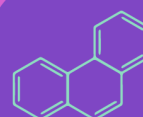


CIRCULARITY

The New Shape
Of Chemistry

2024



Symposium 'Circularity: The New Shape of Chemistry'

A symposium of T.S.V. 'Jan Pieter Minckelers'

Eindhoven University of Technology
Auditorium Building

21st of May 2024



**T.S.V.
'JAN PIETER
MINCKELERS'**

WELCOME

Dearest participant,

On behalf of the entire Symposium Committee 2024, I would like to welcome you to our symposium; 'Circularity: The New Shape of Chemistry'!

Circularity is a topic that is becoming more mainstream by the moment, as dwindling resources and increasing awareness of climate change grip chemists, chemical engineers and society as a whole. There are many different ways how circularity can be introduced and worked on in the chemical industry and research, and the importance of these possibilities is exactly why it was chosen to host a symposium about it!

As such, these possibilities will be discussed by 8 interesting guest lectures, ranging from academia to industry, and from chemistry to engineering! These will introduce aspects of circularity that can be researched and implemented, and the challenges that are faced in this process. Certain important questions will be asked, and answered by the guest lecturers, such as: Are different recycling methods possible for plastics? Can the way we make plastics today be different? How can we increase the rate of the Energy Transition? How can we use AI and other computational methods to aid in circularity? How can we implement circularity in existing plants by the means of advanced process design? And so much more!

I hope today will give you a broader view of what circularity means, and what can be done with it. Additionally, I hope that today will inspire you to strive for circularity in every branch of chemistry and chemical engineering, so we can create a sustainable, circular future for the next generations!

Enjoy the symposium, please ask any questions you have and share your ideas!

Ynse Sterkenburgh

Chairman of the Symposium Committee 2024



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PROGRAM OF THE DAY

9:00-9:30	Welcome and walk-in
9:30-10:00	Opening and introduction
10:00-10:45	Presentation by Fabian Eisenreich <i>Sustainable polymers in circular harmony</i>
10:45-11:30	Presentation by Bernhard von Vacano <i>Circularity for polymeric materials with complementary recycling processes and design</i>
11:30-11:50	Coffee break
11:50-12:35	Presentation by Jo Peters and Céline Fellay <i>Dimensions in (energy and circular) transitions</i>
12:35-13:20	Presentation by Sipke Wadman <i>Circular chemicals in Shell</i>
13:20-14:00	Lunch break
14:00-14:05	Presentation by KNCV
14:05-14:50	Presentation by Katrien Bernaerts <i>From lignin derived building blocks to covalent adaptable networks and recyclable materials</i>
14:50-15:35	Presentation by Aaldrik Haijer <i>Energy efficiency, production effectiveness and sustainability strategy</i>
15:35-15:55	Coffee break
15:55-16:40	Presentation by Süleyman Er <i>Exploring the chemical space through computational screening and AI to discover molecules for energy storage</i>
16:40-17:25	Presentation by Jaap den Doelder and Melissa Dunkle <i>The pillars of circularity</i>
17:25-17:40	Closure



Chairman of the day Antoni Forner-Cuenca



Antoni (Toni) Forner-Cuenca is an associate professor at the Eindhoven University of Technology (TU/e). Toni studied chemical engineering at the University of Alicante (Spain) and obtained his PhD from ETH Zurich and the Paul Scherrer Institute (Switzerland) in the field of hydrogen fuel cells in 2016. He then moved to Boston for his postdoctoral fellowship at the Massachusetts Institute of Technology (US), where he worked in the field of redox flow batteries for large scale energy storage. In 2019, he started his independent academic career at TU/e as faculty member. He is internationally recognized as a young leader in the science and engineering of electrochemical systems, and has been awarded the Hydrogen Europe Young Scientists Award, the ETH Zurich Medal, the Electrochemical Society Energy Technology Graduate Student Award, the NWO Veni and recently an ERC Starting Grant (FAIR-RFB).

Antoni leads the Electrochemical Materials and Systems (EMS) group in the Department of Chemical Engineering and Chemistry at TU/e. The EMS group aims to accelerate the deployment of transformative energy technologies into the real world. Furthermore, we educate the next generation of engineers and scientists in developing the independent and critical thinking skills needed to solve challenging problems facing modern society. The group employs fundamental principles at the interface of (electro)chemical engineering, materials science, and physical chemistry to design, synthesize, characterize, and simulate materials and reactors. Current areas of interest include large-scale energy storage with flow batteries, energy conversion through hydrogen fuel cells and electrolyzers, and decarbonization of the chemical industry through efficient chemical conversions and separations.



