoly(2-oxazoline)s in Binary Water-Ethanol Mixtures
Journal of Polymer Science Part a-Polymer Chemistry 48 (14), 3095-3102

C. Pietsch, A. Vollrath, R. Hoogenboom, U. S. Schubert
A Fluorescent Thermometer Based on a Pyrene-Labeled Thermoresponsive Polymer
Sensors 10 (9), 7979-7990

C. R. Becer, K. Kokado, C. Weber, A. Can, Y. Chujo, U. S. Schubert
Metal-Free Synthesis of Responsive Polymers: Cloud Point Tuning by Controlled "Click" Reaction
Journal of Polymer Science Part a-Polymer Chemistry 48 (6), 1278-1286

C. Ulbricht, C. R. Becer, A. Winter, U. S. Schubert
RAFT Polymerization Meets Coordination Chemistry: Synthesis of a Polymer-Based Iridium(III) Emitter
Macromolecular Rapid Communications 31 (9-10), 827-833

C. Weber, C. R. Becer, W. Guenther, R. Hoogenboom, U. S. Schubert
Dual Responsive Methacrylic Acid and Oligo(2-ethyl-2-oxazoline) Containing Graft Copolymers
Macromolecules 43 (1), 160-167

E. Altuntas, K. Kempe, A. Crecelius, R. Hoogenboom, U. S. Schubert
ESI-MS & MS/MS Analysis of Poly(2-oxazoline)s with Different Side Groups
Macromolecular Chemistry and Physics 211 (21), 2312-2322

E. F. J. Rettler, J. M. Kranenburg, H. M. L. Lambermont-Thijs, R. Hoogenboom, U. S. Schubert
Thermal, Mechanical, and Surface Properties of Poly (2-N-alkyl-2-oxazoline)s
Macromolecular Chemistry and Physics 211 (22), 2443-2448

F. Schlutter, A. Wild, A. Winter, M. D. Hager, A. Baumgaertel, C. Friebe, U. S. Schubert
Synthesis and Characterization of New Self-Assembled Metallo-Polymers Containing Electron-Withdrawing and Electron-Donating Bis(terpyridine) Zinc(II) Moieties
Macromolecules 43 (6), 2759-2771

H. M. L. Lambermont-Thijs, F. S. van der Woerdt, A. Baumgaertel, L. Bonami, F. E. Du Prez, U. S. Schubert, R. Hoogenboom
Linear Poly(ethylene imine)s by Acidic Hydrolysis of Poly(2-oxazoline)s: Kinetic Screening, Thermal Properties, and Temperature-Induced Solubility Transitions
Macromolecules 43 (2), 927-933

I. Perevyazko, A. Vollrath, S. Hornig, G. M. Pavlov, U. S. Schubert
Characterization of Poly(methyl methacrylate) Nanoparticles Prepared by Nanoprecipitation Using Analytical Ultracentrifugation, Dynamic Light Scattering, and Scanning Electron Microscopy
Journal of Polymer Science Part a-Polymer Chemistry 48 (18), 3924-3931

I. Y. Phang, N. Aldred, X. Y. Ling, J. Huskens, A. S. Clare, G. J. Vancso
Atomic force microscopy of the morphology and mechanical behaviour of barnacle cyprid footprint proteins at the nanoscale
Journal of the Royal Society Interface 7 (43), 285-296

J. Bonilla-Cruz, C. Guerrero-Sanchez, U. S. Schubert, E. Saldivar-Guerra
Controlled "Grafting-from" of poly[styrene-co-maleic anhydride] onto polydienes using nitroxide chemistry
European Polymer Journal 46 (2), 298-312

J. C. Ribot, C. Guerrero-Sanchez, R. Hoogenboom, U. S. Schubert
Aqueous gelation of ionic liquids: reverse thermo-responsive ion gels
Chemical Communications 46 (37), 6971-6973

J. C. Ribot, C. Guerrero-Sanchez, R. Hoogenboom, U. S. Schubert
Thermoreversible ionogels with tunable properties via aqueous gelation of an amphiphilic quaternary ammonium oligoether-based ionic liquid
Journal of Materials Chemistry 20 (38), 8279-8284

J. Hummel, A. Winter, A. Baumgaertel, N. Risch, U. S. Schubert
New Ditopic Ligands Containing 2,2 ':6 ',2 ''-Terpyridine and a Rigid U-/S-Shaped Terpyridine
Synlett (1), 61-66

J. Perelaer, M. Klokkenburg, C. E. Hendriks, U. S. Schubert
Microwave Flash Sintering of Inkjet-Printed Silver Tracks on Polymer Substrates
Advanced Materials 21 (47), 4830-+

