



Annual Report

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Organisation 2021

Supervisory Board

- Dr. Jacques. Joosten, Chair
- Prof.dr. Frank Baaijens
- Anton van Beek, MSc
- Bernie van Leeuwen, MSc
- Dr. Erik Van Praet

Executive Board

- Ernst Jan van Klinken, MSc Managing Director, Chair
- Vacancy Scientific Director

Programme Managers and Business Development

- Dr. Claude Bostoen Polyolefins
- Dr. Denka Hristova-Bogaerds Performance Polymers
- Pooja Jagadeesh, MSc Business Development
- Ronald Korstanje, MSc Polymers for Oil and Gas Circular Plastics Initiative





Scientific Programme Chairs

- **Prof.dr. Costantino Creton** Performance Polymers
- Prof.dr. Bernhard Rieger Polyolefins

Organisation Staff

- Jeanne van Asperdt (left in 2021) Finance
- Arie Brouwer, MSc (left in 2021) Programme Manager Seafront
- Leon Damen Project Administration Finance
- Renée Hoogers-Valken
 Secretariat
- Peter Kuppens AA Controlling
- **Eylem van Mierlo** (successor Jeanne van Asperdt) Finance
- Rosanne Peters
 Manager HR&O
- Christianne Scharff-Bastiaens Communications
- Linda de Wit Project Administration



DPI - Shaping polymer innovation

DPI fundamental programme

DPI's pre-competitive research programme currently embraces three programmes. Companies and knowledge institutes can participate in one or more of these programmes, each of which encompasses a substantial number of projects. The participating companies jointly define the programme content for the programmes in which they participate. PhD students and postdocs from our partner knowledge institutes perform their research in close collaboration with scientists from our industrial partners. Shaping that collaboration between industry and academia is the key to building a coherent community that delivers research results to the envisaged high standard and prepares our scientists for their future careers, in industry or elsewhere.

Pre-Competitive programme

Polyolefins	Performance Polymers	Polymers for Oil and Gas
18 projects 34 researchers	23 projects 37 researchers	5 projects 5 researchers
Industry	Industry	Industry
Borealis Braskem Dow Benelux ExxonMobil Reliance SABIC SIBUR SCG Chemicals	DSM Hutchinson Kingfa SABIC Saudi Aramco Shell SKF Teijin Aramid	Shell SNF Floerger
Academia	Academia	Academia
CPE Lyon Eindhoven University of Technology Ghent University Japan Advanced Institute of Science and Technology Leibniz-Institut für Polymerforschung Dresden Lomonosov Moscow State University National Technical University of Athens University of Chemistry and Technology Prague University of Groningen University of Konstanz University of Naples Federico II University of Perugia University of Salerno University of Turin University of Wisconsin-Madison Utrecht University	ENSAM Paris Delft University of Technology Eindhoven University of Technology ESPCI Paris Foundation for Research and Technology Hellas Ghent University IFREMER JOANNEUM RESEARCH KTH Montanuniversität Leoben National Technical University of Athens Polymer Competence Center Leoben Radboud University Shanghai Jiao Tong University Sichuan University Southwestern University of Finance and Economics The University of Manchester University of Bologna University of Nottingham University of Oxford University of Twente University of Twente University of Twente University Savoie Mont Blanc	Clausthal University of Technology Université de Bordeaux University of Groningen University of Twente

DPI development programme

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

Circular Plastics Initiative

Towards a responsible, circular value chain in plastics We live in a 'plastic age' where society thrives thanks to developments in polymer science and technology. At the downside, plastic litter can be found all around the globe. As a society, we need to rethink plastic. It is too valuable to be treated as waste. And it can serve as the feedstock for circularity. This calls for concerted action, in particular, to tackle plastic waste and ensure its recycling.

The mission of the Circular Plastics Initiative is to boost circularity in plastics on an industrial scale. We address the entire value chain from an international perspective and focus on the technological, logistic, and societal challenges lying ahead.

Efforts to reduce the use of plastics will contribute to solving its associated problems. However, for many purposes plastics offer advantages to other materials. They often combine high performance with reduced weight and thus help reduce the use of energy. It is therefore equally important to develop a strategy for their responsible use. Circularity will have to be at the heart of this strategy.

At the Circular Plastics Initiative, we work towards a fully circular value chain, from production and use via collecting and sorting towards re-use and recycling. This is done in a concerted action involving all relevant players and addressing all relevant issues. The focus will be in particular on plastics used in food packaging, as these confront us with the most pressing problems. They are prone to irresponsible disposal, they are difficult to sort and it's quite a challenge to bring them back to the beginning of the value chain. Achieving circularity in plastics for food packaging will therefore lead the way to achieving plastics circularity in general.

