PROCEEDINGS

of the XVII Postgraduate Summer School on Green Chemistry

7 July - 11 July 2025 Venice, Italy





Green Sciences For Sustainable Development Foundation

COLLECTION OF ABSTRACTS

Editors: Francesco Trotta, Fabio Aricò, Aurelia Visa and Mirabbos Hojamberdiev

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XVII Postgraduate Summer School on Green Chemistry,

7 July - 11 July 2025, Venice, Italy

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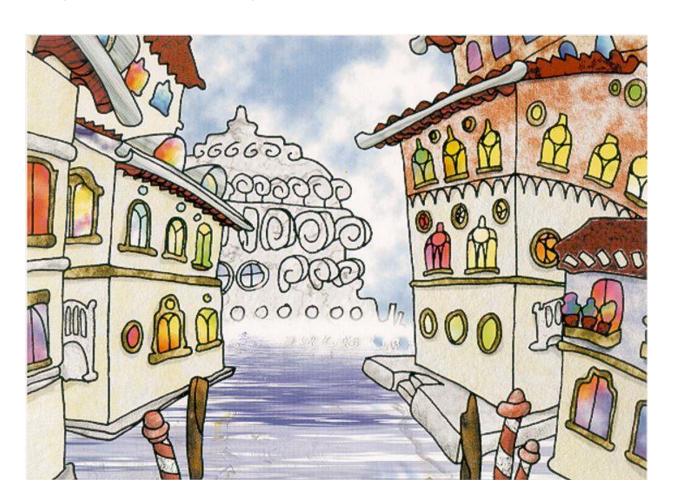






GREEN SCIENCES FOR SUSTAINABLE DEVELOPMENT FOUNDATION

The Summer School was an international initiative organized and managed by the new-born **Green Sciences for Sustainable Development (GSSD) Foundation** (<u>www.gssd-foundation.org</u>), a non-profit Foundation established in February 2020 and based in Venice, Italy.



The Foundation was constituted, pursuant to Article 14 and following the Italian Civil Code, on February 17th, 2020.

The Foundation has legal personality since it was registered at the Prefecture of Venice on May 28th, 2020, as a non-profit organization. Any proceeds, annuities, and profits deriving from the performance of the activities are used exclusively to pursue the purposes of the Foundation.

The Foundation is based in the Municipality of Venice. In order to pursue the statutory purposes, with the resolution of the Board of Directors, secondary offices, agencies, and branches may also be established, also abroad.

The Foundation facilitates the participation in its activity of public bodies and administrations and private subjects, developing and increasing the necessary network of national and international relations functional to achieve its goals.



PURPOSES

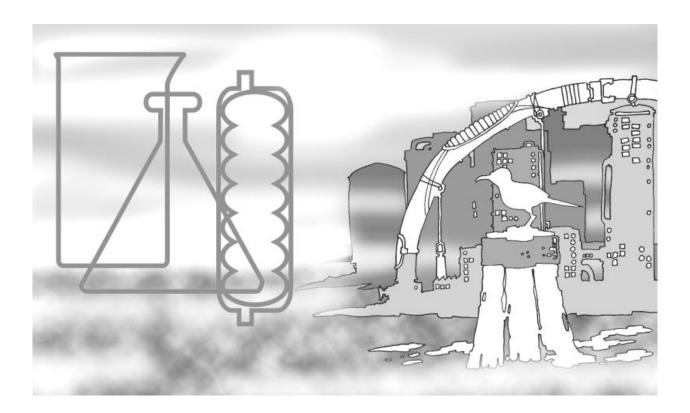
The main aims of the Foundation are:

- a) to encourage the development of scientific education and the dissemination of knowledge in the national and international fields of the sciences of a chemical, physical and environmental order and of the disciplines that care and promote sustainability with particular regard to Sustainable and Green Chemistry and their applications;
- b) to support and disseminate scientific, technological and cultural development in Sustainable Development in accordance with the 17 Goals of the United Nations, in the sectors of the use of renewable resources, energy saving, intrinsically clean processes and products, with low or no environmental impact, not harmful to health and green remedies for climate change;
- c) to promote initiatives supporting the transfer of research results, the protection of intellectual property and the birth of new entrepreneurship;
- d) to promote the involvement and collaboration of public or private, local, national, EU, foreign or international subjects in pursuing the aims of the Foundation itself;
- e) to promote the internationalization of teaching and research activities through the management of specific services and participation in joint initiatives with other subjects, public or private, national, EU or international.



ACTIVITIES

- a) to organize and manage national and international Congresses and Conferences, education, specialization, and updating courses and other advanced training activities such as Summer Schools, Forums, and International Thematic Workshops, also in collaboration with other private and public institutions; the sub-Saharan African continent will be paid particular attention;
- b) to publish books and magazines with their own ISBN;
- c) to create and manage any laboratories or research centers also together with other public or private entities;
- d) to participate in the operational management of scientific and/or technological structures of other foundations, structures, and research bodies;
- e) to enter into agreements, contracts, agreements, or understandings with other subjects, public or private;
- f) to promote and organize the collection of private and public funds and the request for local, national, European, and international public and private contributions to be used for the purposes of the Foundation.



XVII POSTGRADUATE SUMMER SCHOOL ON GREEN CHEMISTRY 7 July - 11 July 2025

BOOK OF ABSTRACTS

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WELCOME MESSAGE FROM THE CHAIR OF THE SUMMER SCHOOL



Dear Colleagues and Students,

I am Francesco Trotta, Full Professor Industrial Chemistry-University of Turin (IT) and President of Green Sciences for Sustainable Development Foundation.

It is with great pleasure that I welcome you to the 17th edition of the Postgraduate Summer School on Green Chemistry (GCSS 2025).

This year's edition marks a significant milestone, as it will be the first one not chaired by Professor Pietro Tundo, the founder of this esteemed Summer School, who sadly passed away last year. I had the honor of knowing Professor Tundo personally, as he was my PhD supervisor

at the University of Turin, where I now lead my research group. His illustrious career as a professor and mentor left a lasting impact on many generations of students and scientists across the globe.

In recognition of his immense contributions, the board of the Green Science for Sustainable Development Foundation and I have decided to continue his legacy by organizing this highly regarded international Summer School. Our aim is to build on the success of previous editions by inviting distinguished educators, leaders from major chemical industries, and outstanding postgraduate students.

One of the key highlights this year was the generous support from our sponsors, which allowed us to offer scholarships to outstanding students from developing countries. These scholarships enabled participation, either on-site or virtually, ensuring that talented students had access to this unique learning and networking opportunity, regardless of cultural barriers. Many of these students will their research during our Virtual and In-person Poster Sessions, contributing to vibrant and innovative discussions.

Postgraduate students will also have the chance to showcase their research in both virtual and in-person poster sessions. The best posters will be awarded during our Closing Ceremony.

GCSS 2025 will provide an exceptional platform for postgraduate students from various countries to interact with renowned scientists and educators in the field of Green Chemistry. It will offer students the chance to exchange ideas, build international research networks, and develop lasting friendships with peers from around the world.

At last but not least, I would like to thank all of the teachers who contributed to making the 17th Postgraduate Summer School on Green Chemistry such a memorable and impactful event. Your active participation, energy, and creativity ensured that this year's edition was not just a continuation of past success, but a step forward in advancing the important work that Professor Tundo started.

As we look to the future, I hope that the bonds formed during the Summer School will continue to strengthen, leading to future collaborations and advances in Green Chemistry. I encourage all of you to remain involved, to build on the knowledge and connections you've gained, and to be ambassadors for sustainable science in your own communities and institutions.

Thank you all once again for your dedication, and I look forward to seeing what we can achieve together in the future.

Francesco Trotta
Chair of the Summer School

FOREWORD BY THE FIRST DEPUTY CEO PJSC PhosAgro



At PhosAgro we understand that supporting science and education is a long-term investment in the future. For this reason, we have been helping young scientists from all over the world thanks to our close collaboration with UNESCO and IUPAC in the field of green technology.

The Postgraduate Summer School on Green Chemistry is a key project for PhosAgro and IUPAC.

Our unique project was brought to life thanks to Professor Pietro Tundo, a talented educator, a true friend, and a great researcher who was one of the pioneers of green chemistry.

Professor Tundo, a giant in the field and author of countless groundbreaking works in organic chemistry and environmental impact reduction, was truly a man with a big heart. He put everything he had into helping young people and played a huge role in educating the next generation of top scientists. And it was Professor Tundo who invited PhosAgro to become a long-term partner of the IUPAC Summer School in Green Chemistry. Professor Tundo's name is printed in bold letters in the annals of chemistry. His memory will forever remain in his legacy, his accomplishments and his students.

Siroj Loikov First Deputy CEO, PJSC PhosAgro

FOREWORD BY THE LOCAL ORGANIZING COMMITTEE IN VENICE



Dear students and teachers of the Postgraduate Summer School on Green Chemistry 2025,

It is an honor for me to welcome you to this 17th edition of the school, which is once again held in the wonderful setting of Venice, which has been, and it is still nowadays a crossroads of peoples and cultures.

This is my tenth Summer School, my seventh one as part of the Organizing committee representing Ca' Foscari University. I still vividly remember my first participation at the Summer School. It happened after returning from my experience abroad in America as a post-doctoral fellow when I was invited by

Prof Tundo - then director of the Interuniversity Consortium "Chemistry for the Environment (INCA) and creator of the event - to take part in the 2005 edition of the School held in San Servolo, a small island in the Venetian Lagoon. I remember the high quality of the teachers' presentations, the excitement of the young students, and the constant buzz of questions, laughter, and conversations about Green Chemistry. Most of the 2005 Summer School students are now grown-up scientists, teachers, and professors that still happily remember the School as an amazing opportunity to broaden their knowledge and create new collaborations and friendships for what has then become their future careers. Almost 20 years later I still recognize in the students' eyes the same excitement and the desire to explore issues related to Green Chemistry and sustainability nowadays even more intertwined with the world's social and economic growth.

The 2025 edition of the Postgraduate Summer School on Green Chemistry is most probably the most emotionally demanding as it is the first one without its founder Prof Pietro Tundo who has also been my mentor for more than 10 years. It was a quite challenging task to guarantee the high quality of the teachers and of the school as Pietro has envisaged over the years, although I am sure he will be very proud of the result we were able to achieve.

This year's topics range from benign synthetic routes to green catalysts, alternative solvents, renewable and green materials, green energy, and green chemistry education. These topics have been selected as they encompass actual, new, or emerging issues related to the green and sustainable development of society and the scientific community.

As in every edition of the Summer School, each student had to present a scientific poster highlighting his actual research topic and interest. The number and the high quality of this year's poster presentations have been overwhelming, and I cannot wait to see how this young scientist will evolve in the future generation of scientific experts that will guide the world toward a greener future.

Fabio Aricò

Professor of Organic Chemistry Ca' Foscari University, Member of the Organizing Committee of the Postgraduate Summer School on Green Chemistry 2025

SUMMER SCHOOL COMMITTEES

CHAIR OF THE SUMMER SCHOOL

• Francesco Trotta, President of Green Sciences for Sustainable Development Foundation, Venice, Full Professor of Industrial Chemistry, University of Turin, Italy

ORGANIZING COMMITTEE

- Prof. Fabio Aricó, Ca' Foscari University of Venice, Italy
- Dr. Aurelia Visa, Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry, Timisoara, Romania
- **Prof. Mirabbos Hojamberdiev**, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark
- Dr. Graziana Gigliuto, Green Sciences for Sustainable Development Foundation, Italy
- Dr. Aleksander A. Antonov, Director, Department of International Development & Projects, PhosAgro

INTERNATIONAL JURY FOR THE POSTER SESSIONS IN PRESENCE AND ONLINE FOR THE

"Green Sciences for Sustainable Development Foundation Students Online Awards"

Coordinator of the Posters Evaluation: Aurelia Visa, Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry – Timisoara, Romania

- Alberto Figoli, Director of the Institute on Membrane Technology of the National Research Council of Italy, ITM-CNR
- Eduardo Garcia-Verdugo Cepeda, Professor at University Jaume I, Castellon, Spain
- Marcello Baricco, Department of Chemistry and NIS INSTM University of Turin, Italy
- **Jonathan Forman,** Science and Technology Advisor in the Global Security Technology and Policy Group under the National Security Directorate of Pacific Northwest National (PNNL), United States
- Christopher Brett, Full professor of chemistry, University of Coimbra, Portugal
- **Philip Jessop,** Full Professor and Canada Research Chair of Green Chemistry at the Department of Chemistry, Queen's University in Kingston, Canada
- Luigi Vaccaro Full Professor of Organic Chemistry, Università degli Studi di Perugia, Italy
- **Vânia Zuin Zeidler,** Professor at Institute of Sustainable Chemistry, School of Sustainability, Leuphana University of Lüneburg, Germany
- Maia Sokolova, Scientific officer, B1 Chemistry Unit, Directorate of Prioritization and Integration, European Chemical Agency, Helsinki, Finland
- Marco Sangermano, Professor at Politecnico di Torino Department of Applied Science and Technology, Turin, Italy
- Mirabbos Hojamberdiev, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark
- Alberto Cugnetto, Expert in Viticulture and Enology, Academy of Agriculture of Turin, Italy

SUMMER SCHOOL 2025

The School was held in collaboration with the academic institution of Ca' Foscari University of Venice and University of Turin.

The event was endorsed by UNESCO Chair Aid4GEA, by the Gruppo Interdivisionale di Green Chemistry of Società Chimica Italiana (SCI), by the Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry, by Mads Clausen Institute, University of Southern Denmark and Data-centric Environmental Studies Center.

The Summer School was sponsored by PhosAgro-Russia, the Organization for the Prohibition of Chemical Weapons-OPCW, the International Union of Pure and Applied Chemistry (IUPAC), and Sasol-South Africa.

Thanks to the participation of these Sponsors, 10 postgraduate students attending in presence and online coming from developing countries have been awarded scholarships.

This year, the number of applications coming from developing countries students was 100.

During a strict selection made in March by the Organizing Committee, the scholarship applicants were evaluated based on their CVs, their list of publications, the recommendation letters from their Tutors, and their motivations to attend the Summer School 2025.

The total number of students attending the 17th IPSSGC 2025 was 75; 40 of them were in-person in Venice and 35 students were online, coming from 33 different countries.

The rigorous selection of the participants contributed to forming a class of high cultural level students, who certainly find themselves at a point in their life where they are ready to invest their talents and scientific know-how for their future professional careers maturely and responsibly. The top-level and diverse range of lectures offered at the Summer School, provided them the chance to look around, exchange their scientific knowledge, and establish important links with other participants and professors for fruitful joint projects and research activities.

Green Chemistry has proven to be a compelling field for young scientists, as demonstrated by the Summer Schools held from 1998 to 2025, with over 1500 students participating. This interest is evident as around 6 alumni have returned as teachers, showing the program's significant impact on their careers and their commitment to the field. Green Chemistry's interdisciplinary nature provides a unique perspective, encouraging students to think creatively about sustainable solutions. The Summer Schools offer a valuable opportunity for students to explore various scientific disciplines and understand the importance of environmentally responsible practices.

The Summer School hosted 7 lecture sessions and 2 poster sessions on the following main topics:

- 1. Exploitation of renewable resources
- 2. New reaction pathways
- 3. Energy saving
- 4. Food safety
- 5. Sustainable Polymers
- 6. Climate Change
- 7. Health

After the Summer School, all participants received a certificate of attendance

This Summer School held in person and remotely, was joined in person and online for those who cannot come to Venice yet. We engaged the participants with the outstanding scientific quality of the teachers, involving themin the discussion of the lectures and, not less importantly, through the poster sessions.

From the outcomes of these hybrid Summer Schools, the GSSD Foundation has learned how to manage future events, which they hope will become a permanent feature in Venice due to their long-standing tradition and high scientific value.

Among various Summer Schools and similar educational events, the Green Chemistry Summer School in Venice stands out as a model of good practice for several reasons. First, the careful selection process ensures a class of top international students passionate about green chemistry and eager to contribute to its research. Second, the program attracts an exceptionally high caliber of teachers, including Nobel Prize winners and top-ranked global scientists. Third, the unique setting of Venice adds a profound dimension to the school, as the city itself is a symbol of sustainability and resilience, offering a fitting backdrop for discussions on environmental stewardship.

During the XVII International Postgraduate Summer School on Green Chemistry in 2025, the teachers provided an in-depth overview of their current scientific work over the five days of the program. They also evaluated the students' research, offering valuable feedback and suggestions for improvement, further enhancing the educational experience.