J. Perelaer, P. J. Smith, D. Mager, D. Soltman, S. K. Volkman, V. Subramanian, J. G. Korvink, U. S. Schubert
Printed electronics: the challenges involved in printing devices, interconnects, and contacts based on inorganic materials
Journal of Materials Chemistry 20 (39), 8446-8453

J. T. Delaney, A. R. Liberski, J. Perelaer, U. S. Schubert
A Practical Approach to the Development of Inkjet Printable Functional Ionogels-Bendable, Foldable, Transparent, and Conductive Electrode Materials
Macromolecular Rapid Communications 31 (22), 1970-1976

J. T. Delaney, A. R. Liberski, J. Perelaer, U. S. Schubert
Reactive inkjet printing of calcium alginate hydrogel porogens-a new strategy to open-pore structured matrices with controlled geometry
Soft Matter 6 (5), 866-869

J. T. Zhang, G. Wei, T. F. Keller, H. Gallagher, C. Stotzel, F. A. Muller, M. Gottschaldt, U. S. Schubert, K. D. Jandt
Responsive Hybrid Polymeric/Metallic Nanoparticles for Catalytic Applications
Macromolecular Materials and Engineering 295 (11), 1049-1057

K. Kempe, A. Baumgaertel, R. Hoogenboom, U. S. Schubert
Design of New Amphiphilic Triblock Copoly(2-oxazoline)s Containing a Fluorinated Segment
Journal of Polymer Science Part a-Polymer Chemistry 48 (22), 5100-5108

K. Kempe, A. Vollrath, H. W. Schaefer, T. G. Poehlmann, C. Biskup, R. Hoogenboom, S. Hornig, U. S. Schubert
Multifunctional Poly(2-oxazoline) Nanoparticles for Biological Applications
Macromolecular Rapid Communications 31 (21), 1869-1873

K. Kempe, R. Hoogenboom, S. Hoeppener, C. A. Fustin, J. F. Gohy, U. S. Schubert
Discovering new block ter-polymer micellar morphologies
Chemical Communications 46 (35), 6455-6457

K. Kempe, S. Jacobs, H. M. L. Lambermont-Thijs, M. M. W. M. Fijten, R. Hoogenboom, U. S. Schubert
Rational Design of an Amorphous Poly(2-oxazoline) with a Low Glass-Transition Temperature: Monomer Synthesis, Copolymerization, and Properties
Macromolecules 43 (9), 4098-4104

K. Knop, B. O. Jahn, M. D. Hager, A. Crecelius, M. Gottschaldt, U. S. Schubert
Systematic MALDI-TOF CID Investigation on Different Substituted mPEG 2000
Macromolecular Chemistry and Physics 211 (6), 677-684

K. Knop, R. Hoogenboom, D. Fischer, U. S. Schubert
Poly(ethylene glycol) in Drug Delivery: Pros and Cons as Well as Potential Alternatives
Angewandte Chemie-International Edition 49 (36), 6288-6308

L. I. Majoros, B. Dekeyser, R. Hoogenboom, M. W. M. Fijten, J. Geeraert, N. Haucourt, U. S. Schubert
Kinetic Study of the Polymerization of Aromatic Polyurethane Prepolymers by High-Throughput Experimentation
Journal of Polymer Science Part a-Polymer Chemistry 48 (3), 570-580

L. Wehder, G. Ernst, A. C. Crecelius, O. Guntinas-Lichius, C. Melle, U. S. Schubert, F. von Eggeling
Depicting the Spatial Distribution of Proteins in Human Tumor Tissue Combining SELDI and MALDI Imaging and Immunohisto-chemistry
Journal of Histochemistry & Cytochemistry 58 (10), 929-937

M. Chiper, R. Hoogenboom, U. S. Schubert
New terpyridine macroligands as potential synthons for supramolecular assemblies
European Polymer Journal 46 (2), 260-269

M. M. Bloksma, D. J. Bakker, C. Weber, R. Hoogenboom, U. S. Schubert
The Effect of Hofmeister Salts on the LCST Transition of Poly(2-oxazoline)s with Varying Hydrophilicity
Macromolecular Rapid Communications 31 (8), 724-728

M. M. Bloksma, M. M. R. M. Hendrix, U. S. Schubert, R. Hoogenboom
Ordered Chiral Structures in the Crystals of Main-Chain Chiral Poly(2-oxazoline)s
Macromolecules 43 (10), 4654-4659