The Circular Plastics Initiative is co-founded by ISPT and DPI.



Institute for Sustainable Process Technology

The projects focus on:

- Analysis of the composition of the mixed plastic waste stream and of contaminants therein
- Evaluation of sorting technology
- Evaluation for chemical processing (pyrolysis & gasification) in terms of quality and scalability (beyond 100 kt/a)
- Evaluation of the opportunities and pitfalls in using the pyrolysis oil as feed for plastic production



economic activity within the foreseeable future (i.e. no later than two to five years after completion of the project). DPI's role is to actively assist in establishing the collaboration and to coordinate the project. DPI's role can also be limited to acting as coordinator of a project. DPI provides a model framework for the collaboration, but the detailed rules are agreed between the members of the consortium.

Current projects:

- Towards Improved circularity of polyolefin-based packaging
- InReP An integrated approach towards Recycling of Plastics
- LEmPlaR- Losses & Emissions in Plastic Recycling

Summary of financial data 2021

Key Performance Indicators DPI fundamental programme

Income	(x EUR million)	%
Contributions from industrial partners	2.54	60.5
Revenue Patents	0.13	3.1
Contributions from knowledge institutes	0.01	0.2
Subsidy of TKI Toeslag	1.32	31.4
Value Chain	0.13	3.1
Business Development	0.07	1.7
Total income	4.20	100

Expenditure	(x EUR million)	%
By nature		
Personnel costs	3.89	82.8
Depreciation	0.02	0.4
Other costs	0.79	16.8
Total expenditure	4.70	100
By Programmes		
Polyolefins	1.56	33.2
Performance Polymers	1.39	29.6
Polymers for Oil and Gas	0.24	5.1
Organisation and support	0.95	20.2
Value Chain	0.19	4.0
Business Development	0.37	7.9
Total expenditure	2.86	100

Number of industrial participations

Number of partner knowledge institutes (universities, etc.)

2020	32
2021	38

Track record DPI researchers

Research output	2020
Unknown	
Employed by non-partner industrial compan	y or start-up
Employed by partner industrial company	
Employed by non-partner knowledge institu	te
Employed by partner knowledge institute	
Left in total	

Scientific publications	39
PhD theses	4
Average journal impact factor	4.69





Partners Industry 2021

involved in DPI fundamental programme

Europe

Borealis	BOREALIS Keep Discovering
Hutchinson	
SIBUR	SIBUR
SKF	5KF
SNF Floerger	SNF FLOERGER



The Netherlands

Dow Benelux	Dow
DSM	Øрги
SABIC	لیابک عالماند
Shell	
Teijin Aramid	ΤΕΙͿΙΝ

North and South America, Asia

Braskem	Braskem
ExxonMobil	ExonMobil
Kingfa	KİNGFA
Reliance	Reliance Industries Limited
Saudi Aramco	aramco 隆
SCG Chemicals	SCG





Partners knowledge institutes 2021

involved in DPI fundamental programme



Europe

ENSAM Paris	Arts et Métiers
Clausthal University of Technology	W TU Clausthal
CPE Lyon	
ESPCI Paris	ESPCI 🖲 PARIS
Foundation for Research and Technology - Hellas (new in 2021)	FORTH
Ghent University	GHENT UNIVERSITY
IFREMER	Ifremer
JOANNEUM RESEARCH (new in 2021)	JOANNEUM RESEARCH
KTH (new in 2021)	٢
Leibniz-Institut für Polymerforschung Dresden	Leibniz-Institut Gr. Paymerforschung Vielden
Lomonosov Moscow State University	
Montanuniversität Leoben (new in 2021)	
National Technical University of Athens	NATIONAL TECHNICAL UNIVERSITY OF ATHENS
Polymer Competence Center Leoben	PCCL

The Netherlands



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The University of Manchester	MANCHESTER 1824 The University of Manchester
University of Bordeaux	Université BORDEAUX
University of Chemistry and Technology Prague	UNIVERSITY OF CHEMISTRY AND TECHNOLOGY PRAGUE
University of Crete (new in 2021)	IANERISTIMIO KPITHE UNIVERSITY OF CRETE
University of Konstanz (new in 2021)	Universität Konstanz
University of Naples Federico II	UNDERSTANCE STUD or NAYCU FEDERACO II
University of Nottingham	University of Nottingham
University of Oxford	WINNERSOFT OF OXFORD
University of Patras (new in 2021)	UNIVERSITY OF PATRAS
University of Perugia	UNIVERITA DEGLI STUDI
University of Salerno (new in 2021)	UNVERSTÀ DECLI STUDI DI SALERNO
University of Turin	UNIVERSITÀ DEGLI STUD DI TORINO
University Savoie Mont Blanc	UNIVERSITÉ SAVOIE MONT BLANC
Universiy of Bologna	