TEACHERS AND LECTURES

(According to the Summer School Programme Order)

1. CHRISTOPHER BRETT

Department of Chemistry, University of Coimbra, Portugal

Deep Eutectic Solvents and Electrochemical Applications: A Green Materials Approach

2. ALBERTO FIGOLI

Institute on Membrane Technology, National Research Council of Italy, Rende (CS) Italy Green Strategies for Membrane Preparation

3. GIACOMO TRAPASSO

Department of Environmental Science Informatic and Statistics, Ca' Foscari University of Venice, Italy Metrics for Green Syntheses: Two Case Studies in Biorefinery

4. AURELIA VISA

Romanian Academy, "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania Greener Approaches to the Synthesis and Application of Metal-Organic Frameworks

5. PHILIP JESSOP

Department of Chemistry, Queen's University, Canada How Chemists Can Use Life Cycle Assessment to Guide Our Research

6. MARCELLO BARICCO

Department of Chemistry and NIS – INSTM, University of Turin, Italy **Hydrogen for Energy Transition**

7. EDUARDO GARCÍA-VERDUGO

Departamento de Química Inorgánica y Orgánica, Universidad Jaume I, Castellon, Spain **Que c'est verte Venise**

8. FABIO ARICÒ

Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Italy

The Reactions of Organic Carbonates

9. MARCO SANGERMANO

Department of Applied Science and Technology, Politecnico di Torino, Italy Polymers and Plastics the Route to Sustainability

10. MIRABBOS HOJAMBERDIEV

Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark Green Hydrogen Generation from Solar Water Splitting over Metal Oxynitrides

11. VÂNIA ZUIN ZEIDLER

Institute of Sustainable Chemistry, School of Sustainability, Leuphana University of Lüneburg, Germany Green and Sustainable Chemistry and The Future of Food

12. PETER LICENCE

School of Chemistry, The University of Nottingham, Nottingham, United Kingdom

Green Chemistry Translation: A Design for Life!

13. POLINA YASENEVA

Department of Chemical Engineering, UCL and Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom

Designing Green – Leveraging Life Cycle Assessment for Sustainable Chemistry

14. MAIA SOKOLOVA

Chemistry Unit, Directorate of Prioritization and Integration, European Chemicals Agency (ECHA) Chemical Safety Through Science, Collaboration and Knowledge

15. LUIGI VACCARO

Laboratory of Green S.O.C., Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Italy

Novel Technologies for Green Synthesis and Catalysis

16. ELISA MORETTI

Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia, Italy

Aid4GEA – A Bridge Across the World: When Hard Science Fertilizes Sustainable Development

17. ANAMARIA TODEA

Politehnica University Timisoara, Faculty of Chemical Engineering, Biotechnology and Envoironmental Protection, Biocatalysis and Green Chemistry Group, Romania

Biocatalytic Strategies for Green Synthesis of Bio-Based Oligoesters

18. ALBERTO CUGNETTO

Socio ordinario dell'Accademia di Agricoltura di Torino, Italy

Innovations in Sustainable Agriculture with a Special Focus on Wine and Viticulture

19. GIULIA FIORANI

Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Italy Catalytic Strategies for Non-Reductive CO₂ Valorization

20. ANDREA SPOLAOR

Institute of Polar Sciences, National Research Council of Italy, Italy

The Climate Change in the Arctic

21. FRANCESCO TROTTA

Department of Chemistry, University of Turin, Italy **Exploitation of Renewable Resources in Polymer Chemistry**

22. JONATHAN E. FORMAN

Pacific Northwest National Laboratory, Seattle, USA

Eliminating the Chemicals of War and the Challenges of Chemical Security: Does Green Chemistry Make a Difference?

17th Edition of the Green Chemistry Postgraduate Summer School 2025

FRIDAY 11-July	0PCW	9:30- Frances co Trotta University of Turin, Italy	10:30- Jonathan Forman		of Pacific Northwest National		11:35 Coffee Break	11:35-	12:30 CLOSING CEREMONY AND POSTER AWARDS													
	9:00	8, 5	i i	11		;	1 11	11	15:													
THURSDAY 10-July	IUPAC	Luigi Vaccaro University of Perugia,	Italy	Elisa Moretti Ca' Foscari University of	Venice, Italy	Coffee Bresk	A T I	Politehnica University of	Timişoara, Romania	Albania Carretta	onaugh on age	Academy or Agriculture of Turin, Italy	dearri	uaum.	Giulia Fiorani	Venice Italy	Andrea Spolaor	Institute of Polar Science (CNR-ISP), Italy	POSTER SESSION 2	-	Coffee break	
	9:00-9:30	9:30- 10:30		11:15		11:15-	11:35	12:20	Ì	12:20-	13:05		13:05 -	14:30	14:30-	CT:CT	15:15-	16:00	16:00-	17:30		
WEDNESDAY 9-July	GSDD Fundation	Vania Zuin Leuphana University.	Germany	Peter Licence	Nottingham, UK	88 SF 2885-55	Coffee break	Polina Yaseneva	University of Cambridge, UK		Maia Sokolova	European Chemical Agency, Finland		Lunch					SOCIAL EVENT:			
	9:00-9:30	9:30-	10.30	10.30-		11:15-	11:35	11:35-			13:05		13:05-	14:30					18:00	THE STATE OF THE S		
TUESDAY 8-July	Phosagro	Philp Jessop Queen's University, Canada	Marcello Baricco	University of Turin, Italy	Coffee Break		Eduardo García-Verdugo	University Jaume I, Spain	Fabio Aricò	Ca' Foscari University of	Venice, Italy	Lunch	-	Polytechnic University of	Turin, Italy	Mirabbos Hojamberdiev	University of Southern Donmark Donmark	POSTER SESSION 1	+		Coffee break	
	9:00-9:30	9:30-	10.30	11:15	11:15-	11:35	12:20		12:20-	13:05		13:05-	200	15:15		15:15-	16:00	16:00-	1/30			
MONDAY 7-July	Registration at the Summer School		OPENING CEREMONY		Lunch	Christopher Brett,	University of Coimbra,	Alboro Eigeli	National Research Council	of Italy (ITM-CNR), Italy	Giacomo Trapasso	Ca' Foscari University of	Vernice, Italy	Coffee break	Aurelia Visa	"Coriolan Drăgulescu"	Institute of Chemistry,	Nomania				
	9:00-		11.00-	12:00-	13:30	13:30-	14:30	14.20	15:15		15:15-	16:00	3	16:00	16:30-	17:15						



CEST TIME Central European Summer Ti

THE SUMMER SCHOOL 2025 PROGRAMME

MONDAY, 7 JULY 2025, MORNING

REGISTRATION

OPENING CEREMONY

PRESENTERS:

Francesco Trotta, Chair of the Green Chemistry Summer Schools and President of GSSD Foundation, University of Turin, Italy

Luigi Brugnaro (letter), Major of Municipality of Venice.

Siroj Loikov (video message), First Deputy CEO PJSC PhosAgro.

Fabio Aricò, Board Member GSSD Foundation, Ca' Foscari University of Venice.

Graziana Gigliuto, Green Sciences for Sustainable Development Foundation, Venice.

MONDAY, 7 JULY 2025, AFTERNOON

1st LECTURE SESSION:

Moderator: Fabio Aricò, Full Professor of Organic Chemistry, Ca' Foscari University of Venice, Italy

CHRISTOPHER BRETT, Professor, Department of Chemistry, University of Coimbra, Portugal

Lecture title: Deep Eutectic Solvents and Electrochemical Applications: A Green Materials

Approach

ALBERTO FIGOLI, Profesor, *Institute on Membrane Technology, National Research Council of Italy, Rende (CS), Italy*

Lecture title: Green Strategies for Membrane Preparation

GIACOMO TRAPASSO, Researcher, Department of Environmental Science Informatics and Statistics, Ca' Foscari University of Venice, Italy

Lecture title: Metrics for Green Syntheses: Two Case Studies in Biorefinery

AURELIA VISA, Senior Researcher, Romanian Academy, "Coriolan Dragulescu" Institute of Chemistry, Timişoara, Romania

Lecture title: Greener Approaches to the Synthesis and Application of Metal-Organic Frameworks

TUESDAY, 8 JULY 2025, MORNING

SPONSORS AND INSTITUTIONS

PHOSAGRO

PRESENTER:

Alexander Antonov – Director, Department PJSC PhosAgro International Projects

2ND LECTURE SESSION:

Moderator: Francesco Trotta, Professor at the Department of Chemistry, University of Turin, Italy

PHILIP JESSOP, Professor, Department of Chemistry, Queen's University, Canada Lecture title: How Chemists Can Use Life Cycle Assessment to Guide Our Research

MARCELLO BARICCO, Professor, Department of Chemistry and NIS – INSTM, University of Turin, Italy

Lecture title: Hydrogen for Energy Transition

3rd LECTURE SESSION:

Moderator: Aurelia Visa, Senior Researcher Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry, Timisoara, Romania

EDUARDO GARCÍA-VERDUGO, Professor, *Departamento de Química Inorgánica y Orgánica, Universidad Jaume I, Castellon, Spain*

Lecture title: Que c'est verte Venise

FABIO ARICÒ, Professor, Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Italy

Lecture title: The Reactions of Organic Carbonates

TUESDAY, 8 JULY 2025, AFTERNOON

4TH LECTURE SESSION:

Moderator: Giacomo Trapasso, Researcher, Ca' Foscari University of Venice, Italy

MARCO SANGERMANO, Professor, Department of Applied Science and Technology, Politecnico di Torino, Italy

Lecture title: Polymers and Plastics the Route to Sustainability

MIRABBOS HOJAMBERDIEV, Professor, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark

Lecture title: Green Hydrogen Generation from Solar Water Splitting over Metal Oxynitrides

IN-PERSON POSTER SESSION 1, 16:00-17:30 (16 Posters)

WEDNESDAY, 9 JULY 2025, MORNING

SPONSORS AND INSTITUTIONS

GREEN SCIENCES FOR SUSTAINABLE DEVELOPMENT FOUNDATION

PRESENTERS:

Francesco Trotta – President, Green Sciences for Sustainable Development Foundation Fabio Aricò – Board Member, Green Sciences for Sustainable Development Foundation

5th LECTURE SESSION:

Moderator: Eduardo Garcia-Verdugo Cepeda, Professor at University Jaume I, Castellon, Spain

VÂNIA ZUIN ZEIDLER, Professor, *Institute of Sustainable Chemistry, School of Sustainability, Leuphana University of Lüneburg, Germany*

Lecture title: Green and Sustainable Chemistry and The Future of Food

PETER LICENCE, School of Chemistry, The University of Nottingham, Nottingham, United Kingdom Lecture title: Green Chemistry Translation: A Design for Life!

6th LECTURE SESSION:

Moderator: Mirabbos Hojamberdiev, Professor, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark

POLINA YASENEVA, Professor, Department of Chemical Engineering, UCL and Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom

<u>Lecture title</u>: Designing Green – Leveraging Life Cycle Assessment for Sustainable Chemistry

MAIA SOKOLOVA, Officer, Chemistry Unit, Directorate of Prioritization and Integration, European Chemicals Agency (ECHA), Finland

Lecture title: Chemical Safety Through Science, Collaboration and Knowledge

FREE AFTERNOON

SOCIAL DINNER

THURSDAY, 10 JULY 2025, MORNING

SPONSORS and INSTITUTIONS

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY (IUPAC)

PRESENTER:

Buxing Han, Chair of the Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD), IUPAC

7th LECTURE SESSION:

Moderator: Jonathan Forman, Science and Technology Advisor in the Global Security Technology and Policy Group under the National Security Directorate of Pacific Northwest National (PNNL), United States

LUIGI VACCARO, Professor, *Laboratory of Green S.O.C.*, *Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Italy*

Lecture title: Novel Technologies for Green Synthesis and Catalysis

ELISA MORETTI, Professor, Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia, Italy Lecture title: Aid4GEA – A Bridge Across the World: When Hard Science Fertilizes Sustainable Development

8th LECTURE SESSION:

Moderator: Jonathan Forman, Science and Technology Advisor in the Global Security Technology and Policy Group under the National Security Directorate of Pacific Northwest National (PNNL), United States

ANAMARIA TODEA, Professor, Politehnica University Timisoara, Faculty of Chemical Engineering, Biotechnology and Envoironmental Protection, Biocatalysis and Green Chemistry Group, Romania Lecture title: Biocatalytic Strategies for Green Synthesis of Bio-Based Oligoesters

ALBERTO CUGNETTO, Consultant, *Socio ordinario dell'Accademia di Agricoltura di Torino, Italy* **Lecture title:** Innovations in Sustainable Agriculture with a Special Focus on Wine and Viticulture

THURSDAY, 10 JULY 2025, AFTERNOON

9th LECTURE SESSION:

Moderator: Aurelia Visa, Senior Researcher Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry, Timisoara, Romania

GIULIA FIORANI, Professor, Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, Italy

Lecture title: Catalytic Strategies for Non-Reductive CO₂ Valorization

ANDREA SPOLAOR, Senior Researcher, *Institute of Polar Sciences, National Research Council of Italy, Italy*

Lecture title: The Climate Change in the Arctic

IN-PERSON POSTER SESSION 2, 16:00-17:30 (15 Posters)

FRIDAY, 11 JULY 2025, MORNING

SPONSORS and INSTITUTIONS

ORGANISATION FOR THE PROHIBITION OF CHEMICAL WEAPONS (OPCW)

PRESENTER:

Jonathan Forman - Science and Technology Advisor Threat Prevention and Resilience Group Pacific Northwest National Laboratory

10th LECTURE SESSION:

Moderator: Giulia Fiorani, Professor at Ca' Foscari University of Venice, Italy

FRANCESCO TROTTA, Professor, Department of Chemistry, University of Turin, Italy Lecture title: Exploitation of Renewable Resources in Polymer Chemistry

JONATHAN E. FORMAN, Senior Scientist, *Pacific Northwest National Laboratory, Seattle, USA*<u>Lecture title</u>: Eliminating the Chemicals of War and the Challenges of Chemical Security: Does Green Chemistry Make a Difference?

CLOSING CEREMONY AND POSTER AWARDS:

PRESENTERS:

Francesco Trotta, President of Green Sciences for Sustainable Development Foundation, Venice, Italy Fabio Aricò, Professor of Organic Chemistry, Ca' Foscari University of Venice, Italy

Aurelia Visa, Senior Researcher, Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry, Timisoara, Romania

Mirabbos Hojamberdiev, Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark

Graziana Gigliuto, Ca' Foscari University, Venice, Italy

XVII Postaraduate	Summer School	l on Green Chemistry	7 July - 11 July 2025	Venice Italy

ABSTRACTS OF LECTURES

(according to the Summer School Programme Order)

Deep Eutectic Solvents as a Greener Materials Approach and Electrochemical Applications

CHRISTOPHER BRETT

Department of Chemistry, University of Coimbra, Portugal

Deep eutectic solvents (DES) are a greener and lower-cost alternative to ionic liquids and conventional organic solvents and are being investigated for use in a number of fields [1]. They rely on strong interactions between a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD) to give an electrically conducting liquid solvent, by mixing of solid components. The properties of DES will be reviewed, and compared with those of ionic liquids, including natural DES (NADES) and therapeutic DES (TADES). Applications of DES in polymer science as solvents or functional additives, in extraction, in metal processing (electrodeposition and electroless deposition), in nanomaterials science and in sensors [2] will be described. The predominant HBA is the non-toxic choline chloride, vitamin B4, and amongst the HBD some of the most used are urea, ethylene glycol and glycerol. For electrochemical applications, ethaline (with ethylene glycol) has a relatively low viscosity that enables easier diffusion of electroactive species.

Recent research on the preparation of electrochemical nanomaterial-polymer film sensors in binary and ternary (two HBD) DES will be shown. The search for HBDs less toxic than ethylene glycol whilst retaining the lower viscosity has led to the investigation of ternary DES (two HBD) as media for the preparation of polymer-modified electrodes, e.g. [3,4]. especially including HBD with low eco-toxicity, the starting point being components of NADES already identified. Future perspectives for the application of such electrochemical sensors and biosensors in monitoring of key analytes in the areas of health, foods and the environment will be discussed.

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Green Strategies for Membrane Preparation

ALBERTO FIGOLI

Institute on Membrane Technology, National Research Council of Italy, Via P. Bucci 17c, Rende (CS) Italy *Corresponding author: a.figoli@itm.cnr.it

The transition toward more sustainable practices in membrane separation technology is accelerating, driven by increasingly stringent environmental and health regulations. In this context, membrane fabrication is undergoing a transformative evolution, inspired by the principles of Green Chemistry [1] and guided by the European framework of Safe and Sustainable by Design (SSbD) [2], which promotes the development of inherently safer and environmentally friendly polymeric membranes. To address the limitations of conventional membrane fabrication, still reliant on toxic solvents such as N, N-dimethylformamide (DMF), N, N-dimethylacetamide (DMAc), and N-methyl-2-pyrrolidone (NMP) [3], new classes of bio-based solvents will be presented. Among these, dihydrolevoglucosenone (CyreneTM), dimethyl isosorbide (DMI), methyl-5-(dimethylamino)-2-methyl-5-oxopentanoate (Polarclean) and N-butylpyrrolidone (commercially known as Tamisolve) and have shown great promise for dissolving conventional polymers such as poly (vinylidene fluoride) (PVDF) and polyether sulfone (PES) for the fabrication of flat-sheet membranes.

These green solvent systems will also be explored for their ability to support the electrospinning of nanofibrous membranes with tailored morphologies. Electrospinning is a versatile and scalable technique that enables the production of continuous fibers with diameters in the micro- to nanoscale range, offering enhanced surface area, tunable porosity, and morphological control.