M. M. Bloksma, S. Rogers, U. S. Schubert, R. Hoogenboom
Secondary structure formation of main-chain chiral poly(2-oxazoline)s in solution
Soft Matter 6 (5), 994-1003

N. Herzer, J. H. K. van Schaik, S. Hoeppener, U. S. Schubert
Contact Angle Analysis During the Electro-oxidation of Self-Assembled Monolayers Formed by n-Octadecyltrichlorosilane
Advanced Functional Materials 20 (19), 3252-3259

N. Herzer, S. Hoeppener, U. S. Schubert
Fabrication of patterned silane based self-assembled monolayers by photolithography and surface reactions on silicon-oxide substrates
Chemical Communications 46 (31), 5634-5652

R. Hoogenboom, C. R. Becer, C. Guerrero-Sanchez, S. Hoeppener, U. S. Schubert
Solubility and Thermo-responsiveness of PMMA in Alcohol-Water Solvent Mixtures
Australian Journal of Chemistry 63 (8), 1173-1178

R. Siebert, A. Winter, B. Dietzek, U. S. Schubert, J. Popp
Dual Emission from Highly Conjugated 2,2 ':6 ':2 ''-Terpyridine Complexes - A Potential Route to White Emitters
Macromolecular Rapid Communications 31 (9-10), 883-888

S. Gunes, A. Wild, E. Cevik, A. Pivrikas, U. S. Schubert, D. A. M. Egbe
Effect of shifting of aromatic rings on charge carrier mobility and photovoltaic response of anthracene and thiophene-containing MEH-PPE-PPVs
Solar Energy Materials and Solar Cells 94 (3), 484-491

T. Erdmenger, C. Guerrero-Sanchez, J. Vitz, R. Hoogenboom, U. S. Schubert
Recent developments in the utilization of green solvents in polymer chemistry
Chemical Society Reviews 39 (8), 3317-3333

T. Erdmenger, I. Perevyazko, J. Vitz, G. Pavlov, U. S. Schubert
Microwave-assisted synthesis of imidazolium ionenes and their application as humidity absorbers
Journal of Materials Chemistry 20 (18), 3583-3585

T. S. Druzhinina, S. Hoeppener, U. S. Schubert
Microwave-Assisted Fabrication of Carbon Nanotube AFM Tips
Nano Letters 10 (10), 4009-4012

V. V. Rajan, B. Steinhoff, I. Alig, R. Waber, J. Wieser
In-Line Analysis of the Influence of Monomeric and Oligomeric Hindered Amine on the Hydrolysis of Poly-carbonate in a PC/ABS Blend
Journal of Applied Polymer Science 118 (6), 3532-3538

V. V. Rajan, R. Waber, J. Wieser
Online Monitoring of the Thermal Degradation of POM During Melt Extrusion
Journal of Applied Polymer Science 115 (4), 2394-2401

Filed patent applications

#502: J.T. Delaney, A. Liberski, U.S. Schubert
Miniaturized hydrogel structures

#502: A. Liberski, J.T. Delaney, U.S. Schubert
Method for preparing microar-rays of single cells

#502: A. Liberski, J.T. Delaney, U.S. Schubert
Preparation of hydrogen-based 3D scaffolds

#502: A. Liberski, J.T. Delaney, A.M. Liberska, J. Perelaer, U.S. Schubert
Custom circuit prototyping using nanoparticle-loaded substrates

#502: J.T. Delaney, A. Liberski, H. Schäfer, U.S. Schubert
Method for preparing single cell culture

#502: J.T. Delaney, J. Perelaer, A. Liberski, U.S. Schubert
Method for preparing microstructured patterns of superconductive materials

Reported inventions

#502: A. Liberski, J.T. Delaney, U.S. Schubert
Method for preparing micro-arrays of single cells

#502: A. Liberski, J.T. Delaney, U.S. Schubert
Preparation of hydrogen-based 3D scaffolds

#502: A. Liberski, J.T. Delaney, A.M. Liberska, J. Perelaer, U.S. Schubert
Custom circuit prototyping using nanoparticle-loaded substrates

#502: J.T. Delaney, A. Liberski, H. Schäfer, U.S. Schubert
Method for preparing single cell culture

#502: J.T. Delaney, J. Perelaer, A. Liberski, U.S. Schubert
Method for preparing micro-structured patterns of super-conductive materials

Bio-Inspired Polymers

Projects

#587: Keratins as cheap feed-stock 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 bio-mineralization: Self-Organizing and Mineralization- Directing Block Copolymers