North and South America, Asia

Japan Advanced Institute of Science and Technology	AAIST JAN ER HYTTITE OF SEINE AND HEINOLOGY
Shanghai Jiao Tong University	ど 済え大学 SILAGGIAN JUAN TONG UNIVERTY
Sichuan University (new in 2021)	m m 小大学 Sichuan University
Southwestern University of Finance and Economics (new in 2021)	西南射徑大學
University of Wisconsin-Madison	

Computing circularity: How digitalisation ignites innovation in the polymer community

Uniting the polymer ecosystem during the DPI Annual Meeting 2021

We all know that the road towards achieving the global sustainability goals can be challenging to navigate. Understanding polymer applications and gaining clear insight into material behaviours are becoming some of the most important focal points in questions of circularity. During DPI's Annual Meeting 2021, leaders from industry and academia came together to discuss the next steps in polymer expertise and innovation. "You can't solve these challenges alone. A solid community is the starting point. And an interdisciplinary approach is the way forward."

Digital enabling technologies to reach optimal strategies for circularity

The Annual Meeting, which opened with an inspiring keynote speech from ESA astronaut and physician André Kuipers, addressed two main topics: digital enabling technologies for material innovation and polymer excellence, such as artificial intelligence and quantum computing, and strategies for circularity in which industry and science can play a leading role. Two pressing topics that demand attention from everyone in the community and require a new approach.

> "The traditional way of doing research is incremental," Adham Hashibon (University College London) pointed out. "We can reverse this and start by looking at what kind of properties and values our products should have. To do this, however, we need to harvest our entire range of knowledge, for that clever balance between having our circularity goals as a starting point and taking all possible information into consideration. Starting with the target material properties and then adding polymer informatics to the mix means that we can accelerate development and innovation'



Data-driven material science. Knowing precisely what we bring and return to market

With the growing complexity of the combinations of circularity and performance demands, collaborations between physicists, chemists, and computing experts become increasingly important. As polymer scientists deal with many interconnected variables, quantum computing allows for an insight into all the atomic interactions and molecular structure of the materials from an algorithmic point of view. This means it can be mobilised to create better, more sustainable, and more flexible polymers. "For this, we definitely need creative scientists and industry professionals to think outside of the box," mentioned Constantino Creton (ESPCI Paris/Scientific Chair DPI). "Now, thanks to digital enabling technologies, we can really take polymer science to the next level. Optimising a material for a particular property can be complicated and relatively costly. But with better data treatment and clever AI applications, organisations enable themselves to do this on a higher pace and innovate faster." All around us, in every industry, we see that the demand for computing expertise is increasing, and the material and chemical industries are no exception. "The technologies are there, and they are already in use." Jerome Claracq (Dow Chemical) explained. "We now need to generate atom models that are applicable to our industry. Tomorrow's science is built on today's. In collaboration with partners from both industry and science, we develop the necessary algorithms, and within ten years - but hopefully sooner! -, we will truly see that impact of these technologies."

"Sharing knowledge in the community is key."

A fresh look: new strategies allow for new collaborations on an international scale

A critical look into how circularity can be achieved is important, and it needs to be approached holistically. As Henk Pool (Cefic) explained: "'Is my material circular?' is not really the right question. People must reflect on something bigger: 'Will the use of my material be circular and how much of the material will be recycled and brought back into the market?' The end-of-life strategy needs to be taken into consideration. That is a first metric point."

Roelof Westerbeek (Highsun Holding Group) concurred: "We have been running the industry by completely different metrics in the past than the ones we need today. It has mostly been about cost and efficiency, which is what the whole industry is tailored to right now. We need to turn around, put the focus on other priorities, and design for recyclability. And in this, we

"If you want to change perspectives and if you want to push borders you need dreamers, thinkers, technicians, and daredevils." should not wait for legislation; we can teach them." "The momentum is changing. That's for sure," Jaqueline Vaessen (ChemistryNL) brought to the table. "Between deed and dreams, there are laws and practical objections, as a famous Flemish writer once uttered. We have to make sure that legislation is not going to prevent us from going into the direction we would like to go in." Of course, there is a great task for regulators to drive circularity, but scientists and industry experts need to be leading the way. The key is that the regulations are harmonised. "And a level playing field is necessary," Henk Pool added. "We know we will have it in Europe but achieving it on a global scale is incredibly complex. We need to keep focussing on this."