SYMPOSIUM COMMITTEE



f.l.t.r. Brendon, Sanne, Ynse, Vanina, Sofia

Ynse Sterkenburgh

Chairman

Sanne Litjens

Secretary

Vanina Valkova

Treasurer

Brendon Bocarro

*Coordinator of
External Affairs*

Sofia Shakolina

Coordinator of Promotion





Fabian Eisenreich

*Assistant Professor at TU/e
Polymer Performance Materials group*

Sustainable Polymers in Circular Harmony

Reducing the need for virgin plastic production and diverting plastic waste from landfills or natural ecosystems are major challenges for our society. Establishing a circular plastic economy offers a solution to these issues, relying on the development of innovative polymers and recycling technologies. In this context, chemical recycling of polymers plays a crucial role as it enables the breakdown of polymers into their monomers, which in turn can be used to create fresh polymers without compromising the material quality.

Our research team has recently developed new types of polymers specifically designed for closed-loop recycling. The scaffold of these polymers contains imine moieties that can selectively be deconstructed under mild and energy-efficient conditions. In addition, we incorporated bio-based building blocks into the polymer architecture to further enhance the sustainability. With this strategy, we created not only compact polymers with tunable properties but also highly porous and ultra-lightweight polymer networks with thermal superinsulation characteristics. Overall, our research efforts aim to make significant contributions to the progress of circular polymers.





Bernhard von Vacano

Senior Research Fellow at BASF

Circularity for polymeric materials with complementary recycling processes and design

In a sustainable circular economy, polymers need to transition to recycled and biobased feedstock and CO₂ emission neutrality. Structural polymers are in most cases fundamentally suited for recycling, as they can be reprocessed with relatively low energy input as a material, cleaved back into their monomers or converted back to feedstock. Today, however, these approaches still fall short in quantitatively diverting waste towards material reuse.

Recycling back into high value applications requires a portfolio of existing and emerging technology solutions: Sustainable design of products and polymers, recycling technologies, appropriate business models, and enabling technologies. These building blocks need to be developed and combined, and finally implemented at scale. Examples from industry range from tailored additives to enable polypropylene mechanical recycling over several cycles, depolymerization of cross-linked materials such as polyurethane foams, or design for recycling on the system or product level.



GRADUATED? JOIN THE VSI/E!

Do you want to stay in touch with your fellow students after graduation? Would you like to expand your network? Are you interested in staying up-to-date with the CE&C faculty? Do you enjoy participating in fun activities? If so, you might consider joining the alumni association.

The VSI/e (Vereniging Scheikundige Ingenieurs Eindhoven) has been organizing activities for CE&C alumni since 1994 and has approximately 500 members. Our primary goals are to enhance networking among engineers from Eindhoven and to foster connections between graduates and the TU/e and chemical engineering & chemistry faculty.

We achieve these goals by hosting a variety of activities, ranging from scientific lectures to social events like reunions. This provides excellent opportunities to stay informed about scientific developments, connect with our faculty, and reunite with old study friends.

Check our website, www.vsi-eindhoven.nl, where you can also join us!





Jo Peters

*Ambassador and Chair of Chemelot
Circular Hub*

Chair of Supervisory Board of Solarge



Céline Fellay

*Program Manager Transition Scenario's
and System Integration at Brightside*

Dimensions in (Energy and Circular) Transitions

The Circular Transition, its dimensions, and its relation to the Energy Transition in the context of Chemelot Circular Hub and Brightside will be discussed during the presentation.

Chemelot Circular Hub is a triple helix alliance of stakeholders (Government, Industry, Education) situated at the Chemelot Campus in Sittard-Geleen (Limburg). Its aim is to power and accelerate the circular transition by benefitting from the vibrant ecosystem that exists on and around the campus. To this end we have created a CEAP (Circular Economy Action Plan) with 21 Flagship projects (some 100 project in total). The aim is for the site and the region to be fully circular by 2050.

The hub (CCH) is based on four pillars in and across which above mentioned projects take place: Innovation, People, Infrastructure and Society. Brightside was founded by Brightside Chemelot Campus, Maastricht University, TNO and Sitech Services and aims to identify and develop novel technology that is required for the circular transition. It releases a yearly BTO (Brightside Transition Outlook) in which main dimensions of required feed and product streams are identified.





Sipke Wadman

Senior Researcher and Principal Science Expert at Shell

Circular Chemicals in Shell

In this lecture he will talk about the role of carbon in the Shell energy transition scenarios. These energy scenarios describe possible futures and allow us to think about projects and technologies in different possible futures. In any of these scenarios, renewable energy will play an increasingly important role in the primary energy mix.