In particular, membranes based on poly (vinylidene fluoride-co-hexafluoropropylene) (PVDF-HFP), processed with CyreneTM-based ternary solvent mixtures including dimethyl sulfoxide (DMSO) and dimethyl carbonate (DMC), have demonstrated high porosity, controlled fiber structure, and excellent functional properties [4]. The integration of graphene-based fillers such as graphene oxide (GO) and graphene nanoplatelets (GNPs) will be shown to enhance membrane performance in membrane distillation, particularly in terms of hydrophobicity, liquid entry pressure, and salt rejection efficiency. Results concerning solvent formulation, fiber morphology, surface properties, and membrane distillation performance will be discussed. Particular attention will be given to the interplay between green processing routes and final membrane functionality, as well as the broader implications for the design of environmentally responsible membrane systems.

This contribution will illustrate how the synergy between green solvents, advanced materials, and membrane configurations (both flat-sheet and electrospun membranes) can enable the next generation of sustainable separation technologies, with reduced environmental impact and uncompromised performance.

Keywords Sustainable membrane preparation, green solvents, electrospinning technique, phase inversion technique

Acknowledgements

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Metrics for Green Syntheses: Two Case Studies in Biorefinery GIACOMO TRAPASSO

Department of Environmental Science Informatic and Statistics, Ca' Foscari University of Venice, Scientific Campus

Via Torino 155, 30170 Venezia Mestre, Italy

*Email: giacomo.trapasso@unive.it

Green metrics is a relatively new concept in Green Chemistry. The application of rigorous green metrics must go along with the experimental validation of synthetic procedures; this is necessary to give precise guidelines so to define a green synthetic approach and avoid misunderstanding and pretentious claims originating from subjective rather than objective evaluations.

5-(hydroxymethyl)furfural (HMF) has been labelled as the "sleeping giant" of the bio-based platform-chemicals realm, due to its versatility and being the starting point for endless chemical transformations into novel monomers for producing bio-based polymers. Among HMF derivatives, 2,5-Furandicarboxylic acid (FDCA) has been extensively studied as monomer for the production of polyesters such as polyethylene furanoate (PEF), considered as one of the most valuable bio-based substitute of the petroleum-derived polyethylene terephthalate (PET). However, the sustainability of the synthetic procedures leading to HMF and its derivatives represent a key aspect that must be addressed in order to foster their entrance into the bio-based plastic market. In this scenario, green metrics such as the environmental factor (E-factor) and the process mass intensity (PMI) represent an useful tool towards this goal.¹

From these premises, the present contribution reports an alternative synthetic procedure for the production of 2,5-furandicarboxylic acid dimethyl ester (FDME) starting from galactaric acid via dimethyl carbonate (DMC) chemistry. Both sulfonic resins and an iron-based Lewis acid showed to promote the one-pot formation of FDME. The pure product was retrieved as a white crystalline solid with an isolated yield of up to 70%. Based on the different intermediates identified, a possible reaction mechanism was proposed, which highlights the essential contribute of DMC in the product formation.² This presentation is also focusing on some key points inherent to the IUPAC project 2017-030-2-041: Metrics for Green synthesis. Thus, the greenness of the herein discussed synthetic procedure was evaluated using the most common green metrics and compared with other available synthetic pathways.

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Acknowledgements:

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Greener Approaches to the Synthesis and Application of Metal-Organic Frameworks

AURELIA VISA

Romanian Academy, "Coriolan Dragulescu" Institute of Chemistry, 24 M. Viteazul Ave, Timişoara - 300223, Romania, Email: apascariu@yahoo.com

Green chemistry research is guided by the Twelve Principles of Green Chemistry, which aim to design chemical processes that minimize environmental impact and promote sustainability [1]. There is an urgent need to develop innovative materials, approaches, and systems that minimize or completely prevent the usage and production of harmful substances.

Conventional and unconventional metal-organic frameworks (MOFs) represent a well-studied category of structured porous materials, characterized by the arrangement of various central metal nodes interconnected by organic linkers. These materials have received significant attention for their diverse environmental applications. The complexity and diversity of the architectural structures of MOFs confer unique properties, including high thermal, chemical, and mechanical stability, which make them suitable for a wide range of applications addressing pollution remediation issues. These applications encompass the removal of heavy metal contaminants from water, the treatment of effluents from the textile and dye industries, catalysis, gas storage, solar energy conversion, and drug delivery.

A prominent area of focus in MOF research is the development of innovative synthetic routes that employ non-hazardous reagents and operate under mild synthetic conditions. Such approaches aim to minimize waste and reduce environmental impact. Alternative green synthesis methods include energy-efficient techniques, solvent-free synthesis, solvent minimization or the utilization of water as a solvent. These advancements not only enhance the sustainability of MOF production but also align with the principles of green chemistry, contributing to more environmentally friendly practices in material synthesis.

This talk will provide some illustrative examples of how MOFs can be synthesized using greener alternative reaction pathways. Several two-component metal-VP or three-component metal-HEDP-Im (metal = Co, Ni, Zn, Cu; VP= vinylphosphonic acid, HEDP = 1-hydroxyethylidene-1,1-diphosphonic acid; Im = imidazole) synthesis and their applications in catalysis, as adsorbent materials for water pollution remediation and their electrochemical activity of metal phosphides toward the oxygen evolution reaction (OER), oxygen reduction reaction (ORR), and hydrogen evolution reaction (HER) [2-5].

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How Chemists Can Use Life Cycle Assessment to Guide Our Research

PHILIP JESSOP

Queen's University, Dept. of Chemistry, 90 Bader Lane, Kingston, Ontario, K7L 3N6, Canada *e-mail: jessop@queensu.ca

Green chemistry researchers throughout the world, including the author, are motivated to use our research to benefit the environment, reduce harm, and help society become more sustainable. However, not all research projects are equally helpful to the environment. Assuming that harm reduction is the priority, we should prioritize projects that should maximize the benefit. Improving a process or product that causes very little harm is not an effective use of the time and resources of a green chemistry lab. However, it is not a trivial exercise to determine which processes, or which parts of processes, are causing significant harm. Several tools are available to green chemistry researchers to help us identify problems and therefore prioritize our research efforts.

Life cycle assessment (LCA) is a particularly powerful tool, because it not only allows us to compare different processes (or different products), but it also gives us detailed information about the *hotspots*. A hotspot is a part of a process (or an ingredient in a product) that causes more harm than other parts of the process/product. If we know the hotspots, then we can use our energy, creativity, and lab time to find better alternatives. That's much more effective than spending time greening a part of the process that isn't a hotspot.

Other tools include emissions databases that track chemical emissions from different industries, as well as impact-based metrics.

This presentation will describe how research chemists and chemical engineers can use LCA, emissions databases, and impact-based metrics to prioritize their research projects and maximize the resulting benefit to the environment.

Keywords: Life Cycle Assessment; Green Metrics; Research strategy

Hydrogen for Energy Transition MARCELLO BARICCO

Department of Chemistry and NIS – INSTM, University of Turin – TORINO, Italy

European investments plan to support hydrogen as a carrier in the energy transition. Hydrogen can be produced in different ways, often joined with its colour. Grey hydrogen is produced with the standard technology, which is based on the steam reforming of methane. Blue hydrogen is obtained when, after the production of grey hydrogen, CO₂ is captured and stored. Green hydrogen is produced by electrolysis of water, by using renewable energy. After production and before the use in different applications, hydrogen may need to be purified, transported, compressed and stored, so suitable hydrogen handling approaches, based on low-cost, safe, highly efficient and sustainable systems and operating close to ambient temperature and pressure, are needed. Then hydrogen can be used as a feed of fuel cells, to produce electrical energy, or can be burned like a classical fuel, and in both cases water is the only product. Of course, hydrogen can be also use for the so called "hard to abate" production technologies, to promote the decarbonisation. An overview on the state of the art of current technologies for hydrogen production, handling and use will be provided. Some case studies using metal hydrides as hydrogen carrier will be presented. A small scale H₂ refuelling station developed to provide hydrogen for a FCdriven drone will be described. The HyCARE project, funded by FCH JU - H2020 and focussed on the development of an efficient metal hydride-based system for the storage of renewables energies, with a quantity of about 50 kg of stored hydrogen, will be presented. The next step, linked to the REMEDHYS EU project, which aims to the development to low cost and low impacting production of hydrogen carrier, will be shown. The Life Cycle Assessment (LCA) methodology to evaluate the environmental impacts associated with developed systems will be shortly described. Finally, main open challenges linked to hydrogen technologies will be outlined, suggesting possible approaches for their overcoming.

Que c'est verte Venise

EDUARDO GARCÍA-VERDUGO

Departamento de Química Inorgánica y Orgánica. Universidad Jaume I. Campus del Riu Sec, E-12071, Castellon, Spain.

Green chemistry offers transformative strategies for designing chemical processes that minimize environmental impact while maintaining industrial viability. This presentation illustrates key principles of green chemistry through three case studies. First, the synthesis of terephthalic acid monomers via supercritical fluids and in particular supercritical water (scH2O₂) demonstrates how alternative reaction media can replace traditional organic solvents: scH2O₂) not only dissolves reagents effectively but also facilitates rapid product separation and solvent recycling, reducing waste and energy consumption. Second, the production of biomass-derived terephthalate analogues showcases the valorization of renewable feedstocks; by converting bio-based 5-hydroxymethylfurfural into furan-dicarboxylic acid (FDCA), chemists obtain monomers analogous to petroleum-based counterparts, closing the carbon loop and lowering greenhouse-gas emissions. Third, we focus on innovative methodologies for chemical recycling and upcycling of end-of-life polymers. A standout example is the use of ionic liquids (ILs) as non-innocent solvent to depolymerize polyurethane waste under mild, organocatalytic conditions. These ILs not only cleave the urethane linkages selectively—yielding high-purity polyol. This approach minimizes energy input and solvent waste, closes the material loop, and illustrates how green-chemistry tools transform "end-of-life" plastics into feedstocks for next-generation polymers rather than landfillbound residues.

Together, these examples underscore how catalysis, alternative solvents, and renewable feedstocks—core components of green chemistry—can be integrated from laboratory research to industrial application. By adopting these tools, chemical engineers and researchers can design processes that are not only economically competitive but also environmentally responsible. This presentation aims to equip students with concrete illustrations of how green chemistry drives sustainable innovation in the chemical industry and highlights the critical path from bench-scale discovery to commercial implementation.

The Reactions of Organic Carbonates

FABIO ARICÒ

Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice,
Via Torino 155, 30170 Venezia Mestre (IT)
*Corresponding author: Fabio.arico@unive.t

The integration of basic sciences into sustainable development is a key focus for many global initiatives, including the International Year of Basic Sciences for Sustainable Development and the United Nations Agenda 2030, which highlights 17 Sustainable Development Goals (SDGs). Organic synthesis plays a crucial role in addressing sustainability challenges such as using non-harmful reagents, minimizing energy and waste, and promoting recycling. These principles are central to the efforts of numerous international organizations, including the International Union of Pure and Applied Chemistry (IUPAC).

The discovery, development, and application of new organic synthesis methods, along with an understanding of their reaction mechanisms, is an essential area of research. In this context, dialkyl carbonates (DACs) have gained significant attention over recent decades due to their benign nature. Dimethyl carbonate (DMC), in particular, has become a vital substitute for chlorine-based chemicals in various chemical reactions. While halogen-based molecules are more reactive, they often lack selectivity in chemical reactions. In contrast, DACs tend to offer high selectivity in alkylation reactions despite their lower reactivity. Green syntheses using DMC have been reported in the production of anti-inflammatory drugs, polymers, fragrances, and solvents. DACs are also utilized as fuel additives, lithium battery solvents, and in the manufacture of pharmaceuticals, pesticides, plastics, coatings, electronics, and agrochemicals.

This lecture focuses on the use of DMC and other DACs as alternatives to halogen-based compounds in the synthesis and derivatization of bio-based platform chemicals such as isosorbide, galactaric acid and furanic compounds derived from D-Fructose.² Assessments of the greenness of the abovementioned procedures were evaluated via Green metrics.

Keywords: Bio-based platform chemicals, , Isosorbide, Galactaric acid, HMF, Green Metrics

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Polymers and Plastics the Route to Sustainability MARCO SANGERMANO

Politecnico di Torino Department of Applied Science and Technology, C.so Duca degli Abruzzi 24, 10129 Torino, Italy

Polymers and plastics are integral to modern life, but their reliance on fossil-based feedstocks poses significant environmental challenges. This talk explores the transition from fossil-derived to biobased polymeric materials, highlighting key advances in renewable feedstocks, biodegradable alternatives, and circular economy strategies. We will examine innovations in biopolymer synthesis, challenges in scalability, and the role of policy and industry collaboration in driving sustainable solutions. By bridging science, technology, and sustainability, this discussion aims to outline a feasible roadmap toward a greener future for polymer materials.

Green Hydrogen Generation from Solar Water Splitting over Metal Oxynitrides

MIRABBOS HOJAMBERDIEV

Mads Clausen Institute, University of Southern Denmark, Sønderborg, Denmark *Corresponding author: mirabbos@mci.sdu.dk

Although hydrogen is a zero-emission energy carrier, its current global production still heavily relies on fossil fuels. Current momentum on renewable energy and environmental remediation is unprecedented because of fast climate change. We all know that the world is hurrying up to achieve the United Nations Sustainable Development Goals (SDGs) by 2030 without pausing even during the COVID-19 pandemic. One of the important SDGs is Goal 7: Affordable and Clean Energy. As a replica of natural photosynthesis, a semiconductor-based artificial photosynthetic system is regarded as one of the most economically viable, highly efficient, and environmentally benign chemical processes to generate green hydrogen energy from solar water splitting. However, to harness solar energy efficiently, it is necessary to enhance the visible-light-driven photocatalytic performance of the existing materials and to discover novel visible-light-active materials. Mixed-anion compounds offer new opportunities in this regard. As a 600 nm-class photocatalyst, BaTaO₂N has received particular attention due to its small bandgap ($E_g =$ 1.9 eV), suitable band edge positions for visible-light-induced water splitting, chemical stability, and nontoxicity. BaTaO₂N is routinely synthesized by a two-step method: (i) the synthesis of a corresponding oxide precursor and (ii) its high temperature nitridation under an NH₃ atmosphere for a prolonged period. This two-step method leads to the formation of various defects that negatively affect the water splitting performance.

Therefore, we have (i) applied an NH₃-assisted direct flux growth approach to reduce the defect density of BaTaO₂N, (ii) engineered the bandgap by cation substitution, and (iii) explored the effects of the altered morphology, size, and porosity on the visible-light-induced water oxidation activity and photoelectrochemical performance of BaTaO₂N. The findings revealed that the photocatalytic activity and photoelectrochemical performance of BaTaO₂N were significantly influenced by its morphology, size, porosity, substituent type, and substitution concentration. Particularly, the BaTaO₂N crystal structures obtained by nitridation of oxide precursor without KCl flux exhibited a higher surface area and high anodic photocurrents compared to the BaTaO₂N crystal structures obtained by nitridation of oxide precursor with KCl flux due to the high number of dangling bonds acted as a nucleation centers for the highly dispersed CoO_x cocatalyst nanoparticles. Also, an NH₃-assisted direct flux growth approach reduced the density of intrinsic defects in BaTaO2N crystals, leading to the substantial enhancement in water oxidation activity. The Mg-substituted BaTaO₂N and Al-substituted BaTaO₂N independently exhibited the highest amounts (in 5 h) of evolved O₂ (503.6 µmol) and H₂ (117.4 µmol), respectively, whereas the Zr-substituted BaTaO₂N showed the high photocatalytic activities in both O₂ (446.8 μmol) and H₂ (80.4 µmol) half-reactions due to the altered potentials of the valence and conduction bands and an increased density of charge carriers.

Keywords:

Metal Oxynitride; BaTaO₂N; Solar water splitting; Green hydrogen; Photocatalysis

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Green and Sustainable Chemistry and The Future of Food

VANIA ZUIN ZEIDLER

Institute of Sustainable Chemistry, School of Sustainability, Leuphana University of Lüneburg, Germany * Corresponding author: vania.zuin@leuphana.de

Green and Sustainable Chemistry has as main objectives the reduction of the total amount and unnecessary complexity related to substances, materials, products, processes (including waste or losses) and energy flows, from local to global level¹. This also implies that the origin of products, their composition, forms of collection, extraction, transformation, reduction, reuse or recycling, associated risks and benefits, costs and gains, flows, functions and services are perceived as a system, such as in the food sector². In fact, this sector is composed of sub-systems (e.g., farming, waste management, input supply systems, etc.) and interacts with other key systems (e.g., energy, trade, health ones, etc.), in which chemistry and related areas play an important role. In this invited lecture, the connections between Green and Sustainable Chemistry for the design and implementation of more Sustainable Food Systems will be discussed³. We seek to reflect on the production (and consumption) of healthier and more nutritious foods in order to achieve food security in the present and future.

Keywords: Green Chemistry; Sustainable Chemistry; Systems Thinking, Sustainable Food Systems; Heath and Food Security.

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Green Chemistry Translation: A Design for Life!

PETER LICENCE

^aSchool of Chemistry, The University of Nottingham, Nottingham, UK NG72RD. *Corresponding author: pete.licence@nottingham.ac.uk

The translation of novel ideas, experiments or materials from the laboratory towards industry or into manufacturing at scale is a landmark event that should be recognised, celebrated and heralded as a prime indicator of success. However, realisation of this dream is not always easy, and when achieved, the pathway is often challenging or blocked by unsurmountable barriers that are not always obvious until far too late in the day!