The right incentives. Taking polymers to the next level for end-to-end circularity

Polymer science is 'mature'. Consequently, as Bernhard Rieger (TU Munich/Scientific Chair DPI) pointed out, an established, cost-driven industry player, using a product that 'does the trick' sufficiently won't feel a pressing need to change its ways. But it is ever so necessary to have academic scientists connect with those industry experts in their daily work to point out where industry can improve as well: "The entire chain of knowledge needs to be activated, from science to engineering and even all the way down to marketing. For us academics, the industry is our friend. A solid innovation community consisting of both industry and academic experts can take polymer innovation to new heights."

"It's not only about the education of young minds. We also have the possibility and the tools to teach politicians."

The main takeaway? It is all about making those connections of process, manufacturability, and life cycle at the start of a project. A next step would be interoperability and potentially a standardised way of connecting the dots. Ernst Jan van Klinken mentioned: "The key is to focus on polymer circularity, linked to performance materials. We don't want to waste our time, our students, our expertise, or our money by working on an incoherent case-by-case basis. With our community, we can make polymer innovation and circularity happen on a truly interdisciplinary scale."



Polyolefins

The Polyolefins research programme encompasses the entire spectrum of the knowledge chain. The aim is to create the knowledge base needed to support the ever-expanding range of applications.

Polyolefin-based materials can be customised for many different applications: from ultra-rigid thermoplastics to high-performance elastomers. This wide performance scope is achieved through a variety of polyolefin molecular structures, whose common features are high atom economy in their synthesis, low cost, excellent properties, a long-life cycle and ease of recycling.

The mission of the Programme is to support and coordinate integrated pre-competitive or explorative research projects on polyolefins along the whole chain of knowledge, from (homogeneous and heterogeneous) catalyst synthesis and immobilization, through catalytic olefin polymerization, down to polyolefin characterization, processing and end-use evaluation. Care for materials and process sustainability in the perspective of a Circular Economy is a pervasive characteristic of the research Programme.

Sub-programmes

Circular Economy solutions for Polyolefins

Key fields are mechanical recycling and chemical recycling processes, Non-chemical recycling and non-mechanical methods of recycling while preserving quality and purity of recyclates. It aims at developing new concepts in design for recycling based on polyolefins, among others to circumvent the multilayer complexity of PET/EVOH/PE composites either through polymer design or specific processing steps, with adjusting 02/C02 barrier properties. Polyolefin modification based on renewable sources is another route to establishing these circular economy targets.

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.

Catalysis

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

Facts and figures

Partners from industry

- Borealis
- Braskem
- Dow Benelux
- ExxonMobil
- Reliance
- SABIC
- SIBUR
- SCG Chemicals

Partners from the research world

- CPE Lyon
- Eindhoven University of Technology
- Ghent University
- Japan Advanced Institute of Science and Technology
- Leibniz-Institut für Polymerforschung Dresden
- Lomonosov Moscow State University
- National Technical University of Athens
- University of Chemistry and Technology Prague
- University of Groningen
- University of Konstanz
- University of Naples Federico II
- University of Perugia
- University of Salerno
- University of Turin
- University of Wisconsin-Madison
- Utrecht University



Budget and organisation

In 2021 there were 34 researchers (PhDs and postdocs) working within the 18 projects of the Polyolefins programme, 3 new projects started with a total budget of €1.31 Million. Prof.dr. Bernhard Rieger was Scientific Chair and Dr. Claude Bostoen was Programme Manager.

Publications and inventions

This programme generated 13 reviewed papers and 3 theses in 2021.

For details, see page 18

Performance Polymers

Performance Polymers possess superior chemical, mechanical and physical properties, especially beyond ambient conditions. They are usually used as multi-component polymeric systems consisting of various polymers, reinforcements and additives.

The research focus of the Programme Performance Polymers is to enhance the performance of different polymeric systems by combining Chemistry, Physics and Engineering Science. This leads to a better understanding of the "structure versus performance" relation on all length scales - from molecular to macroscopic. Via the generated knowledge, the Performance Polymers programme provides opportunities for responding to the new sustainability challenges posed to the industrial sectors of automotive, aerospace, electronics, oil & gas transport, energy and construction.