Next to the energy transition a carbon transition will be necessary; currently virtually all carbon-based products are oil derived, and intimately linked to the energy infrastructure. Not only would they serve as energy carrier in hard to electrify sectors, but roughly 20% of the oil is destined for non-energy products. We will discuss alternative carbon sources in the light of scale, timeframe and technical feasibility.

Two specific projects will be highlighted in which we explore those sustainable carbon sources. In one of these projects, non-technical aspects drove us to halt further development. The other project is currently under construction at the Shell Moerdijk chemicals park.






BECOME **1** of us

Covestro is one of the world's largest polymer companies. Our business activities are focused on the manufacture of high-tech polymer materials and the development of innovative solutions for products used in many areas of daily life. You can find us e.g. in lightweight vehicles, comfortable mattresses, energy efficient houses and wind energy parks.

In the Netherlands Covestro focuses on the production of sustainable coatings that are applied amongst others in decorative paints, inks for the printing industry and protective coatings for fibre optic cables. Innovation and sustainability are the driving forces behind the continuous development of our products, processes and facilities.

Covestro aims to achieve climate neutrality in its operations by 2035 and wants to fully focus on the Circular Economy as a guiding principle in its company strategy. This means we want to completely move away from fossil energy and fossil raw materials and focus all our R&D efforts on new and innovative chemical recycling routes for our end products. With these high ambitions we see ourselves as a shaping force for the entire plastics industry. **Would you like to become 1 of us?**



Then don't hesitate to check our vacancies at www.covestro.career.com or to reach out to us via NederlandHR@covestro.com!



Katrien Bernaerts

*Associate Professor at Maastricht University
Sustainable Polymer Synthesis group*

From lignin derived building blocks to Covalent Adaptable Networks and Recyclable Materials

In response to the escalating challenges associated with traditional polymer materials, the following integrated study demonstrates innovative approaches towards sustainable polymer synthesis and application. The collective research endeavors delve into the realms of covalent adaptable networks (CANs) derived from biomass sources, with a particular focus on lignin-derived building blocks. The overarching objective is to address pressing environmental concerns by exploring green and low-carbon feedstock, eco-friendly preparation processes, and effective material recycling. As such, this work contributes to the ongoing transition towards a circular economy.

Three distinct approaches to sustainable polymer synthesis as well as different application pathways are explored. First, the utilization of lignin-derived vanillin in the production of circular plastics is investigated through water-borne emulsion polymerization. The resulting polymethacrylates, based on 2-(methacryloyloxy)ethyl vanillin and 2-octyl acrylate, exhibit imine functionality for the creation of recyclable vitrimers. The emphasis on water-borne synthesis aims to minimize environmental impact. A second approach focuses on addressing the environmental concerns associated with acrylic photopolymer resins in stereolithographic 3D printing. Biobased, photo-cross-linkable molecules are synthesized from vanillin and dimer fatty diamine, yielding imine based vitrimers that contribute to the development of recyclable 3D-printed resins. The study demonstrates their rapid crosslinking under UV light and subsequent reprocessing capabilities. Finally, the third example involves the catalyst-free synthesis of imine based covalent adaptable networks (CANs) directly from lignin. The tunable mechanical properties of the CANs, along with their chemical recyclability and potential application as repairable, self-cleaning, removable and degradable coatings will be demonstrated.





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Aaldrik Haijer

CEO of Water Energy Solutions



Water Energy Solutions is a company focussing on energy efficiency, production effectiveness and sustainability strategy.

Aaldrik will take listeners on a tour of sustainable production and show why moving towards biobased products can only be achieved by raising circularity in our feedstock and production chains.

Water & Energy Solutions is a technical firm with strong roots in chemical engineering. Process optimisation being their area of expertise, they will provide an insight into the role circularity plays in it. They provide industrial clients with new optimization opportunities to greatly reduce production costs by increasing water and energy efficiency while maximizing process throughput. As a result, their ideas help companies to become high-performing businesses.



Advanced recycling for plastics

ExxonMobil

ExxonMobil is strengthening the circularity of plastics through Exxtend™ technology for advanced recycling. Advanced recycling can turn more of the plastics we use every day into valuable products. Less than 10% of plastics are recycled today. Advanced recycling complements mechanical recycling and helps address plastic waste by enabling the breakdown of more kinds of plastic and converting them back into the molecules needed to make new products. It's also helping users of plastic such as packaging manufacturers, beverage companies, and restaurants meet their sustainability goals. It's a proven technology that can be used around the

world, significantly improve recycling rates and support a more circular economy.

Our large-scale advanced recycling facility in Baytown, Texas, has been operating since December 2022, capable of processing 80 million pounds of plastic waste per year. This facility is already helping to meet rising demand for circularity, with sales in the United States, Canada, Thailand and Australia, among others. We plan to increase our global capacity to 1 billion pounds per year by the end of 2026, with advanced recycling facilities in Europe, the United States, and Asia Pacific.