This lecture will give an insight into 2 short vignettes – both of which are based upon the foundational teachings of Anastas and Warner's agenda setting book "Green Chemistry: Theory and Practice". The Principles of Green Chemistry provide a rationale that underpinned the design of 2 distinct families of chemical process, one is historical, the second contemporary. I will use these Green Chemistry stories to explore some of the challenges and indeed opportunities that can be experienced along the path to application.

The discussion will explore the importance of ideas, the benefits of multidisciplinarity and the essential requirement for luck and serendipity. The conclusion of my talk is simple, for our chemistry to really make a difference, it must be put to work. We are not going to turn the tide on global scale challenges unless we deliver cleaner processes, smarter materials and better science today.

Tomorrow will always be a day too late!

Keywords: Flow Chemistry, Process, Industry, Plasma Chemistry, Supercritical Fluids, Story Telling.

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Designing Green – Leveraging Life Cycle Assessment for Sustainable Chemistry POLINA YASENEVA^{1,2}

¹Department of Chemical Engineering, UCL

²Department of Chemical Engineering and Biotechnology, University of Cambridge

p.yaseneva@ucl.ac.uk

The manufacture of chemicals underpins nearly every aspect of modern technological society. Chemical substances play a critical role in ensuring public health, food security, and the conveniences of daily life. Over the past few decades, the use and production of chemicals have grown steeply, mirroring the expansion of global industrialization and consumer demand.

However, the majority of chemicals today are still produced from fossil-based feedstocks through linear manufacturing systems. This approach not only depletes non-renewable resources but also significantly contributes to climate change and environmental pollution and degradation. In light of these challenges, there is an urgent need to transition toward a circular and sustainable model of chemical manufacturing. This transition entails a holistic optimization of the entire chemical production life cycle—from raw material sourcing and process efficiency to waste management and end-of-life considerations.

A critical component of this transition is the identification of the most sustainable production pathways for specific chemical products. To support this effort, Life Cycle Assessment (LCA) serves as the primary analytical tool. LCA enables a comprehensive evaluation of the environmental impacts associated with all stages of a product's life cycle. It is widely used by major chemical companies—to assess the environmental performance of alternative materials and processes, and to guide sustainable design and decision-making.

This lecture presents a step-by-step methodology for conducting Life Cycle Assessment, with a focus on its application to the chemical manufacturing sector. The principles and practices of LCA are illustrated through two detailed case studies centered on the production of bio-based chemicals and materials.

- The first case study investigates waste treatment scenarios in the production of cellulose nanocrystals, a promising biomaterial derived from woody biomass. This analysis highlights the environmental trade-offs associated with different waste management strategies.
- The second case study examines alternative production pathways for the terpene-derived pharmaceutical intermediate, nopinone, focusing on process design optimisation. It demonstrates how LCA can be used to identify the more sustainable option based on energy use, emissions, and resource efficiency.

Together, these examples showcase the practical relevance of LCA in enabling a more sustainable future for chemical manufacturing.

Chemical Safety Through Science, Collaboration and Knowledge

MAIA SOKOLOVA

Scientific officer, B1 – Chemistry Unit, Directorate of Prioritization and Integration

<u>maia.sokolova@echa.europa.eu</u>

<u>echa.europa.eu</u>

P.O. Box 400, FI-00121 Helsinki, Finland

Green chemistry does not operate in a vacuum: robust chemical legislation provides the framework needed to drive safer, non hazardous chemical design, save production, and save use. This lecture will introduce students to the role of modern regulatory schemes, exemplified by the European Union's most comprehensive Regulation REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals), industry obligations toward sustainable objectives.

First, we will outline the scope and mechanisms of REACH, including its requirements for manufacturers and importers to register chemical substances, evaluate their hazards, and deal with restrictions and authorizations for uses of substances of very high concern (SVHC). Further highlighting mail goals: promoting transparency, reducing human and environmental risks, and incentivizing innovation in safer alternatives.

Next, we will explore some case studies - such as restriction and substitution of hazardous PFAS under regulatory pressure or addressing microplastic, illustrating how REACH deals with legal obligations to deliver both compliance and competitive advantage. Finally, we will examine REACH's enforcement tools (e.g., inspections by the competent authorities - "no data, no market" provisions).

By the end of this lecture, students will understand how legislative frameworks can facilitate the development and adoption of sustainable chemical technologies, ensuring that green chemistry flourishes not only in the laboratory but throughout the entire lifecycle of chemical products.

Novel Technologies for Green Synthesis and Catalysis

LUIGI VACCARO

Laboratory of Green S.O.C., Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Via Elce di Sotto, 8 – Perugia; Web: http://greensoc.chm.unipg.it; luigi.vaccaro@unipg.it

Our approach to modern green chemistry is focused on the general idea that green/efficient processes are those designed to minimize the waste by the rational combination of different technologies and the use of specific metrics needed to quantify the advance in terms of sustainability.

Our research program is mainly committed to the definition of efficient and sustainable synthetic tools by combining the development of several crucial areas of investigation: i) use of safer reaction media, ii) preparation and use of nanostructured heterogeneous and reusable catalytic systems; iii) definition of continuous-flow reactors allowing a minimal waste production and high productivity; iv) applications of metrics and LCA to assess the overall sustainability of the results.^[1]

Among the different projects, we are currently dedicated attention to the valorisation of waste for the preparation of recoverable catalytic systems and electrodes to define efficient protocols based on the use of continuous-flow reactors and electrochemistry.

In this contribution it will be presented an overview of our vision and ongoing research in the field.



Keywords:

Green solvents, continuous-flow technologies, heterogeneous catalysis

Acknowledgements:

Part of this work has been funded within the following programs, EU ECS00000041 – VITALITY; Marie Sklodowska-Curie entitled STiBNite (N_ 956923), PRIN-PNRR 2022 project "P2022XKWH7 – CircularWaste.

References

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Aid4GEA – A Bridge Across the World: When Hard Science Fertilizes Sustainable Development

ELISA MORETTI

Ca' Foscari University of Venice, Via Torino 155, 30172 Venezia, Italy. elisa.moretti@unive.it * Chairholder of the UNESCO Chair AID4GEA

The UNESCO Chair Aid4GEA on Technologies and Materials for Green and Energy Applications has just been established at the Ca' Foscari University of Venice, Italy, and at the Luleå University of Technology, Sweden. It aims to strengthen awareness of the key role of advanced materials and technologies to promote sustainable development, especially in developing countries. Materials and production technologies are central to sustainable development: they improve the quality of life and at the same time can offer solutions for environmental restoration and the efficient use of energy sources. A circular life cycle is needed, in which the reuse and recycling of waste are central. Aid4GEA promotes this awareness through capacity building at the local level, creating a network of teaching/research institutions and the most authoritative global companies in the sector. North-South-South and South-South cooperation includes the exchange of students and researchers, support for doctoral and post-doctoral researchers from developing countries, the definition of joint research and training projects, the sharing of knowledge through symposiums and multilateral workshops. Aid4GEA aims to increase awareness at a societal level through specific actions involving the public, stakeholders, and policy makers. The focus is on needs-driven requests from developing country partners. In the long term, Aid4GEA will impose a new vision of the use and reuse of materials in society through education and the development of skills towards sustainable development.

Biocatalytic Strategies for Green Synthesis of Bio-Based Oligoesters

ANAMARIA TODEA

Politehnica University Timisoara, Faculty of Chemical Engineering, Biotechnology and Envoironmental Protection, Biocatalysis and Green Chemistry Group, Vasile Pârvan 6, 300223 Timisoara, Romania

*Corresponding author: anamaria.todea@upt.ro

As the global demand for environmentally friendly materials grows, polymer science research is increasingly focusing on developing bio-based alternatives to replace fossil-derived polymers [1]. This requires the discovery of renewable monomers and innovative synthesis strategies that adhere to the principles of green chemistry.

One of the most promising strategies is using enzymes to polymerise sustainable building blocks into functional materials. Biocatalysis offers a versatile, eco-friendly way of producing a variety of polymer architectures, particularly polyesters and polyesteramides, by making use of the natural selectivity and efficiency of enzymes [2].

Biocatalysis is emerging as a powerful tool for addressing sustainability challenges. Enzymes can catalyze the synthesis, functionalization and degradation of polymers under mild, environmentally friendly conditions with high selectivity. Unlike conventional chemical methods, enzymatic approaches allow for targeted transformations without the need for harsh solvents or extreme temperatures. Hydrolase enzymes, such as lipases and cutinases, are widely used for the in vitro polycondensation of bio-based diacids and polyols to produce biodegradable polyesters with well-defined structures and adjustable properties [1,2]. At the same time, several research groups have demonstrated their ability to degrade existing polyesters, showing potential for closing the loop in polymer life cycles.

The correlation between polymer structure and enzyme activity provides exciting opportunities for designing next-generation materials. Tailoring the composition of polymers to match the specificity of selected enzymes could enable the creation of fully biodegradable materials compatible with natural ecosystems, particularly marine environments [3,4]. The development of these bio-based, biodegradable materials exemplifies how green chemistry and biotechnology can collaborate to promote sustainable innovation in polymer science [4,5].

Keywords: Bio-based oligoesters, Enzymes, Biocatalysis, Ecodesign

Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 101029444 (RenEcoPol)

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Innovations in Sustainable Agriculture with a Special Focus on Wine and Viticulture

ALBERTO CUGNETTO

Socio ordinario dell'Accademia di Agricoltura di Torino, Italy

Sustainable agriculture management today faces critical challenges: climate change, the emergence of new pathogens, and the need to reduce environmental impact without compromising farm profitability, particularly in areas with low gross margins per hectare. Technological and biotechnological innovations offer valuable tools to address these challenges. Advanced genetic techniques such as TEAs, precision agriculture, soil biodiversity management, and the use of remote sensors and decision support systems (DSS) contribute to improving both productive and ecological sustainability. The integration of drones, autonomous tractors, and modern machines for spreading plant protection products, combined with the use of low-impact chemicals and new biotechnological preparations, represents an innovative approach that optimizes operational management, reduces risks, costs, and ensures both safety and productivity. The presentation will showcase practical applications of innovative technologies, with a particular focus on wine production and viticulture, highlighting how an interdisciplinary approach is essential for developing a modern agriculture that is sustainable from economic, environmental, and social perspectives.

Catalytic Strategies for Non-Reductive CO₂ Valorization

GIULIA FIORANI

Department of Molecular Sciences and Nanosystems, Ca' Foscari University of Venice, via Torino 155, 30172 Venezia (VE), Italy

*Email: giulia.fiorani@unive.it

Carbon dioxide (CO₂) is an anthropogenic waste product, as well as the most abundant greenhouse gas in Earth's atmosphere. Catalytic methodologies for non-reductive CO₂ chemical valorisation represent a growing research field, allowing for the upgrading of CO₂ as an abundant, cheap, non-toxic, and readily available C¹ building block. The most well-known example of non-reductive CO₂ transformation include carboxylation,² and insertion reactions,³ which are atom economical processes highly desirable from a green chemistry perspective. Particularly, the synthesis of cyclic organic carbonates (COCs) via CO₂ insertion into epoxide rings has quickly become a cornerstone in chemical valorisation of CO₂. This communication showcases three distinct approaches towards the design of new, sustainable catalytic systems active towards CO₂ insertion reactions. This field represents an exciting area of research, with significant implications for both the chemical industry and climate change mitigation efforts.

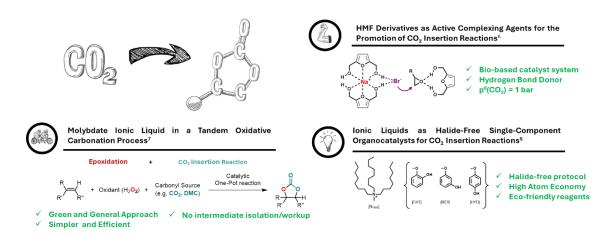


Figure 1: Catalytic systems for non-reductive CO₂ valorisation.

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The Climate Change in the Arctic

ANDREA SPOLAOR

Institute of Polar Sciences, National Research Council of Italy, Via Torino 155, (I) 30172 Venezia-Mestre (VE), Italy

Climate change driven by anthropogenic activities is causing a rise in global temperatures, sea level rise, alterations in environmental processes, and the presence of contaminants in remote areas through longrange transport mechanisms. In this context, the Arctic region is particularly vulnerable, with temperatures rising up to three times faster than the global average. This phenomenon, known as Arctic Amplification, is a complex cascade of feedback mechanisms involving various components of the Arctic environment. The main driver of Arctic Amplification is the reduction of sea ice, which decreases the surface albedo, i.e., the ability of the ice-covered surface to reflect solar radiation and, increases the absorption of sunlight, further enhancing regional warming. However, understanding Arctic Amplification requires a broader perspective that includes atmospheric dynamics, the retreat of ice sheets, increased ice melt, the greening of the Arctic (the expansion of vegetation over formerly icecovered areas), and permafrost thaw, which releases greenhouse gases such as methane and exacerbates coastal erosion while threatening the stability of built infrastructure. The role of the oceans is also significant: the northward transport of increasingly warmer water masses further contributes to Arctic warming and inhibits sea ice formation during winter. Moreover, the Arctic is a region of our planet where direct human impact is limited due to the absence of large industrialized areas. In this context, the Arctic serves as an optimal location to study global pollution caused by human activities and to identify the background levels of target contaminants. The Arctic is a rapidly changing and highly complex system that can serve as a "time machine" to help us understand and partially predict how mid-latitude regions may evolve in response to climate change. Studying the Arctic is not an end in itself, changes occurring in this region have far-reaching consequences, directly impacting both environmental conditions and daily life in lower-latitude areas.

Exploitation of Renewable Resources in Polymer Chemistry

FRANCESCO TROTTA

Department of Chemistry, University of Turin. Via Pietro Giuria 7, 10125 Torino, Italy

To face severe environmental and health concerns, limit greenhouse effects and improve the management of the foreseeable depletion of fossil resources, over the last decades, chemistry has moved towards the use of renewable resources for the production of energy and the synthesis of chemicals. Unlike materials deriving from fossils, which are often concentrated in a limited part of the world, renewable raw materials can be produced and utilized theoretically everywhere. These renewable raw materials come from various value chains, such as vegetable oils, fats, cellulose, starch, wood and biomass. It is important to underline that, where possible, renewable raw materials coming from agricultural and forestry products should not be used for food or feed but expressly employed for the production of materials, heat, electricity or fuel. Today many products are made from renewable raw materials, which often require less energy consumption and use safer and eco-friendly synthetic routes. These include textiles, cosmetics, medicines, building materials, dyes, lubricants, intermediates and (bio)-polymers [1].

Of particular interest is the production of polymer materials using renewable resources. In fact, polymers have a wide range of applications and are of crucial importance in modern society. In 2015 a global production of 322 million tons of different polymers was recorded. However, only 1% is actually related to bio-polymers although a constant growth has been detected.

In this lesson I would like to share the results obtained over the last decades on the use of some starch derivatives i.e. cyclodextrins and linear dextrins to produce both cross-linked and branched polymers with an impressive number of applications [2]. Toxic solvent-free production and even solvent-free synthesis are possible, thus making these new materials particularly appealing.

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Eliminating the Chemicals of War and the Challenges of Chemical Security: Does Green Chemistry Make a Difference?

JONATHAN E. FORMAN, Ph.D.

Science and Technology Advisor Threat Prevention and Resilience Group

Pacific Northwest National Laboratory 1100 Dexter Ave N, Suite 500, Seattle, WA 98109 USA jonathan.forman@pnnl.gov

Harmful properties of chemicals have been exploited for weaponization throughout the history of warfare, culminating into industrial scale usage in the first world and the buildup of military stockpiles of toxic chemical weapon arsenals in the 20th Century. In 1992 after nearly twenty years of deliberation and negotiation, world states reached a landmark agreement to eliminate chemical weapons entirely. This agreement, the Chemical Weapons Convention (CWC), entered-into-force in 1997, obligating all States Party to the agreement (which currently number over 190) to declare and permanently destroy their chemical weapon stockpiles under international oversight. Twenty-six years later in 2023, a milestone was achieved, the last of the declared stockpiles of chemical weapons being forever destroyed. It must, however, be appreciated that international arms control, disarmament, and non-proliferation treaties are politically negotiated and reflect where world States have agreed to certain legally binding obligations, in the case of the CWC this includes destroying chemical weapon stockpiles, allowing international oversight of chemical activities within the borders of a state, cooperation among States Parties to counter chemical threats, and never again developing, possessing, or proliferating chemical weapons. In this presentation we will look at what the States actually negotiated and committed themselves to, including how a "chemical weapon" is defined and how that translates into operational destruction of arsenals and reporting obligations, look at the 26 year history of the stockpile destruction and what it entailed (including the chemical processes it required), and consider what this milestone of declared stockpile elimination truly means for past, present, and future chemical security and countering the use of chemical weapons. Finally, we will consider how the concepts and outputs of Green Chemistry intersect with chemical security issues, appreciating that even benign chemicals can be used in intentionally harmful ways, independent of the types of processes that were used in their production.