Focus areas

Advanced modelling & experimental strategies for enhanced durability & performance

- Early detection of de-bondig at interfaces
- Surface treatment for enhanced polymer performance
- Composites fatigue: prediction of damage and correlation to lifetime
- Impact mechanisms in polymer composites
- Extending durability / lifetime of performance polymers
- Advances in solid-state NMR for polymeric systems

Processing – Structure – Performance relationship

- Flow instability and processing of filled polymeric melts
- Linking rheology to the molecular and macroscopic structure of polymers

Polymers for electronics and energy

- Informed design of electrically conductible composites
- Polymers and composites under high voltage conditions
- Polymers as high-barrier materials for gas (H2) storage/ transportation

Recycling / Reprocessing / Recovery of performance polymers

- Reversible bonds for re-use/recycling of composites and thermosets
- Composites recycling / re-processing

Facts and figures

Partners from industry

- DSM
- Hutchinson
- Kingfa
- SABIC
- Saudi Aramco
- Shell
- SKF
- Teijin Aramid

Partners from the research world

- ENSAM Paris
- Delft University of Technology
- Eindhoven University of Technology
- ESPCI Paris
- Foundation for Research and Technology Hellas
- Ghent University
- IFREMER
- JOANNEUM RESEARCH
- KTH
- Montanuniversität Leoben
- National Technical University of Athens
- Polymer Competence Center Leoben
- Radboud University

Shanghai Jiao Tong University

- Sichuan University
- Southwestern University of Finance and Economics
- The University of Manchester
- University of Bologna
- University of Crete
- University of Nottingham
- University of Oxford
- University of Patras
- University of Twente
- University Savoie Mont Blanc

Polymers for oil and gas

Polymers find broad application in the recovery, transport and utilisation of oil and gas, e.g. as oil field chemicals or as lightweight materials with superior durability properties. The aim of the Polymers for Oil and Gas programme is to generate tools and new insights into existing and new polymers for utilisation in the exploration, production and transport of oil and gas. Two main areas of study are distinguished: firstly, the use of polymers in fluids for enhanced oil recovery (EOR) and other sub surface drilling/recovery applications. Secondly, the behaviour of polymers in functional materials used under extreme/adverse conditions (in close collaboration with the Performance Polymers programme).

Sub-programmes

Structure-property relationships and the design of new model macromolecules

Controlled radical polymerisation techniques will be employed to investigate the effects of macromolecular topology, for example branching, on polymer solution properties and on viscosity and/or visco-elasticity. These novel structures are evaluated in core flow experiments to determine their injectivity and impact on the recovery of oil in porous media.

> The effects of polymeric surfactants, i.e. high molecular weight amphiphilic structures that have the potential to decrease the interfacial tension and enhance oil recovery compared with that obtained with the current polymer flooding applications, are also being investigated.







Budget and organisation

In 2021 there were 37 researchers (PhDs and postdocs) working within the 23 projects of the Performance Polymers programme, 7 new projects started with a total budget of €1.58 Million.

Prof.dr. Costantino Creton was Scientific Chair and Dr. Denka Hristova-Bogaerds was Programme Manager of the Performance Polymers programme.

Publications and inventions

This programme generated 13 reviewed papers and one thesis in 2021.

For details, see page 20

Relating polymer rheology to apparent viscosity in porous media

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

Facts and figures

Partners from industry

- Shell
- SNF Floerger

Partners from the research world

- Clausthal University of Technology
- Université de Bordeaux
- University of Groningen
- University of Twente

Budget and organisation

In 2021 there were 5 researchers (PhDs and postdocs) working within the 5 projects of the Polymers for Oil and Gas, 1 new project started with a total budget of €0.14 Million. Ronald Korstanje acted as Programme Manager.

Publications and inventions

This programme generated 2 reviewed papers and one thesis in 2021.