Thesis

I. van der Meulen
Polyesters from natural macrolactones for biomedical applications

Scientific publications

H. Teles, P. J. Skrzeszewska, M. W. T. Werten, J. van der Gucht, G. Eggink, F. A. de Wolf
Influence of molecular size on gel-forming properties of telechelic collagen-inspired polymers
Soft Matter 6 (19), 4681-4687

J. Vitz, N. P. Yevlampieva, E. Rjumtsev, U. S. Schubert
Cellulose molecular properties in 1-alkyl-3-methylimidazolium-based ionic liquid mixtures with pyridine
Carbohydrate Polymers 82 (4), 1046-1053

P. J. Skrzeszewska, J. Sprakel, F. A. de Wolf, R. Fokkink, M. A. C. Stuart, J. van der Gucht
Fracture and Self-Healing in a Well-Defined Self-Assembled Polymer Network
Macromolecules 43 (7), 3542-3548

S. Jabbari-Farouji, P. van der Schoot
Competing Templated and Self-Assembly in Supramolecular Polymers
Macromolecules 43 (13), 5833-5844

R. Deumens, A. Bozkurt, M. F. Meek, M. A. E. Marcus, E. A. J. Joosten, J. Weis, G. A. Brook
Repairing injured peripheral nerves: Bridging the gap
Progress in Neurobiology 92(3) 245-276

P. J. Skrzeszewska, F. A. de Wolf, M. A. C. Stuart, J. van der Gucht
Kinetics of network formation by telechelic polypeptides with trimeric nodes
Soft Matter 6(2) 416-422

A. Wild, S. Hornig, F. Schlutter, J. Vitz, C. Friebe, M. D. Hager, A. Winter, U. S. Schubert
Complexation of Terpyridine-Containing Dextrans: Toward Water-Soluble Supramolecular Structures Macromolecular Rapid Communications 31 (9-10) 921-927

Filed patent applications

#608: I. van der Meulen, A. Heise, R. Duchateau, C.E. Koning
Polyesters based on macrolactones

#608: I. van der Meulen, R. Deumens, A. Heise, C.E. Koning, M.A.E. Marcus, B. Joosten
Polyesters based on macro-lactones

Reported inventions

#608: I. van der Meulen, A. Heise, R. Duchateau, C.E. Koning
Polyesters based on macro-lactones

#608: I. van der Meulen, R. Deumens, A. Heise, C.E. Koning, M.A.E. Marcus, B. Joosten
Polyesters based on macro-lactones

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 inter-layers 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

Scientific publications

J. C. Kuhlmann, P. de Bruyn, R. K. M. Bouwer, A. Meetsma, P. W. M. Blom, J. C. Hummelen
Improving the compatibility of fullerene acceptors with fluorene-containing donor-polymers in organic photovoltaic devices
Chemical Communications 46 (38), 7232-7234

B. F. Bory, S. C. J. Meskers, R. A. J. Janssen, H. L. Gomes, D. M. de Leeuw
Trapping of electrons in metal oxide-polymer memory diodes in the initial stage of electroforming
Applied Physics Letters 97 (22), -

G. Aresta, P. A. Premkumar, S. A. Starostin, H. de Vries, M. C. M. van de Sanden, M. Creatore
Optical Characterization of Plasma-Deposited SiO2-Like Layers on Anisotropic Polymeric Substrates
Plasma Processes and Polymers 7 (9-10), 766-774

M. A. Baklar, F. Koch, A. Kumar, E. B. Domingo, M. Campoy-Quiles, K. Feldman, L. Y. Yu, P. Wobkenberg, J. Ball, R. M. Wilson, I. McCulloch, T. Kreouzis, M. Heeney, T. Anthopoulos, P. Smith, N. Stingelin
Solid-State Processing of Organic Semiconductors
Advanced Materials 22 (35), 3942-+

R. Z. Rogowski, A. A. Darhuber
Crystal Growth near Moving Contact Lines on Homogeneous and Chemically Patterned Surfaces
Langmuir 26 (13), 11485-11493

Reported inventions

#640: A.A. Darhuber, P. Bloemen, J. van der Veen, A. Jorge, V. Salas
Engineering the morphology of organic (semi-)conductor layers

#618: M. Lu, P.W.M. Blom
Polymer LED's with doped charge transport layer

Corporate Technology

Projects

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

#597: Ultra-performance polymer separations

#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 Chromatograhpy 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

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#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

Thesis

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

Scientific publications

A. Alekseev, A. Efimov, K. B. Lu, J. Loos
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Emerging Technologies

Project

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

Reported invention

#716: D.A.Z. Wever, F. Picchioni, A.A. Broekhuis
Polyacrylamide through atomic transfer radical polymerization

About DPI ...

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

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

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

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

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

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

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

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

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