Keywords:

Chemical Weapon, Chemical Weapons Convention, Stockpile Destruction, Declarations

IN-PERSON POSTER PROGRAM

XVII Postgraduate Summer School on Green Chemistry

Poster session 1, Tuesday, 8th July 2025, 16:00-17:30

Poster	Name	Affiliation and	Title
number		country	
1	JOY SALOME DOTSE	Research Centre for Synthesis and Catalysis, Department of Chemical Science, University of Johannesburg, South Africa	Interaction of cellulose with a new phosphonium salt-lactic acid deep eutectic solvent: Amorphization vs Functionalization
2	SINETHEMBA KABA	Department of Chemistry, Center for Rubber Science and Technology, Nelson Mandela University, Gqeberha 6031, South Africa	Synthesis and application of gadolinium tungstate photocatalyst integrated with pineapple leaf biomass for enhanced wastewater treatment
3	NADIA ANTER	Molecular Chemistry, Materials and Catalysis Laboratory, Faculty of Sciences and Techniques (FST-BM), University of Sultan Moulay Slimane, Morocco	Allylation of Cellulose Microfibers for Hydrosilylation with Various Hydrosilanes and Hydrosiloxanes, and Their Application in Corn-Starch-Mimosa Tannin (CSMT) Adhesive to Improve Particleboard Properties
4	LU LIU	The Centre for Ionics Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya, Malaysia	Salt-controlled dense ultramicropores hard carbon anode with a high-plateau capacity for sodium-ion battery
5	OSCAR EDUARDO CHURIO SILVERA	Dpto. de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria C1428EGA, Buenos Aires, Argentina	Theoretical-Experimental Analysis of Green Carbon-Based Materials for Energy Applications
6	LAUTARO NICOLÁS ACOSTA		
7	SARAHÍ JOSEFINA ESTRADA LOREDO	Instituto de Física, Universidad Autónoma de San Luis Potosí, México	Hydroxyapatite-curcumin nanocomposites: a breakthrough in crop yield improvement

8	KHISHN KUMAR KANDIAH	Higher Institution Centre of Excellence (HICoE), UM Power Energy Dedicated Advanced Centre (UMPEDAC), Level 4, Wisma R&D, Universiti Malaya, Malaysia GSK Carbon Neutral	Transparent, self-cleaning, and spectral response coating for glass substrate and its potential applications in the solar panel industry
9	SOPHIE SHEARLAW	GSK Carbon Neutral Laboratories for Sustainable Chemistry, Nottingham, United Kingdom and Nottingham Trent University, Nottingham, England	Four pillars of environmentally friendly cement
10	RONAN OZDURAL	School of Chemistry, the University of Nottingham, United Kingdom	Enhancing structural representation and inputs for polymer property prediction
11	JAMES BRETT	School of Chemistry, the University of Nottingham, United Kingdom	Thermoresponsive Coatings
12	EDOARDO BAZZICA	Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie Università degli Studi di Perugia, Italy	Biomass-Derivable Feedstock- Compatible Strategy for the Sustainable ortho-Alkylation of Phenols via Cooperative Dual Catalysis
13	KRISTINE MEILE	Latvian State Institute of Wood Chemistry, Dzerbenes Str 27, LV- 1006, Riga, Latvia	Platform chemicals obtained from lignocellulosic biomass by fast pyrolysis
14	MATEA LAUČAN	Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia	Sustainable synthesis of quinuclidine peptidomimetics via Ugi multicomponent reaction
15	MATTIA ANATELLI	Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Italy	Sustainable Strategies for the Synthesis of Cyclic Organic Carbonates: Mechanistic and Catalytic Insights
16	GRETA PALOMBELLA		

IN-PERSON POSTER PROGRAM

XVII Postgraduate Summer School on Green Chemistry

Poster session 2, Thursday, 10th July 2025, 16:00-17:30

Poster	Name	Affiliation and country	Title
number 1		Dongutus out of Dolomo	Dual-Chemical Modification of Corn
1	MUHAMMAD	Department of Polymer Chemistry and Technology,	Starch using Dodecenyl Succinic and
	NASIF	Kaunas University of	Acetic Anhydrides
		Technology, Lithuania	,
2	NAHEL BLANC	Laboratoire des technologies	Additive manufacturing of Li-ions
		innovantes, Avenue des	batteries
		facultés- Le Bailly, Amiens, France	
3	DAVIDE	Department of	Continuous Flow: etherification of Bio-
		Environmental Sciences,	Based Furanic Compounds
	DALLA TORRE	Informatics and Statistics,	•
		Ca' Foscari University of	
4	D.D. 1. E.D. 7. E.	Venice, Italy	G
4	BEATRIZ	Department of Environmental Sciences,	Sustainable Bio-Based Epoxy Thermosets from 2,5-Furan
	CHICHARO	Informatics and Statistics,	Dicarboxylic Acid Derivates
		Ca' Foscari University of	With Tunable Chain Length
		Venice, Italy	S
5	CHAIMAA	Department of	A Greener Approach to 2,5-
	SADRAOUI	Environmental Sciences,	Furandicarboxylate Macrocycles and
		Informatics and Statistics,	Their Subsequent Ring Opening Polymerization
		Ca' Foscari University of Venice, Italy	Forymenzation
6	IMANUEL	¹ BEST – Bioenergy and	Direct and Indirect Utilization of CO2
	WUSTINGER	Sustainable Technology,	for the Production of Sustainable
	WOSTINGLIC	Inffeldgasse 21b, 8010 Graz,	Aviation Fuel in the Fischer Tropsch and
		Austria and	Mixed Alcohol Synthesis
		² TU Wien, Institute of Chemical, Environmental &	
		Bioscience Engineering,	
		Getreidemarkt 9/166, 1060	
		Vienna, Austria	
7	RAMANA PYDI		Plant based ionic liquids as sustainable
		Veterinary Public Health,	synergists in insecticide formulations
		Clinical Department for Farm Animals and Food	
		System Science, University of	
		Veterinary Medicine Vienna,	
		Austria	
8	SARA	¹ CNR-ISSMC, National	Hybrid materials for sustainable water
	AMADORI	Research Council of Italy,	treatment: integrating microalgae
		Institute of Science, Technology and	biomass with inorganic nanomaterials
		Sustainability for Ceramics,	
<u> </u>		Sustainability for Cerunics,	

		Faenza, Italy and	
		² Department of Chemical	
		Science, Life and	
		Environmental Sustainability,	
		University of Parma, Parma,	
9	HANG DETER	Italy Dipartimento di Chimica e	A Comprehensive DFT Study of the
9	HANS PETER	Biologia"A.Zambelli" and	Mechanism of Selective PE Oxidation
	BLOCH	INSTM Research Unit,	with a Ruthenium-Porphyrin Catalyst
		Università degli	with a Ratheman 1 orphythi Catalyst
		Studi di Salerno, 84084	
		Fisciano, SA, Italy	
10	MOUNA	¹ Institute on Membrane	Bio-Hydroxyapatite and TamiSolve
	MEKKI	Technology, National	NxG sustainable solvent integration for
	MEKKI	Research Council of Italy	green PES mixed matrix membrane
		(CNR-ITM), Italy and	development
		² Dipartimento di Chimica e	
		Tecnologie Chimiche (CTC),	
		Università della Calabria,	
		87036 Rende, CS, Italy	
11	GIULIA SINESI	Department of Earth and	Sustainable Polymer Modifications for
		Environmental Sciences	Microplastic Replacement
		DISAT, University of Milano-	
		Bicocca, Milan, Italy and	
		² Department of Biotechnology and	
		Biosciences, University of	
		Milano-Bicocca, Milan, Italy	
		³ INTERCOS S.p.A., Agrate	
		Brianza (MB), Italy	
12	AQSA	¹ Institute of Membrane	Green solvents in membrane
	MANSOOR	Technology (ITM-CNR), Italy	preparation: CyreneTM in a sustainable
		and ² Department of	solvent system for flat sheet and
	KHAN	Environmental Engineering,	electrospun nanofiber membranes
		University of Calabria, Via	
		P.Bucci-cube 44/A 87036	
	,	Rende (CS), Italy	
13	VINÍCIUS DE	CICECO – Aveiro Institute of	Mild-condition dissolution-based
	PAULA	Materials, Department of	recycling of ABS with renewable
		Chemistry, University of	solvents
14	TONIDITAL	Aveiro, Portugal Department of Chamistry	Green synthesis of a saylaring
14	TONI DIVJAK	Department of Chemistry, Faculty of Science,	Green synthesis of α-acylamino acetamides
		University of Zagreb,	acciannucs
		Horvatovac 102a, Zagreb,	
		Croatia	
15	ANTONIO	Laboratory of Green S.O.C.	Direct symmetric synthesis of
		- Dipartimento di Chimica,	triarylamines via acceptorless
	VELLA	biologia e Biotecnologie,	dehydrogenative coupling from phenol-
		Università degli Studi di	derived compounds
		Perugia, Italy	*

ONLINE POSTER PROGRAM

XVII Postgraduate Summer School on Green Chemistry

Poster number	Name	Affiliation and country	Title
1	AHMAD SAIFUDDIN MOHAMAD ARSHAD	Centre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia	Copper-Catalyzed Synthesis of 9-Aryl- β-Carbolines through Tandem Oxidative Aromatization and Ullmann- Type C–N Cross-Coupling Reactions
2	SIMRAN SAINAND REVANKAR	Department of Chemistry, JSS Science and Technology University, Mysuru, 570 006, Karnataka, India	Lead- free Cs ₃ Bi ₂ Br ₉ @EVA Nanocomposite based Triboelectric Nanogenerator for Energy Harvesting and Tactile Sensing
3	ARPITA DEVI	Department of Chemical Sciences, Tezpur University, India	Using C1 and C2 Alcohols to Activate Peroxymonosulfate Over a CuO Catalyst to Synthesize 3,3'-Bis (Indolyl)Methane
4	DANIEL BAIER	Department of Molecular Chemistry, Materials and Catalysis (MOST); Institute of Condensed Matter and Nanosciences (IMCN), UC Louvain, Belgium	Mechanochemical Deracemization: A Fast and Solvent-Minimized Approach to Enantiopurity
5	TSHEGOFATSO MOLAPO	Molecular Science Institute, University of the Witwatersrand, South Africa	Synthesis and Evaluation of Nitrogen- Chelated Mn(I) Complexes for (De)Hydrogenation Catalysis: Applications in Hydrogen Storage and Sustainable Chemistry
6	SOCHI CHINAEMEREM OSIGWE	Department of Chemistry, Orebro University, Sweden	Assessment of PFAS contamination in selected consumable liquids: method development, validation, and application to market basket samples
7	BRYLE MATTHEW BACATAN	Green Chemistry and Sustainability Program, Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand	Upcycling PET waste into Bimetallic Terephthalate Metal Organic Framework
8	SAFA NOUAA	Laboratoire de Chimie Appliquée et Environnement Département de Chimie, Faculté des Sciences, Marroco	Eco-Friendly Competitive Adsorption of Binary Dyes Using Moroccan Cactus Peel: A Green Approach to Wastewater Treatment
9	BRYAN LEONARDO MORALES ESPINO	Dipartimento di Chimica "Giacomo Ciamician", Ravenna Campus, University of Bologna, Italy	Lycopene extraction from tomato waste using sustainable solvents

XVII Postgraduate Summer School on Green Chemistry, 7 July - 11 July 2025, Venice, Italy

10	HUMPHREY SAMUEL	¹ Computational Astrochemistry and Bio- Simulation Research Group, Federal University Wukari, Wukari, Taraba State, Nigeria and ² Department of Chemical Sciences, Federal University Wukari, Wukari, Taraba State, Nigeria	Sustainable Green Chemistry Approach to Structure-Based Drug Discovery of Soursop (AnnonaMuricata) Bioactive Compounds: Anticancer Efficacy through Quantum Chemical Calculations, Molecular Docking, and ADMET Studies with 7SA9 and 4ZFI Proteins		
11	MARIA- IULIANA CHIRICA	National Institute of Materials Physics, 405A Atomistilor Street, Magurele, Romania	Acid modified MXenes for catalytic PET depolymerization		
12	OLAWALE DABO	Department of Pure and Applied Chemistry, Ladoke Akintola University of Technology, Ogbomoso, Nigeria	Green Synthesis and Optimization of ZnO-Loaded Adsorbent for Malachite Green Removal		
13	ANKITA SARKAR	Department of Chemistry, National Institute of Technology Nagaland, Nagaland 797103, India	Catalytic performance optimization of agro-waste derived solid acids using statistical approach		
14	AYESHA GHAZANFAR	Tallin University of Technology, Estonia	Lignin-based Advance Fillers to Thermoplastic for Printing		

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ABSTRACTS OF STUDENTS

(alphabetical order of surnames)

Hybrid Materials for Sustainable Water Treatment: Integrating Microalgae Biomass with Inorganic Nanomaterials

AMADORI Sara*^{1,2}, Zanoni Ilaria¹, Brigliadori Andrea¹, Costa Anna Luisa¹, Ortelli Simona¹, Giacò Pierluigi³, Baldisserotto Costanza³, Pancaldi Simonetta³, Blosi Magda¹

¹CNR-ISSMC, National Research Council of Italy, Institute of Science, Technology and Sustainability for Ceramics, Faenza, Italy

²Department of Chemical Science, Life and Environmental Sustainability, University of Parma, Parma, Italy ³Department of Environmental and Prevention Sciences, University of Ferrara, Ferrara, Italy

The unregulated release of pollutants from urbanization and industrialization into the water compartment is a rising global concern. In response to the need for more effective and sustainable water treatment technologies we present a new class of hybrid nanomaterials suitable for downstream processes and prepared with a safe and sustainable by-design approach. We present the preparation of hybrid nanomaterials obtained combining inorganic nanomaterials (NMs) with organic phase based on microalgae biomass to advance the nanoremediation technology.

The coupling of adsorption properties of microalgae (Neochloris oleoabundans and Phaeodactylum tricornutum) with the photocatalytic action of TiO₂/SiO₂ nanoparticles allowed us to explore a new challenging frontier in the bio-nanomaterial design. The use of non-living microalgae enabled us to leverage their biosorption properties while enhancing overall processability. Biomass was coupled with inorganic NPs through a colloidal process followed by cold granulation to produce reactive, easily handled granules.

The materials were widely characterized using physicochemical methods, and two key functional aspects were evaluated: adsorption of heavy metals and organic pollutants on simulated and real urban wastewater, and photocatalytic activity through the degradation of Rhodamine B (RhB) dye. The results showed a positive synergistic effect in the hybrid samples, attributed to better biomass dispersion in the inorganic phase, highlighting their potential for use in nanoremediation technologies.

Keywords:

- Hybrid-nanomaterials
- Wastewater
- Synergistic effect

Sustainable Strategies for the Synthesis of Cyclic Organic Carbonates: Mechanistic and Catalytic Insights

Mattia ANNATELLI*, Giulia FIORANI

Ca'Foscari University of Venice
Department of Molecular Sciences and Nanosystems Ca'Foscari University of Venice,
Via Torino 155, 30172 Venezia Mestre, Italy
*E-mail: mattia.annatelli@unive.it

The most common cyclic organic carbonates (COCs) are five-membered compounds, such as ethylene carbonate (EC), mainly used as polar aprotic solvents due to their high boiling points.[1] COCs also serve as industrial lubricants, electrolytes for lithium-ion batteries, co-reagents in polymer synthesis, monomers for polycarbonates, fuel additives, and solvents in pharmaceutical and fine chemical applications.[2] COCs are not limited to fivemembered rings; larger-ring variants, known as macrocyclics, can also be synthesized. A key example is trimethylene carbonate (TMC), a monomer used to produce bioabsorbable polymers for medical applications. TMC enables the creation of flexible homo- and copolymers that degrade in the body within approximately five months. The increasing use of resorbable sutures highlights the need for more cost-effective and environmentally friendly TMC synthesis routes.[3] However, macrocyclic COCs are more challenging to synthesize due to their low product stability, which often leads to side reactions and limited yields. The most common route to TMC still involves the reaction of phosgene with 1,3-propanediol (1,3-PDO), a method that relies on a highly toxic reagent and produces hazardous byproducts.[4] This study explores the synthesis of COCs with six or more ring atoms via intramolecular transcarbonation of diols and linear carbonates. Specifically, 1,3-PDO was reacted with various linear carbonates in acetonitrile under pseudo-high dilution conditions, using basic organocatalysts such as TBD and DBU. With DBU (1 equiv.) and diphenyl carbonate (DPC), TMC was obtained in 98% yield (NMR). When dimethyl carbonate (DMC) was used, the yield decreased to 43% due to byproducts. TBD exhibited excellent selectivity, achieving 99% yield with DPC in just 2 hours. Preliminary tests with DBU@PS, a heterogeneous organocatalyst, were also promising. This work contributes to the development of sustainable synthetic strategies for macrocyclic carbonates.

Keywords

Cyclic Organic Carbonates; Transcarbonation; Intramolecular transcarbonation; Heterogeneous catalyst; Green chemistry; Sustainable methodologies

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Allylation of Cellulose Microfibers for Hydrosilylation with Various Hydrosilanes and Hydrosiloxanes, and Their Application in Corn-Starch-Mimosa Tannin (CSMT) Adhesive to Improve Particleboard Properties

Nadia Anter ^{a*}, Mohamed-Yassine Guida ^a, Ahlam Chennani ^a, Abdelghani Boussetta ^b, Amine Moubarik ^c, Abdellatif Barakat ^{d.e}, Abdelouahid Medaghri-Alaoui ^{a.f}, Abdellah Hannioui ^{a.f}

^d UMR IATE, University of Montpellier, Agro Institute of Montpellier, France.