For details see page 21

Output

Polyolefins

Projects

#801: Predictive modelling of mechanical anisotropy in oriented semi-crystalline polymers directly from morphological characteristics

#803: HEat Management in Polymerization Reactors (HEMPR)

#804: From homogeneous to "colloidal" olefin polymerization catalysts: effects of mass transport limitations on reaction kinetics and polymer microstructure

#810: Online Polyolefin structuring during Cast Film Extrusion

#813: Multi-scale investigation of silicasupported ethylene polymerization catalysts during the early stages of the reaction

#814: Control of crystallisation, chain entanglement and rheology via process conditions

#815: Augment the macroscopic PROperties of i-PP composites by controlling the microscopic Fiber-matrix Interactions via Transcrystallization

#816: Correlation between processinduced crystallization and mechanical properties in injection molded isotactic polypropylene (iPP)

#817: An inter-disciplinary highthroughput approach to olefin block copolymers

#830: Electrostatic charging of polyolefin powders on the level of particles

#831: Molecular modelling of stretchinduced crystallization in polyethylene and polypropylene layers

#832: Quality model for COntaminated **Recycled Polyolefins**

#834: RHEOlogical determination of POLyolefin ARchitectures

#835: Quantitative Structure-Activity Relationships (QSAR) in Post-Metallocene-Based Olefin Polymerizations Using Chemically Meaningful Computational Descriptors

#836: Practical, High Throughput Quench Labeling Techniques for Information-Rich Analysis of Alkene Polymerization Catalysts

#846: In-Chain Functionalized Polyethylenes from Controlled Free-Radical Polymerization under Benign Conditions (started in 2021)

#847: A microstructural insight in polyethylene based bioriented monomaterials: from fundamental to processing (started in 2021)

#848: Ziegler-Natta Catalysts for Polypropylene with Temperature-Controlled ID/ED Compositions (started in 2021)

Theses

Evan Milacic Studying liquid injection in fluidised beds through

Gaia Urciuoli Structural Characterization of Olefinbased Multiblock Copolymers by Chain Shuttling Technology

Ruben Demets The assessment of quality and substitution potential of recycled plastics

Publications

A. Piovano, M. Signorile, L. Braglia, P. Torelli, A. Martini, T. Wada, G. Takasao, T. Taniike and E. Groppo Electronic Properties of Ti Sites in Ziegler-Natta Catalysts Acs Catalysis 11 (15) 9949-9961

A. Piovano, T. Wada, A. Amodio, G. Takasao, T. Ikeda, D.Z. Zhu, M. Terano, P. Chammingkwan, E. Groppo and T. Taniike Formation of Highly Active Ziegler-Natta Catalysts Clarified by a Multifaceted Characterization Approach

Acs Catalysis 11 (22) 13782-13796

G. Takasao, T. Wada, A. Thakur, P. Chammingkwan, M. Terano and T. Taniike Dataset of energetically accessible structures of MgCl2/TiCl4 clusters for Ziegler-Natta catalysts Data in Brief 34

G. Takasao, T. Wada, A. Thakur, P. Chammingkwan, M. Terano and T. Taniike Insight into structural distribution of heterogeneous Ziegler-Natta catalyst from non-empirical structure determination

Journal of Catalysis 394 299-306

E. Milacic, M.N. Manzano, S. Madanikashani, G.J. Heynderickx, K.M. van Geem, A.A.M. van de Greef, A. Richter, S.H.L. Kriebitzsch, K.A. Buist, M.W. Baltussen and J.A.M. Kuipers

Experimental study on the temperature distribution in fluidised beds Chemical Engineering Science 248

F. Di Sacco, S. Saidi, D. Hermida-Merino and G. Portale

Revisiting the Mechanism of the Meso-to-alpha Transition of Isotactic Polypropylene and Ethylene-Propylene Random Copolymers Macromolecules 54 (20) 9681-9691

M.J. Werny, J. Zarupski, I.C. ten Have, A. Piovano, C. Hendriksen, N.H. Friederichs, F. Meirer, E. Groppo and B.M. Weckhuysen Correlating the Morphological Evolution of Individual Catalyst Particles to the Kinetic Behavior of Metallocene-Based Ethylene Polymerization Catalysts Jacs Au 1 (11) 1996-2008

Y. Spoerer, R. Boldt, R. Androsch and I. Kuehnert Pressure- and Temperature-Dependent Crystallization Kinetics of Isotactic Polypropylene under Process Relevant Conditions Crystals 11 (9)

D. Tammaro, G. D'Avino, S. Costanzo, E. Di Maio, N. Grizzuti and P.L. Maffettone A microcapillary rheometer for microliter sized polymer characterization Polymer Testing 102

G. Urciuoli, A. Vittoria, G. Talarico, D. Luise, C. De Rosa, V. Busico, R. Cipullo, O.R. de Ballesteros and F. Auriemma In-Depth Analysis of the Nonuniform Chain Microstructure of Multiblock Copolymers from Chain-Shuttling Polymerization Macromolecules 54 (23) 10891-10902