Learn more about how Advanced Recycling works:





Süleyman Er

*Head Solar Fuels Department and Group Leader
Autonomous Energy Materials Discovery Group at
DIFFER*

Exploring the chemical space through computational screening and AI to discover molecules for energy storage

Redox flow batteries (RFBs) represent a promising technology for energy storage, offering scalable solutions to integrate renewable energy sources into the electricity grid. However, advancing RFB technologies faces challenges in identifying electroactive compounds that are abundant or easily synthesizable, electrochemically efficient, stable, safe, and in line with circular chemistry principles. A major challenge is to identify compounds from a vast chemical space. High-throughput computational screening, using powerful computational chemistry methods and software tools on high-performance computing, offers a solution. Concurrently, artificial intelligence (AI) models are useful at rapidly predicting material properties and revealing insights from extensive experimental and computational data.

In the presentation, he will introduce research projects that merge AI with computational screening for identifying electroactive molecules for RFBs. Our approach is multi-faceted, involving: 1) Development of theoretical methodologies and AI tools to evaluate redox potentials and solubilities of candidate compounds in water, along with automated chemical space visualization and chemical price search tools for sourcing these molecules from suppliers. 2) Investigation of structure-property relationships and prioritization of compounds, aiming to pinpoint the ideal candidates for practical experiments. 3) Conducting electrochemical tests on safe and easily accessible compounds selected from our virtual library. 4) Developing a computational database of electroactive molecules. In summary, these examples demonstrate how AI and computational science can be coupled to effectively search for promising chemical compounds for energy storage.



Jaap den Doelder

Research & Development Fellow at Dow



Melissa Dunkle

Senior Research Scientist at Dow



The pillars of circularity

For the chemical industry, plastics circularity requires a multifaceted approach, where various recycling routes should be incorporated into the overall strategy. As part of Dow's 2030 goal to transform plastic waste and other forms of alternative feedstocks into 3 million metric tons of circular and renewable solutions annually, both mechanical and chemical (or advanced) recycling options are under investigation.

In this presentation, we will highlight our plastics circularity strategy. We will focus on technology, from challenges to opportunities. We will also highlight the importance of partnerships in this journey.



COMMITTEE OF RECOMMENDATION

This symposium is supported by the following people:

Prof. dr. ir. Kitty Nijmeijer

Dean of the department of Chemical Engineering and Chemistry at Eindhoven University of Technology and professor in the Membrane Materials and Processes research group



Prof. dr. Yvonne van der Meer

*Chairman of the KNCV
(Royal Dutch Chemistry Society)*



Prof. dr. Silvia Lenaerts

Rector Magnificus of Eindhoven University of Technology



Prof. dr. ir. John van der Schaaf

Program director of the department of Chemical Engineering and Chemistry at Eindhoven University of Technology and professor in the Sustainable Process Engineering research group



**Ruud van de Donk**

Interim managing director of the department of Chemical Engineering and Chemistry at Eindhoven University of Technology

**Prof. dr. Željko Tomović**

Professor in the Polymer Performance Materials research group

**Prof. dr. ir. Anja Palmans**

Professor in the Supramolecular Chemistry and Catalysis research group

**Dr. ir. Ivo Filot**

Assistant professor in the Inorganic Materials and Catalysis research group

**Dr. Ghislaine Vantomme**

Assistant professor in the Macro-Organic Chemistry research group





T.S.V. 'JAN PIETER MINCKELERS'

The study association T.S.V. 'Jan Pieter Minckelers', commonly abbreviated as 'Japie', is the study association for the department of Chemical Engineering and Chemistry at the Eindhoven University of Technology. The goals of Japie can be split up into three categories: education, self-development and fun.

Japie has the goal to improve the education at our department by giving the students the opportunity to give their feedback and have regular contact with teachers.

Japie gives its members the opportunity to develop their soft skills. Members can take part in several committees. The committees vary from a freshmen committee, which organizes four smaller activities throughout the year, to a study tour committee, which organizes a trip of four weeks to a foreign country. While taking part in a committee, members can improve their communicative, cooperative or presentational skills. Japie also focuses on preparing its members for their professional career by visits to industrial plants and organizing lectures given by chemical companies.

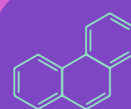
The final goal is quite self-explanatory: fun. Japie organizes a variety of relaxing, sporty or social activities. A casino night and a survival day are the perfect examples of this. Having fun with friends and meeting new people are great ways to re-energize after a long day of studying.



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