^e Mohammed VI University Benguerir Morocco, Morocco.

*Correspondence to: nadia.anter@usms.ma

Recently, Cellulose microfibers (CMF) have garnered significant attention due to their renewability, biode gradability, and unique properties such as high aspect ratio, low density, high strength, stiffness, and distinctive optical properties. These characteristics have been highlighted in publications worldwide. However, the struc ture of CMF is difficult to access with solvents, limiting its dissolution in common organic solvents. The synthesis of CMF–siloxane or CMF–silane hybrid materials from cellulose generally involves several reactions steps, and therefore catalysts. The allylation of CMF is catalyzed by the phase-transfer catalyst tetrabutylammonium bro mide (TBAB), which enables the combination of CMF with allyl. This is followed by a hydrosilylation reaction catalyzed by Karstedt's catalyst, based on platinum (0), to combine the hydrophilic allylated CMF with hydride terminated hydrophobic hydrosilane or hydrosiloxane. Environmentally friendly particleboards were developed using bio-based adhesives composed of corn-starch and Mimosa tannin (CSMT) mixtures. These mixtures included 4, 6, 8, and 10 wt% of CMF, allylated CMF and silylated CMF. The mechanical and physical properties of particleboards, such as modulus of elasticity (MOE), modulus of rupture (MOR), internal bond strength (IB), surface soundness (SS), water absorption (WA) and thickness swelling (TS) were determined.

Keywords: Cellulose; Allylated-cellulose; Phase transfer catalyst; Silylated-cellulose; Wood adhesive Particleboards.

^a Molecular Chemistry, Materials and Catalysis Laboratory, Faculty of Sciences and Techniques (FST-BM), University of Sultan Moulay Slimane (USMS), 23000, Béni-Mellal, Morocco.

^b Materials Science, Energy and Nanoengineering (MSN) Department, Mohammed VI Polytechnic University, Lot 660– Hay Moulay Rachid, 43150 Ben Guerir, Morocco.

^c Laboratory of Chemical Processes and Applied Materials, Polydisciplinary Faculty, Sultan Moulay Slimane University, BP 592, Beni-Mellal, Morocco.

f Department of Chemistry and Environment, Faculty of Sciences and Techniques (FST-BM), University of Sultan Moulay Slimane (USMS), 23000, Béni-Mellal, Morocco.

Upcycling PET Waste into Bimetallic Terephthalate Metal Organic Framework

Bryle Matthew F. BACATAN¹, Wipark ANUTRASAKDA^{2*}, Fuangfa UNOB^{2*}

¹Green Chemistry and Sustainability Program, Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand

²Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand * Corresponding Author, E-mail: <u>fuangfa.u@chula.ac.th</u>, <u>wipark.a@chula.ac.th</u>

Plastic waste is a major global environmental problem. The ASEAN region alone disposes over 31 million tons of plastics annually, but only 26% is recycled [1-2]. This current study looks to respond by upcycling polyethylene terephthalate (PET) waste into monomer ligands as to fabricate Metal-Organic Frameworks (MOFs). Bimetallic MOFs are emerging class of materials that leverages synergistic interactions of two metals towards various applications ³. While two metals affect a material's structure, improvements on the performance in the removal of emerging contaminants like heavy metals and antibiotics are notable [4-5]. As the MOF synthesis is expensive, a waste-based feedstock approach is potentially cost effective. This work reports up to 90% PET waste conversion retrieving the target monomer via alkaline hydrolysis. The successful upcycling is characterized against commercial ligand by Nuclear Magnetic Resonance (NMR) spectroscopy and Fourier Transform Infrared (FTIR) spectroscopy. The subsequent successful synthesis of bimetallic MOF, Fe-Cu MOF crystallinity and porosity is confirmed and compared against the monometallic Fe-MOF through X-ray Diffraction (XRD), and N2 adsorption in 77K, where the PET-Fe-Cu MOF reports the greatest surface area among the synthesized MOFs. This upcycling strategy offers a promising development in the quest for sustainable materials from waste valorization, thereby a circular economy.

Keywords: Bimetallic MOFs, Plastic Upcycling, Contaminant Removal

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Biomass-Derivable Feedstock-Compatible Strategy for the Sustainable ortho-Alkylation of Phenols via Cooperative Dual Catalysis

Benedetta DI ERASMO¹, Edoardo BAZZICA¹, Giulia BRUFANI¹, Chao-Jun LI² and Luigi VACCARO^{*1}

¹Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie Università degli Studi di Perugia, Via Elce di Sotto 8, 06123 – Perugia – Italy

²Department of Chemistry and FRQNT Centre for Green Chemistry and Catalysis

McGill University 801 Sherbrooke Street West, Montreal, Quebec H3A 0B8 – Canada

*Corresponding author: luigi.vaccaro@unipg.it

Functionalized phenols are essential compounds employed across diverse industries, including pharmaceuticals, agriculture, polymers, and biofuels. ¹ While traditionally produced via the Hock process, ² phenols can nowadays be sustainably obtained from lignin, ³ providing structurally diverse derivatives such as guaiacols. Among these, alkylated phenols are particularly valuable, serving as non-ionic surfactants, polymer additives, components in active pharmaceutical ingredients and agrochemicals. Conventional alkylation methods, typically based on electrophilic aromatic substitution, ⁴ face challenges related to regioselectivity and waste generation.

To overcome these limitations, a cooperative dual catalytic system combining heterogeneous Pd/C and the Lewis acid Sc(OTf)₃ has been developed for the selective ortho-alkylation of phenols with primary alcohols. This solvent-free, scalable strategy involves hydrogenation, aldol condensation, and re-aromatization steps, minimizing waste and enabling catalyst recyclability (up to five runs with minimal Pd loss). The protocol also supports continuous-flow synthesis using a tube-in-tube reactor. The system demonstrated excellent yields across a broad range of phenols and alcohols, including the one-step synthesis of amyl-m-cresol, a pharmaceutically relevant molecule. Mechanistic studies suggest a release-and-catch mechanism, wherein Pd catalyzes aldehyde formation and Sc promotes the aldol condensation.

This innovative method offers strong potential for industrial applications, combining a high atom economy, broad substrate compatibility and efficiency in full alignment with green chemistry principles.

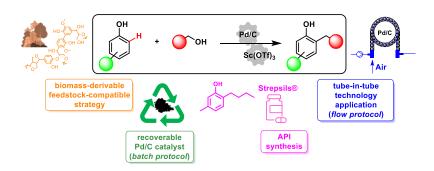


Figure 1. Cooperative dual catalysis for the selective ortho-alkylation of phenols

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Additive Manufacturing of Li-ions Batteries

Nahel BLANC, Jules TOPART, Vincent SEZNEC, Stephane PANIER

Laboratoire des technologies innovantes, Avenue des facultés- Le Bailly, Amiens, France nahel.blanc@u-picardie.fr

Electrification of our modes of transportation and machinery is closely linked to a greener future, making battery research a key field of investment and innovation. While significant progress has been made in the development of improved active materials with lower cost and reduced environmental impact, other aspects still require indepth investigation. One challenge hindering the widespread adoption of electrification is the limited availability of standard battery formats (cylindrical, pouch, prismatic), which are not always optimized for specific applications. 3D printing offers a promising approach to overcome this limitation by enabling the design of batteries tailored to the particular requirements of a device or system. In addition, it allows increased complexity and customization in battery architectures, which can enhance cycling performance.

Another issues in the battery field is the use of PVDF as binder. As a persistant polluant, PVDF must be replaced with more friendly alternatives. In this study, we propose an acrylate based system, wich serves both as a binder and matrix material for 3D printing.

Keywords: Additive manufacturing, Material for energy, Functional printing, Acrylate

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A Comprehensive DFT Study of the Mechanism of Selective PE Oxidation with a Ruthenium-Porphyrin Catalyst

Hans Peter BLOCH^{1,2}, Laura FALIVENE¹, Lucia CAPORASO¹

¹Dipartimento di Chimica e Biologia "A.Zambelli" and INSTM Research Unit, Università degli Studi di Salerno, 84084 Fisciano, SA, Italy

²NEST, Scuola Normale Superiore, Piazza San Silvestro 12, 56127 Pisa, Italy *Corresponding author: hanspeter.blocha@sns.it, lcaporaso@unisa.it

Polyethylene (PE) is one of the most widely used polymers. However, its environmental persistence and poor surface adhesion limit its field of application. A promising strategy to address these problems is selective oxidation, which introduces polar functional groups (–OH and –C=O) into the polymer structure without altering its molecular weight. This modification opens up new possibilities for the use of PE and lays the foundation for creative recycling of polyethylene plastic waste.[1] Furthermore, the presence of isolated C=O groups in the polyethylene chains allows the programmed photodegradation of the polymer, with consequent advantages in terms of sustainability.[2] Ruthenium (Ru)-based catalysts have demonstrated high efficiency in this process.[3] However, the underlying reaction mechanism and the factors responsible for their remarkable selectivity remain poorly understood. In this work we employ Density Functional Theory (DFT) simulations to investigate the electronic structure of a Ru-based catalytic system and elucidate the reaction mechanism involved in polyethylene oxidation. The catalyst precursor, carbonylruthenium(II) tetrakispentafluorophenylporphyrin [Ru^{II}(TPFPP)(CO)], is activated by a stoichiometric oxidant to generate an oxo-ruthenium species. This active species selectively oxidizes polyethylene, introducing only –OH and –C=O functional groups, without promoting undesired side reactions. [4]

Our simulations reveal that the active species is a RuV(TPFPP)(Cl) complex, formed via autooxidation of the solvent. A key finding of this study is that the oxo-ruthenium porphyrin complex follows a concerted reaction mechanism where the C-H bond is cleaved simultaneously with the formation of the C-O and O-H bonds. This pathway proceeds without the formation of radical intermediates, providing a clear rationale for the high selectivity observed experimentally. Notably, this represents the first evidence of a concerted mechanism operating in C-H activation mediated by oxo-ruthenium porphyrin complexes. This study provides crucial insights into the structural and electronic features responsible for the catalyst's performance. It offers guidance for the rational design of more efficient and sustainable catalytic systems for polyethylene functionalization. [5]

Keywords

DFT, Selective PE Oxidation Mechanism, Ruthenium Catalyst

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Thermoresponsive Coatings

James Brett

School of Chemistry, the University of Nottingham, United Kingdom

Thermoresponsive coatings are used to monitor the temperature within an aerospace engine and are essential for assessing their safety, efficiency and durability, and assist in the design process of the complex components. This project investigates ceramic coatings, such as alumina, silica, and titania, that exhibit thermally activated changes in properties such as phase composition, photoluminescence, dopant migration, and surface morphology. These properties will be used to develop coatings with superior performance while reducing the reliance on environmentally hazardous materials which are currently in use.

The coatings are synthesised via sol-gel and related routes. The base materials will undergo structural, spectroscopic and morphological characterisation using X-Ray Diffraction (XRD), scanning/transmission electron microscopy (SEM/TEM), Energy-Dispersive X-Ray spectroscopy (EDX), Fourier Transform Infrared Spectroscopy (FTIR), Ultraviolet-Visible spectroscopy (UV-Vis) and Raman spectroscopy. Post-calcination characterisation will show how these materials respond to heat treatment. Finally, the materials will be heated to engine temperatures (800-1600 °C) and the responses will be used calibrate the materials so that the unknown temperatures within real engines can be estimated.

By creating environmentally benign and non-hazardous thermoresponsive coatings with greater precision and thermal range over the current solutions, engine monitoring can be significantly improved. This technology promises enhanced safety, fuel efficiency, engine longevity and a significant reduction in occupational exposure hazardous materials.

Sustainable Bio-Based Epoxy Thermosets from 2,5-Furan Dicarboxylic Acid Derivates with Tunable Chain Length

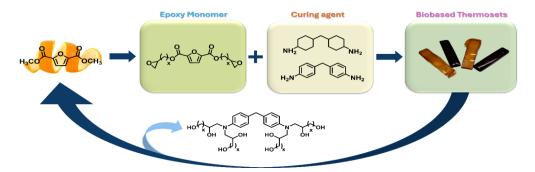
<u>Beatriz CHICHARO</u>, a,b Sami Fadlallah,b* Dumitru Moraru,c Luke Darney,b Marco Sangermano,c Fabio Aricò,a* Florent Allaisb*

^aDepartment of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Via Torino155, 30172 Venezia Mestre, Italy

^bURD Agro-Biotechnologies Industrielles (ABI), CEBB, AgroParisTech, 3 Rue des Rouges-Terres, 51110 Pomacle, France

^cDipartimento di Scienza Applicata e Tecnologia, Politecnico di Torino, 10129 Torino, Italy

Epoxy thermosets (ERTs) play a crucial role in modern life due to their excellent thermal and mechanical properties, outstanding dimensional stability, and resistance to chemical corrosion. However, despite these advantages, epoxy resins have some significant drawbacks, particularly their non-renewable and non-recyclable nature. Most of these resins are derived from petrochemical sources, with approximately 90% of production coming from diglycidyl ether of bisphenol A (DGEBA), a well-known derivative of the fossil fuel-based chemical bisphenol A (BPA). Due to safety concerns associated with bisphenol A-based epoxy thermosets, many European countries have introduced stricter regulations, leading to an increased demand for bio-based alternatives.² In this view, furan-based monomers, such as 2,5-furandicarboxylic acid (FDCA) derived from carbohydrates, have been widely explored as sustainable building blocks for high- performance epoxy resins.^{3,4} However, most studies focused on short-chain FDCA-derived epoxides, like C3-based glycidyl ester derivatives, with little research on FDCA-derived epoxides of varying chain lengths. Building on these premises, this work focuses on synthesizing a new family of bisepoxide FDCA monomers with chain lengths of four, six, and ten carbons. These bio-based monomers were synthesized via oxidation of α . ω -diene ester furan monomers and thus thermally cured using two bisamine hardeners, namely 4,4'-methylenebis(cyclohexan-1-amine) and 4,4'-methylenedianiline leading to FDCA-based epoxy thermosets. Structural analysis confirmed the successful curing and crosslinking of these monomers. Data collected highlighted the influence of the monomer length on the properties of the thermoset materials, with longer bisepoxide monomers exhibiting enhanced thermal stability and flexibility. Furthermore, it was found that the length of the bisepoxide monomer also affected the crosslinking density of the final materials. Interestingly, the bisepoxide FDCA monomer with six-carbons chain cured with 4,4'-methylenedianiline showed the highest crosslinking density, comparable to conventional DGEBA-based thermosets. Finally, a simple methanolysis can efficiently depolymerize the thermoset into its starting monomer, FDCA dimethyl ester, and a polyol offering potential for recycling or the development of new polymers.



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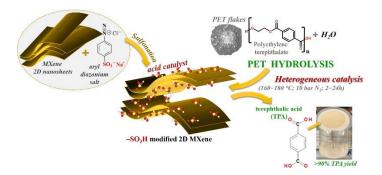
Acid Modified MXenes for Catalytic PET Depolymerization

Maria-Iuliana CHIRICA^{1,2}, Anca MIREA¹, Andrei KUNCSER¹, Stefan NEATU¹, Mihaela FLOREA¹, Michel W. BARSOUM³, Florentina NEATU*

¹National Institute of Materials Physics, 405A Atomistilor Street, Magurele, Romania ²University of Bucharest, Faculty of Physics, 405 Atomistilor Street, Magurele, Romania ³Department of Materials Science and Engineering, Drexel University, Philadelphia, USA *Presenting author: iuliana.m.chirica@gmail.com *Corresponding author: florentina.neatu@infim.ro

Polymer recycling has raised environmental concerns that throw a shadow over the usefulness of these materials in our economy and daily life. Heterogeneous catalysis is essential for recycling waste plastics, but none of these have shown excellent performance, hence no industrial strategy has been developed [1,2]. This work envisages novel solid acids that depolymerize PET to raw materials. MXenes, a recently identified group of two-dimensional (2D) metal carbides-nitrides exhibiting graphene-like structures, have gathered significant interest since their unique properties. These materials are synthesized through the etching of A element from the MAX phase [2,3]. Modulating the surface of MXenes presents a potentially valuable strategy for controlling their catalytic activity. In this scope, we have modified MXene with acid groups by adding sulfanilic acid moieties on the MXene surface [4]. Different levels of sulfanilic acid salt were employed to determine the acid group concentration, named as $Ti_3C_2T_x-SO_3H-y$, where y=(1,3,5,7) and represent the amount of sulfanilic acid introduced. Different techniques (XRD, DRIFT, RAMAN, SEM, TEM) showed that the as-modified MXene structure remains lamellar and did not collapse during sulfonation process. The interlayer spacing of the MXene layers increases following modification as a result of the presence of aryl sulfonate groups attached between them. The presence of -SO₃H groups on the MXene surface has been confirmed by the EDX (SEM) and XPS results. The depolymerization of PET in water occurred with a very good isolated yield in TPA (99%) for the MXene with the highest amount of sulfonic acid groups. The reaction parameters (temperature, pressure, catalyst quantity) indicate that Ti₃C₂T_x-SO₃H-y is a good candidate for environmentally friendly PET up-cycling.