Y. Kim, R. Kubena, J. Axtell, H. Samouei, P. Pham, J.M. Stauber, A.M. Spokoyny and C. Hilty

Dynamic Nuclear Polarization Using 3D Aromatic Boron Cluster Radicals Journal of Physical Chemistry Letters 12 (1) 13-18

Y. Kim, H. Samouei and C. Hilty Polyolefin catalysis of propene, 1-butene and isobutene monitored using hyperpolarized NMR Chemical Science 12 (8) 2823-2828

A. Yakimov, J. Xu, K. Searles, W.C. Liao, G. Antinucci, N. Friederichs, V. Busico and C. Coperet DNP-SENS Formulation Protocols To Study Surface Sites in Ziegler-Natta Catalyst MqCl2 Supports Modified with Internal Donors Journal of Physical Chemistry C 125 (29) 15994-16003

Performance Polymers

Projects

#805: Probing interfacial damage in composites with mechanofluorescence

#806: 2D Material Coatings for Fibres

#811: Reliable Prediction of Residual Structural Integrity and Damage-Evolution During Long-Term Fatigue in Thermoplastic Composites

#812: Physics-based fatigue design tool for matrix cracking and delamination in unidirectional and sandwich composites under multi-axial fatigue loads with arbitrary R-ratio: development, validation and finite element implementation

#819: Controlling electrical percolation in hybrid thermoplastic composites through informed selection of fillers

#822: Processing for enhandced product performance

#823: Modular, designer polydopomine adhesives for facile and versatile surface conjugation of function of polyethylenes

#824: Micromechanical modelling of complex composite systems for improved failure prediction and product design

#825: Development of Hyperpolarized and 1H MAS NMR Spectroscopy for the study of performance polymers

#826: Multi-layered wEar-Resistant Coatings with additional fUnctionality - new stRategies for enhancing the tribologicAl performance of poLymers in demanding environments

#827: Impact Modelling of Polymers: high-Rate Experiments for Solid-state Simulations

#828: Elastomer DEgradation under MEchanical Loading: investigation of coupling effect

#829: Physical and chEmical Ageing of amoRphous polymers by moLecular simulation

#837: Linking rheological material functions to polymer crystallization (started in 2021)

#838: Supramolecular modulation of the network connectivity in vitrimers

#839: Dynamic chemistry for tunable reversible bonding in bulk and at interfaces (started in 2021)

#840: Engineering the rheology ANd processinG-induced structural anisotropy of poLymEr composites with non-Brownian fibrous particles (started in 2021)

#841: Understanding the Rheological Origin of Striped Flow Marks in Injection Molding (started in 2021)

#843: Recyclable high-performance composites with reversible interface bonding (started in 2021)

#844: Modelling and Design of Multiphase Polymeric Materials for High Performance Applications Across Multiple Scales

#845: A joint molecular modelling and experimental approach to developing novel thin-film polymer barriers for gas containment systems

#850: Mechanism of Electrical Aging Caused by Different Structural Defects in Performance Polymer Materials (started in 2021)

#851: Creep Fatigue Interaction in Performance Polymers at High Temperatures (started in 2021)

Theses

Jingwen Chu Application of Raman and photoluminescence spectroscopy in the study of two-dimensional material/fibre hybrid composites

Publications

A.T. Zdvizhkov, M. Van Duin and F. Picchioni *Recycling Behavior of Thermoreversibly Diels-Alder Crosslinked Epm* Rubber Chemistry and Technology 94 (2) 288-297

L.V. Pastukhov and L.E. Govaert Crack-growth controlled failure of short fibre reinforced thermoplastics: Influence of fibre orientation International Journal of Fatigue 143

L.V. Pastukhov and L.E. Govaert Plasticity-controlled failure of fibrereinforced thermoplastics Composites Part B-Engineering 209

A. Aerts, C. Kroonen, J.H. Kamps, R.P. Sijbesma and J.P.A. Heuts *High Molar Mass Polycarbonate via Dynamic Solution Transcarbonation Using Bis(methyl salicyl) Carbonate, an Activated Carbonate* Macromolecular Chemistry and Physics 222 (18)

J.W. Chu, M.A. Bissett and R.J. Young MoS2 Nanosheet-Coated Carbon Fibers as Strain Sensors in Epoxy Composites Acs Applied Nano Materials 4 (9) 9181-9189

H. Ahmadi, M. Hajikazemi and W. Van Paepegem *A computational study about the effects of ply cracking and delamination on the stiffness reduction of damaged lamina and laminate* International Journal of Damage Mechanics 31 (3) 325-347