Tables and Figures



Kevwords

PET, depolymerization, MXene, sulfonation, hydrolysis

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Theoretical-Experimental Analysis of Green Carbon-Based Materials for Energy Applications

Oscar CHURIO a,b, José M. Díaz-Raseroc, Beatriz Ledesmac, Silvia Romanc, Rubén Mirandad, Rubén Ramosc, Veronica M. Sancheza,b, Ezequiel de la Llavea,b

^a Dpto. de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria C1428EGA, Buenos Aires, Argentina.

E-mail: silvera@gi.fcen.uba.ar

The transition toward sustainable energy technologies demands the development of advanced materials with low environmental impact [1]. This work presents a comprehensive and green strategy for the production and analysis of carbon-based nanomaterials derived from lignocellulosic biomass, aimed at their use as electrodes in rechargeable lithium and sodium batteries. The experimental pathway involves hydrothermal carbonization (HTC) of agro-industrial residues, such as peach pit shells, under mild conditions (180–240 °C, 2–8 h), yielding hydrochars with tunable porosity, surface functionalization, and yield [2]. These materials were characterized by FTIR spectroscopy, thermogravimetric analysis (TGA), and calorific value determination, aiming to correlate their structure with electrochemical performance.

Complementarily, a computational methodology was developed using molecular dynamics (MD) simulations with the LAMMPS® [3] package to model the behavior of the electrolyte (LiTfO or NaTfO in monoglyme) confined within slit-shaped carbon pores ranging from 1 to 5 nm, as well as in bulk conditions. Key structural and dynamic properties were analyzed, such as density, ionic diffusion, radial distribution functions, and solvent conformations. The results reveal that confinement within the pores significantly modulates the organization of the electrolyte, inducing conformational changes in the solvent and affecting ionic mobility. This research highlights the importance of integrating green synthesis methods with molecular modeling to design functional materials for electrochemical energy storage. The convergence of sustainability, nanotechnology, and simulation provides a promising pathway toward cleaner and more efficient energy devices.

Kevwords

Green chemistry, biomass, hydrothermal carbonization, sustainable batteries, molecular simulation.

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b CONICET-Universidad de Buenos Aires, Instituto de Química Física de los Materiales, Medio Ambiente y Energía (INQUIMAE), Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria C1428EGA, Buenos Aires, Argentina.

^c Dpto. de Física Aplicada, Escuela de Ingenierías Industriales, Universidad de Extremadura, Avda. Elvas s/n, 06006, Badajoz, España.

^d Dpto. de Ingeniería Química y de Materiales, Facultad de Ĉiencias Químicas, Universidad Complutense de Madrid. Avda. Complutense s/n, 28040 Madrid, España.

^e Centro Iberico de Investigación en Almacenamiento Energético (CIIAE). Polígono 13, Parcela 31, "El Cuartillo", 10004 Cáceres, España.

Green Synthesis and Optimization of ZnO-Loaded Adsorbent for Reactive Black 5 Removal

<u>Olawale S. DABO</u>^a, Abdur-Rahim A. Giwa^a, Kazeem K. Salam^b, Deborah O. Aderibigbe*^a, Mary A. Oladipo^a

^aDepartment of Pure and Applied Chemistry, Ladoke Akintola University of Technology, Ogbomoso, Nigeria ^bDepartment of Chemical Engineering, Ladoke Akintola University of Technology, Ogbomoso, Nigeria Corresponding author: [doaderibigbe@lautech.edu.ng]

The urgent need for environmentally friendly water treatment strategies has prompted the exploration of low-cost, sustainable adsorbents from agricultural biomass. In this study, a novel green adsorbent ZnO nanoparticles loaded onto acid-modified *Pupalia lappacea* (Z-APL) was synthesized using a plant-mediated route and evaluated for its efficiency in removing Reactive Black 5 (RB5) dye from aqueous solutions. The biosynthesized adsorbent was characterized using FTIR, SEM, TEM, and pH-point-of-zero charge. To optimize dye removal, two modeling tools were applied: Response Surface Methodology (RSM) and Adaptive Neuro-Fuzzy Inference System (ANFIS). Key process variables such as solution pH, contact time, initial dye concentration, and adsorbent dosage were used as input factors. RSM identified a statistically significant cubic model (p < 0.0001), confirming that all variables had a strong effect on RB5 uptake. ANFIS analysis revealed the triangular membership function as the most efficient, producing the lowest root mean square error in both training and testing sets. This study highlights how green synthesis and AI-driven modeling enhance the design of sustainable, high-performance adsorbents for wastewater treatment, promoting scalable, eco-friendly solutions aligned with green chemistry principles.

Keywords: ANFIS; Green synthesis; Response Surface Methodology; ZnO nanoparticles; Pupalia lappacea

Continuous Flow: Etherification of Bio-Based Furanic Compounds

Davide DALLA TORRE, a* Giacomo Trapasso, a Fabio Aricò a

^a Department of Environmental Sciences, Informatics and Statistics, Ca' Foscari University of Venice, Scientific Campus Via Torino 155, 30170 Venezia Mestre, Italy.

*Davide Dalla Torre: davide.dallatorre@unive.it

The ultimate goal of the Biorefinery is to move away from a fossil-based business towards a more sustainable industry centred on the use of renewable feedstocks, capable of respecting the principle of the circular economy[1,2]. In this perspective, the so-called Bio-Based Platform Chemicals play an important role. Among them, 5-hydroxymethylfurfural (HMF) and 2,5-bis(hydroxymethyl)furan (BHMF) - achieved by HMF hydrogenation - are two of the most studied representatives. The etherification of these molecules with different alcohols yields 5-(alkoxymethyl)furfurals (AMFs) and 2,5-bis(alkoxymethyl) furans (BAMFs) respectively, both demonstrating potential application as fuel additives [3]. In addition, HMF, when subjected to self-etherification, leads to 5,5'-[oxybis(methylene)]bis-2-furfural (OBMF), another bio-based monomer of growing interest [4]. The presented work focuses on the etherification of HMF and BHMF promoted by a commercially available ion exchange resin - Purolite CT275DR, using a continuous flow apparatus. The reaction conditions were optimized by evaluating key parameters, including catalyst type and quantity, reaction media, temperature, and flow rate for the etherification of BHMF with ethanol and then extended to achieve a library of BAMFs. HMF self-etherification to form OBMF was conducted in the presence of both heterogeneous (CT275DR) and homogeneous acid (methanesulfonic acid - MSA) catalysts using dimethyl carbonate (DMC) as green solvent, with the latter being the most effective. Finally green metrics were calculated for the optimized etherification of BHMF with ethanol and the values were compared to previously published procedures.

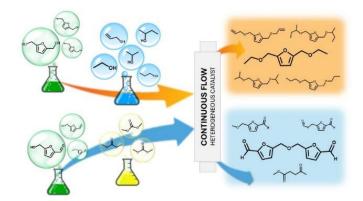


Figure 1: Etherification of furanics via Continuous Flow

Keywords: Bio-Based Platform Chemicals, etherification, Continuous Flow, 2,5-bis(hydroxymethyl)furan (BHMF), 2,5-bis(alkoxymethyl) furans (BAMFs), furanics.

Acknowledgements: This work was supported by the DoE 2023-2027 (MUR, AIS.DIP.ECCELLENZA2023 27.FF project).

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Mild-Condition Dissolution-Based Recycling of ABS with Renewable Solvents

<u>Vinícius DE PAULA</u>*, Paula S. S. LACERDA, Filipe H. B. SOSA, Ana M. FERREIRA, Andreia F. SOUSA

CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal
*Corresponding author: vgmp@ua.pt

Acrylonitrile-butadiene-styrene (ABS) plastics, frequently found in long-life goods such as automotive components, electronic devices, and domestic items, are currently subjected to incineration or landfill disposal [1]. As a sustainable alternative, dissolution-based recycling methods have gained attention for enabling the recovery of high-quality polymer fractions, with renewable solvents standing out due to their promising greeness. In this work, we present an enhanced methodology for the physical recycling of ABS, leveraging renewable solvents in alignment with circular economy principles. A computational screening of renewable solvents - including biobased solvents and eutectic solvents (ESs) - was conducted using the COnductor-like Screening Model for Realistic Solvents (COSMO-RS), which identified ester-functionalized compounds as particularly effective in dissolving styrene-acrylonitrile (SAN), a major constituent of ABS. Subsequent experimental validation confirmed the performance of four bio-based solvents and three eutectic solvents in achieving selective SAN solubilization. The separated fractions, including recovered SAN and residual ABS matrix, were thoroughly characterized by Fourier-transform infrared (FTIR) and nuclear magnetic resonance (NMR) spectroscopy. Furthermore, a preliminary process optimization was carried out through design-of-experiments and kinetic studies, demonstrating that efficient separation can be achieved within one hour under ambient temperature and pressure. These findings position this strategy as a scalable and environmentally responsible solution for the selective recovery of persistent and hard-to-recycle polymeric materials.

Keywords

Acrylonitrile-Butadiene-Styrene, Physical Recycling, Dissolution, Green Chemistry

Acknowledgements

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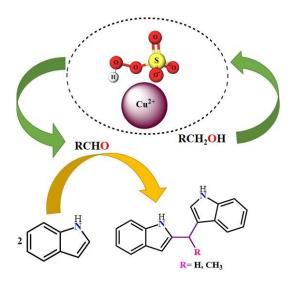
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Using C1 and C2 Alcohols to Activate Peroxymonosulfate Over a CuO Catalyst to Synthesize 3,3'-Bis (Indolyl)Methane

Arpita DEVI1, and Kusum K. Bania1*

¹ Department of Chemical Sciences, Tezpur University, India arpitadevi000hs@gmail.com and *kusum@tezu.ernet.in

Biologically important 3,3'-bis(indolyl)methanes (BIMs) were synthesized using a CuO-peroxymonosulfate (CuO-PMS) as a simpler and greener catalytic system. C1 and C2 alcohols served as the source of the bridging methylene group in the BIMs in contrary to commonly utilised aldehydes like formaldehyde and acetaldehyde, which are extremely volatile and challenging to manage in ambient circumstances. Without the need for any dangerous solvents, the reaction took place under mild and environmental-friendly conditions. The low-cost CuO-PMS system makes the reaction to be highly efficient resulting in very good product yield. The involvement of free radicals in the reaction mechanism was confirmed by radical scavenging test and CV and EPR analysis.



Keywords: C1 and C2 Alcohols, 3,3'-Bis (Indolyl)Methane, CuO-peroxymonosulfate

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Green Synthesis of α-acylamino Acetamides

Toni DIVJAK, Ines PRIMOŽIČ

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia *tdivjak@chem.pmf.hr

In recent years, mechanochemical synthesis^{[1], [2]} and microwave-assisted synthesis^[3] have earned significant attention due to their reduced environmental impact and alignment with the principles of green chemistry. In the Ugi multicomponent reaction^[4] various amines, aldehydes or ketones, carboxylic acids and isocyanides react to form α -acylamino amides. In this work, four new α -acylamino acetamides were synthesized through the Ugi reaction using acetic acid, benzylamine, *tert*-butyl isocyanide and varying four different aldehyde or ketone – paraformaldehyde (1), acetaldehyde (2), benzaldehyde (3) or acetone (4). The Ugi reaction was performed using microwave-assisted synthesis, a ball mill without solvent and with a catalytic amount of solvent (liquid-assisted grinding, LAG) or the classical method of organic synthesis. The mechanochemical synthesis with a catalytic amount of solvent of α -acylamino acetamide 1 showed better yield ($\eta = 65$ %) than mechanochemical synthesis without solvent ($\eta = 40$ %) or the microwave-assisted synthesis ($\eta = 28$ %) or the classical organic synthesis ($\eta = 34$ %). Obtained products were characterized by standard analytical methods (FTIR, 1D NMR, HRMS). The purity of the obtained products was checked by HPLC method.

Keywords: Mechanochemical synthesis, Microwave-assisted synthesis, Ugi reaction.

Acknowledgements: This work was supported by the Croatian Science Foundation under the project number HRZZ-IP-2022-10-9525.

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Interaction of Cellulose with a New Phosphonium Salt-lactic Acid Deep Eutectic Solvent: Amorphization vs Functionalization

Joy S. DOTSE¹ and Banothile C.E. Makhubela^{1*}

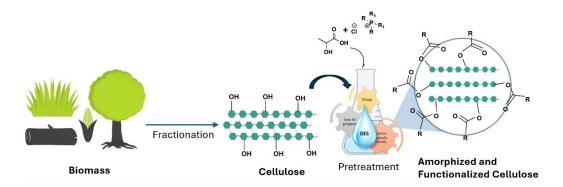
¹Research Centre for Synthesis and Catalysis, Department of Chemical Science, University of Johannesburg.

Kingsway Campus. Auckland Park 2006-Johannesburg, South Africa

*Corresponding Author email: joyd@uj.ac.za

The valorisation of lignocellulosic biomass into platform chemicals is a key step toward a sustainable chemical industry. Ionic liquids (ILs), a class of low-melting organic salts, have gained attention as green solvents for cellulose, offering new opportunities in cellulose chemistry. Despite their potential, limitations such as high solution viscosities and elevated costs hinder their wider application. Deep eutectic solvents (DESs), analogues of ionic liquids, which are considered safer and less toxic than ionic liquids, are composed of two or more components, typically including at least one hydrogen bond donor (HBD) and one hydrogen bond acceptor (HBA), that interact strongly through hydrogen bonding. Using cotton linter cellulose as a model substrate, we assessed the structural modifications induced by a new deep eutectic solvent formed from bis(hydroxymethyl)diphenyl phosphonium chloride and lactic acid. Characterisation techniques such as Powder X-ray Diffraction (PXRD), Fourier-Transform Infrared Spectroscopy (FTIR) and Scanning Electron Microscopy (SEM) were employed to evaluate changes in crystallinity and surface morphology of pre-treated cellulose. Preliminary results showed that the DES system induces partial amorphization and functionalization of cellulose, which may enhance hydrolysis under acidic conditions. These findings provide insight into the design of greener biomass processing strategies, aligning with the principles of green chemistry by promoting safer solvents, energy efficiency, and renewable feedstocks.

Keywords: Deep Eutectic Solvents, Biomass, Cellulose



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Hydroxyapatite - Curcumin Nanocomposite: A Breakthrough in Crop Yield Improvement

<u>Sarahí ESTRADA</u>¹, Daniel SÁNCHEZ¹, Ingrid MEZA¹, Demetrio MENDONZA², Denisse de LOERA³, Daniela SALADO^{1,4}

Hydroxyapatite (HAp) and curcumin (Cur) are materials of growing interest in the agricultural sector due to their unique properties. HAp provides essential nutrients such as calcium and phosphorus, which are fundamental for the structure and metabolic functions of plants, while Cur, a natural polyphenol extracted from Curcuma longa, exhibits antimicrobial and antifungal activity, positioning it as an effective natural biopesticide. Previous studies have demonstrated that the use of HAp nanoparticles (nHAp) improves the overall development of treated seedlings, while turmeric extracts have shown positive results against agronomically significant microorganisms. This study focused on the synthesis and evaluation of an HAp/Cur-based nanofertilizer at different Cur concentrations. HAp and the HAp/Cur compound were synthesized by a microwave-assisted hydrothermal method. Morphological and structural analyses (SEM, XRD, and FTIR) revealed that the incorporation of Cur modified the particle morphology without affecting the monoclinic crystalline phase of HAp. The post-synthesis Cur quantification assessed by UV-Vis confirmed the highest Cur content (93.2%) in the 6.37% formulation. Biological evaluation was performed on Raphanus sativus and Solanum lycopersicum seeds exposed to Cur, HAp, and HAp/Cur at concentrations ranging from 100 to 1000 mg/L. In Raphanus sativus, 100 mg/L of HAp significantly improved germination (80%) and stem elongation, while 250 mg/L of the HAp/Cur compound improved only germination. In contrast, high concentrations of Cur reduced both parameters. In Solanum lycopersicum, no significant improvements were observed, although 1000 mg/L of HAp/Cur generated taller seedlings with more foliage and germination comparable to the control (100%). No toxic effects were detected on root length or dry weight, and treatments with HAp/Cur showed fewer malformations. These results suggest a positive effect of the nanocomposite on early development and its potential application as a bio-stimulant and possible plant protective agent.

Keywords: Nanofertilizer, Hydroxyapatite (HAp), Curcumin (Cur), Germination, Agriculture.

¹ Instituto de Física, Universidad Autónoma de San Luis Potosí, Av. Parque Chapultepec 1570, Privadas del Pedregal, 78295 San Luis Potosí, S.L.P., México.

² Instituto Nacional de Investigaciones Nucleares; Carr. México-Toluca s/n La Marquesa, Ocoyoacac, Edo. de México C.P. 52750, México.

³ Facultad de Ciencias Químicas, Universidad Autónoma de San Luis Potosí, Manuel Nava Martínez 370, 78290 San Luis Potosí, San Luis Potosí, S.L.P., México.

⁴ Investigadoras e Investigadores por México, SECIHTI, Av. Insurgentes Sur 1582, Col. Crédito Constructor, 03940 Alcaldía Benito Juárez, Ciudad de México, México.