C. Breite, A. Melnikov, A. Turon, A.B. de Morais, C. Le Bourlot, E. Maire, E. Schoberl, F. Otero, F. Mesquita, I. Sinclair, J. Costa, J.A. Mayugo, J.M. Guerrero, L. Gorbatikh, L.N. McCartney, M. Hajikazemi, M. Mehdikhani, M.N. Mavrogordato, P.P. Camanho, R. Tavares, S.M. Spearing, S.V. Lomov, S. Pimenta, W. Van Paepegem and Y. Swolfs Detailed experimental validation and benchmarking of six models for longitudinal tensile failure of unidirectional composites Composite Structures 279

C. Breite, A. Melnikov, A. Turon, A.B. de Morais, F. Otero, F. Mesquita, J. Costa, J.A. Mayugo, J.M. Guerrero, L. Gorbatikh, L.N. McCartney, M. Hajikazemi, P.P. Camanho, R.P. Tavares, S.V. Lomov, S. Pimenta, W. Van Paepegem and Y. Swolfs Blind benchmarking of seven longitudinal tensile failure models for two virtual unidirectional composites Composites Science and Technology 202

E. Rashidinejad, H. Ahmadi, M. Hajikazemi and W. Van Paepegem Modeling of geometric configuration and fiber interactions in short fiber reinforced composites via new modified Eshelby tensors and enhanced meanfield homogenization Mechanics of Materials 162 A. Amiri-Rad, M. Hutter, L.E. Govaert and J.A.W. van Dommelen Improved associated flow rule for anisotropic viscoplasticity in thermoplastic polymer systems Mechanics of Materials 163

R.H.M. Mols, G.G. Vogiatzis, L.C.A. van Breemen and M. Hutter *Microscopic Carriers of Plasticity in Glassy Polystyrene* Macromolecular Theory and Simulations 30 (5)

G.G. Vogiatzis, L.C.A. van Breemen and M. Hutter Structural Transitions in Glassy Atactic Polystyrene Using Transition-State Theory Journal of Physical Chemistry B 125 (26) 7273-7289

W. Vogel, M. Hegde, A.N. Keith, S.S. Sheiko and T.J. Dingemans Chemistry and Properties of Cross-Linked All-Aromatic Hyperbranched Polyaryletherketones Macromolecules 55 (1) 100-112

Polymers for Oil and Gas

Projects

#807: Smart brines for minimal surface adsorption in polymer EOR

#808: Adsorption/retention of Polymer in Porous Media

#818: Experimental and Numerical Evaluation of Polymer Viscoelasticity Effects during EOR Applications

#821: New Polymeric Surfactants for Enhanced Oil Recovery

#849: Feasibility study of enhanced oil recovery by Polymer Assisted Water-Alternating-Gas (started in 2021)

Thesis

Bauyrzhan Satken Adsorption/Retention of Polymer Solution in Porous Media

Publications

A. Mohan, A. Rao, J. Vancso and F. Mugele Towards enhanced oil recovery: Effects of ionic valency and pH on the adsorption of hydrolyzed polyacrylamide at model surfaces using QCM-D Applied Surface Science 560

A. Guzik and P. Raffa

Direct synthesis via RAFT of amphiphilic diblock polyelectrolytes facilitated by the use of a polymerizable ionic liquid as a monomer Polymer Chemistry 12 (38) 5505-5517

Newpol

Theses

Ivana Maric

The Quest for Function in Systems with Two Dynamic Covalent Bonds: Supramolecular Self-Assembly, Self-Replication and Hydrogels for Biomedical Applications

Adrian Gonzalez Nelson

Emergent rotational dynamics and optical properties of metal-organic frameworks

Publications

A. Gonzalez-Nelson, C. Joglekar and M.A. van der Veen *Pillared cobalt metal-organic frameworks act as chromatic polarizers* Chemical Communications 57 (8) 1022-1025 A. Gonzalez-Nelson, S. Mula, M. Simenas, S. Balciunas, A.R. Altenhof, C.S. Vojvodin, S. Canossa, J. Banys, R.W. Schurko, F.X. Coudert and M.A. van der Veen *Emergence of Coupled Rotor Dynamics in Metal-Organic Frameworks via Tuned Steric Interactions* Journal of the American Chemical Society 143 (31) 12053-12062

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DPI

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

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

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

DPI provides a unique platform for generating awareness of new technology, in which participating industrial companies, competitors in the market place, communicate on a precompetitive 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 60 researchers (PhDs and Post-Docs) are currently involved in DPI projects at knowledge institutes throughout the world.





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