Lignin-based Advance Fillers to Thermoplastic for Printing

Ayesha GHAZANFAR

Tallin University of Technology, Estonia

We are investigating the valorization of lignin, a renewable by-product of lignocellulosic biomass, as a sustainable filler to enhance polylactic acid (PLA) for 3D printing applications. Lignin was extracted from pinewood and peat using acid-catalyzed ethanol organosolv pretreatment and characterized via FTIR, DSC, and ^31P NMR spectroscopy. PLA-lignin biocomposites were fabricated using solvent casting with varying lignin loadings (5–9%) and mixing times (40–120 minutes), guided by Central Composite Design (CCD) to optimize thermal and mechanical performance. Differential Scanning Calorimetry revealed improved glass transition temperatures (Tg) at optimized compositions—74.6 °C for pine lignin and 74.3 °C for peat lignin—indicating enhanced thermal resistance. Mechanical testing demonstrated increased modulus and tensile strength at specific lignin loadings, confirming effective reinforcement. 3D printing trials using Hot End Deposition Modeling verified filament processability and print quality. Green chemistry metrics indicated relatively high environmental impact, with Efactors of 29.15 (pine) and 23.02 (peat), and Life Cycle Assessment (LCA) revealed significant regional variability, with Estonia showing the highest climate impact due to energy profiles. The study confirms that lignin integration not only improves PLA's performance but also promotes circular economy goals in bio-based material design. Future work will explore lignin purification, chemical functionalization, and broader sustainability assessments.

Mechanochemical Deracemization: A Fast and Solvent-Minimized Approach to Enantiopurity

<u>Job GIELING</u>,^{+,a} Guillaume WÉRY,^{+,a} Chrystal LOPES,^b Joséphine DE MEESTER,^a Clément BRANDEL,^b Yohann CARTIGNY,^b Tom LEYSSENS,^a and <u>Daniel M. BAIER^{a,*}</u>

^a Department of Molecular Chemistry, Materials and Catalysis (MOST); Institute of Condensed Matter and Nanosciences (IMCN), UCLouvain, Louvain-La-Neuve, Belgium

^b Laboratoire SMS, UR 3233, University of Rouen Normandy, Rouen, France

*Corresponding author: daniel.baier@uclouvain.be

Today, over 50 % of pharmaceuticals are chiral and ensuring enantiopurity has become a top priority for the pharmaceutical industry. [1] While significant progress has been made in asymmetric synthesis, many compounds are still produced as racemates, necessitating subsequent resolution steps. Traditional resolution methods are inherently wasteful, often discarding the undesired enantiomer. In contrast, deracemization processes—where the undesired enantiomer is racemized and converted to the desired one—offer a sustainable alternative with a theoretical yield and enantiomeric excess (ee) of 100 %. [2]

Deracemizations require an external energy input. [2] Mechanical energy, as first demonstrated by Viedma [3], offers a solvent-based alternative via grinding of a suspension, whereby racemization in solution is followed by deracemization by crystallization; however, these reactions are limited to racemic conglomerates and require large amounts of toxic solvent and long reaction times. [2]

Mechanochemistry has emerged as a sustainable and versatile alternative to traditional solvent-based reactions. Recently, we reported the first examples of mechanochemical deracemization (MCDR), achieving enantiopurity in hours rather than days with minimal solvent use. [4]

Here, MCDR is introduced as a sustainable and generalizable strategy for obtaining enantiopure compounds. Its broad applicability is demonstrated via deracemization of several key organic functionalities—ketones, isoindolinones, imines, and esters—as well as an inorganic compound. Critical reaction parameters, including milling material, ball number and size, liquid-assisted grinding (LAG), and the use of a bulk material are discussed. Our findings reveal the pivotal role of these parameters in achieving high ee with reaction times reduced by up to 97 % while solvent use can be reduced by as much as 100 %.

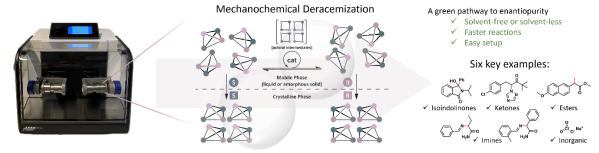


Figure 1: Mechanochemical deracemization (MCDR). MM400 ball mill used for MCDR (left), possible mechanism for MCDR similar to Viedma Ripening (middle), advantages of MCDR and examples studied (right).

Keywords: Mechanochemistry, Ball-Milling, Solvent-Free Synthesis, Chirality, Deracemization, Enantiopurity

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Lead-Free Cs₃Bi₂Br₉@EVA Nanocomposite Based Triboelectric Nanogenerator for Energy Harvesting and Tactile Sensing

<u>Kushal Mohan GOWDA</u> ¹, Yashaswini Veeranapura Lokesh ¹, Manjushree Nagaraju ¹, <u>Simran Sainand Revankar</u> ¹, Rumana Farheen S. M.², Sangamesha Madanahalli Ankanathappa ³, Bhagyashree Mahesha Sachith ⁴, Malgorzata Norek ⁵, Krishnaveni S ², Beejaganahalli Sangameshwara Madhukar ¹*.

Department of Chemistry, JSS Science and Technology University, Mysuru, 570 006, Karnataka, India
 Department of Studies in Physics, University of Mysore, Mysore, Karnataka 570006, India
 Department of Chemistry, The National Institute of Engineering, Mysuru, 570008, Karnataka, India
 Assistant in Research, Department of Physics, Florida State University, Tallahassee, FL, 32306
 Institute of Materials Science and Engineering, Material University of Technology, 2 Kaliskiego Str., 00-908
 Warsaw, Poland

*Corresponding author Email: <u>madhukarbs007@jsstuniv.in</u>

Triboelectric nanogenerators (TENGs) have paved way for groundbreaking advancements in sustainable and efficient energy solutions. In this study, lead-free Cs₃Bi₂Br₉ incorporated Ethylene-co-Vinyl Acetate (EVA) nanocomposites were prepared via green solution casting method. The Cs₃Bi₂Br₉ (CBB) nanoparticles, synthesized through a facile antisolvent reprecipitation technique, serve as non-toxic nanofillers. This was successfully integrated into the EVA matrix at varying concentrations (0.0-4.0 wt/wt %). Characterizations using X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM) verified the uniform distribution of the nanoparticles and resulting enhancement in the modified surface morphology. The differential scanning calorimetry (DSC) showed the increased glass transition temperature (T_o), indicating improved flexibility and stability. The optimised nanocomposite exhibits enhanced surface roughness and water contact angle of the nanocomposite improved the TENG's performance. The TENG, with the 4.0 wt./wt.% Cs₃Bi₂Br₉@EVA (CBB@EVA) nanocomposite achieved a maximum open circuit voltage of 236.06 V, short circuit current of 98.12 µA and power of 261.36 mW. The optimized TENG was used to charge electrolytic capacitors, light commercial LEDs, and power digital watches. Additionally, it displayed promising results as a self-powered, flexible tactile sensor for wearable and portable devices. Integrating lead-free halide perovskites and sustainable polymers, the study demonstrates a green chemistry approach to high performance, multifunctional energy harvesting devices, paving way for next generation environmentally friendly technologies.

Keywords: Lead-free Perovskite, Triboelectric nanogenerator, Cs₃Bi₂Br₉@EVA nanocomposites, Self-powered devices, Tactile sensor.

Synthesis and Application of Gadolinium Tungstate Photocatalyst Integrated with Pineapple Leaf Biomass for Enhanced Wastewater Treatment

Sinethemba KABA*a, Dr Zikhona Tywabi-Ngevab, Dr Bulelwa Ntsendwanac

Water is a vital resource for numerous sectors, including municipal, industrial, agricultural, and power generation, but rapid urbanization and industrial growth have magnified water demand, creating significant challenges in water management and sustainability. A key concern is water pollution, particularly contamination of water by heavy metals and organic pollutants. These pollutants not only threaten aquatic ecosystems but also pose a serious health risks to communities, especially in underserved regions. This project explores the sustainable application of nanotechnology for water remediation, focusing on the synthesis and use of a rare-earth based photocatalyst i.e., gadolinium tungstate for advanced wastewater treatment. The photocatalyst is integrated with an eco-friendly adsorbent derived from pineapple leaf biomass, a widely available agricultural residue in many African regions. The resulting nanocomposite is thoroughly characterized to evaluate its structural, morphological, and optical properties. Its performance is assessed based on the adsorption of heavy metals in wastewater, and the possibility of reusing the spent adsorbent in the photocatalytic degradation of organic pollutants such as organic dyes, aiming to demonstrate enhanced degradation efficiency. Furthermore, the synergistic mechanisms between photoadsorption—are investigated to gain insight into the interfacial dynamics between the photocatalyst and biomass matrix. This work highlights a green, low-cost solution for addressing water pollution in line with circular economy principles.

Keywords: Advanced oxidation processes, Heavy metals, Hybrid treatment technology, Rare-earth nanoparticles, Water pollution

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^a Department of Chemistry, Center for Rubber Science and Technology, Nelson Mandela University, Gqeberha 6031, South Africa

^b Advanced Materials Division/MINTEK, Private Bag X3015, Randburg 2125, Gauteng Province, South Africa *e-mail: (s213289504@mandela.ac.za)

Transparent, Self-Cleaning, and Spectral Response Coating for Glass Substrate and Its Potential Applications in the Solar Panel Industry

Khishn Kumar KANDIAH ^a, A. Syafiq ^a, B. Vengadaesvaran ^a, S. Ramesh ^b, K. Ramesh ^b, Thibeorchews Prasankumar ^{b,c}, Shahid Bashir ^a, N.K. Farhana^b, M. Pershaanaaa ^b, Z.L. Goh ^b, Gerard Ong ^b

^a Higher Institution Centre of Excellence (HICoE), UM Power Energy Dedicated Advanced Centre (UMPEDAC), Level 4, Wisma R&D, Universiti Malaya, Jalan Pantai Baharu, 59990 Kuala Lumpur, Malaysia.
 ^b Centre for Ionics, Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya, Kuala Lumpur, Malaysia

Author (email): khishnkks@gmail.com, amirul90@um.edu.my, venga@um.edu.my, rameshkasi@um.edu.my, prasankumar04@gmail.com, shahidbashirbaig@um.edu.my, khuzaimahaziz@um.edu.my, pershaanaa@gmail.com, gohzhiling56@gmail.com, <a href="mailto:google-parad-95@hotmailto:google-parad-95@hotmailto:google-parad-95@hotmailto:google-parad-95@hotmailto:goo

In this research work, novel combinations of Europium (Eu) doped CaCO₃-based filler have been used to prepare a hydrophobic, transparent, self-cleaning and spectral response coating for glass substrate, which will help improve solar panel efficiency. The filler was synthesized using the solid-state diffusion method, and the coating material was prepared via a simple stirring method. Glass slides were coated by the dip coating method. The coated specimens have been characterized for SEM analysis, wetting behaviour, transparency, self-cleaning test and photoluminescence (PL) test. Results revealed that developed material acts as a down-conversion material and shows transparency of coated glass about 89%, and water contact angle (CA) of $102 \pm 2^{\circ}$. Furthermore, the coated glass exhibits good self-cleaning and thermal properties as well. All the outcomes demonstrated that this coating could be used on solar panel glass covers to filter the high-energy photons and remove dust and dirt on the glass, which blocks the photons from penetrating solar panels. This coating can potentially enhance the efficiency of solar panels and reduce the cleaning cost.

Keywords: photoluminescence; down-conversion; Europium (Eu); self-cleaning coating, solar panel, hydrophobicity; transparency

^c Institute of Power Engineering, College of Engineering, Universiti Tenaga Nasional, 43000 Kajang, Malaysia

Green solvents in Membrane Preparation: CyreneTM in a Sustainable Solvent System for Flat Sheet and Electrospun Nanofiber Membranes

Aqsa. M. KHAN^{1,2,*}, F.Russo¹, F. Macedonio¹, A. Criscuoli¹, A. Figoli¹

¹Institute of Membrane Technology (ITM-CNR), Via P.Bucci 17/C, 87036 Rende (CS), Italy ²Department of Environmental Engineering, University of Calabria, Via P.Bucci-cube 44/A 87036 Rende (CS), Italy

agsamansoor.khan@unical.it *

The growing emphasis on sustainability is pushing the development of new, eco-friendly materials, alternative green solvents and new membrane production patterns to meet the performance demand of industry while reducing the environmental footprints. In this work a greener, bio-degradable Cyrene-based solvent systems was used for the fabrication of flat sheet and electrospun nanofibers (ENMs) membrane. Poly(vinylidene fluoridehexafluoropropylene) PVDF-HFP flat sheet membranes were prepared via phase inversion method. The influence of the additive polyethylene glycol PEG (200) and of the co-solvent triethyl phosphate (TEP) on membrane morphology and properties was investigated. The effect of different coagulation baths (only water and ethanol and water (1:1)) was also studied. Four different membranes were prepared which were further classified as M1, M2, M3, and M4. The prepared membranes were well characterized through pore size, contact angle, porosity, thickness, mechanical test and scanning electron microscopy. The results showed an asymmetric structure with the formation of macrovoids along the cross-section for membrane produced with ethanol and water (1:1) as coagulation bath. The pore size of the membranes was in the microfiltration range (0.09 µm - 0.42 µm), the porosity lied between 80 to 86 % and thickness ranged from 78.5 μm to 106.4 μm. M4 membrane was tested [1] in a lab scale DCMD MCr setup. In addition to the optimization of the NIPS conditions, preliminary electrospinning tests were performed on polymeric solutions of different viscosity. Electrospinning is an emerging technique for the preparation of electrospun fiber membranes, offering high yield and excellent scalability, making it a promising approach aligned with the process intensification [2]. Most of the nanofiber production relies on the use of carcinogenic and toxic solvents. In this work, DMSO (dimethyl sulfoxide), DMC (dimethyl carbonate) and TEP (triethyl phosphate) were explored as a low toxic profile solvent system together with Cyrene to produce PVDF nanofiber membranes. Kynar® PVDF nanofiber membranes were prepared using the electrospinning technique, employing different combinations of green solvents such as CyreneTM, DMSO, DMC and TEP, to explore their impact on nanofibers morphology and membrane performance. Additionally, a small percentage of lithium chloride (LiCl) was incorporated in some formulations to further optimize the polymer solution electro spinnability.

Keywords: Green solvents; flat sheet membranes; electrospun fiber membranes ENMs

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Acknowledgements

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Sustainable Synthesis of Quinuclidine Peptidomimetics via Ugi Multicomponent Reaction

Matea LAUČAN*, Alma RAMIĆ, Ines PRIMOŽIČ

Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia *mlaucan@chem.pmf.hr

The complexity and diversity of chemical synthesis necessitate the development of various greener approaches in our pursuit of sustainable practices. Consequently, several innovative strategies have emerged to address these challenges, including mechanochemical synthesis [1], [2] and microwave-assisted synthesis [3], both of which align well with the principles of green chemistry and offer more environmentally friendly alternatives to traditional synthetic methods. In this work, four novel peptidomimetics were synthesized. Compounds were synthesized via Ugi multicomponent reaction [4] using 3-aminoquinuclidine. Other components used were paraformaldehyde, benzoic acid, and *tert*-butyl isocyanide, benzyl isocyanide, *p*-toluenesulfonylmethyl isocyanide or 4-(2-isocyanoethyl)morpholine as the isocyanide component. Besides the traditional syntheses in the solution, new quinuclidine peptidomimetics were prepared by microwave-assisted synthesis and mechanochemical synthesis without the addition of any solvent. The course of mechanochemical reaction was monitored by ATR-FTIR spectroscopy. The structures of the synthesized compounds were confirmed by 1D and 2D NMR spectroscopy and ATR-FTIR spectroscopy.

Keywords: Mechanochemical synthesis, Microwave-assisted synthesis, Ugi reaction

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Salt-controlled Dense Ultramicropores Hard Carbon Anode with a High-plateau Capacity for Sodium-ion Battery

LU Liu^{1,2}, Shahid Bashir³, Ramesh Kasi², and Ramesh T. Subramaniam²

- 1. Research Center for Clean Utilization Technology Phosphorous Resources, Hubei Three Gorges Polytechnic, 443000 Yichang, Hubei, China
 - 2. The Centre for Ionics Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya 3. Higher Institution Centre of Excellence, UM Power Energy Dedicated Advanced Centre

Currently, various new rechargeable energy storage devices have been proposed, and the sodium-ion battery (SIB) has emerged as a promising option for large-scale energy storage because of its low cost and excellent performance. Yet identifying a suitable anode material with optimal electrochemical performance remains a challenge for SIB commercialization. Here, we focused on preparing hard carbon with abundant pores as the anode material for SIB. We introduced various pore-forming agents, such as zinc salts (zinc acetate, zinc chloride, and zinc gluconate), to facilitate the formation of pores in hard carbon materials. Zinc gluconate exhibited the most effective regulation of the microstructure among these three zinc salts, creating rich pore structures due to its decomposition of zinc gluconate and its interactions with the carbon matrix, particularly pores smaller than 0.7 nm. The optimized hard carbon with dense ultramicropores (< 0.7 nm) shows a high reversible capacity of 402.3 mAh g⁻¹ with a plateau capacity of 277 mAh g⁻¹. Thus, this effort provides fundamental information for the future targeted design of hard carbon materials.

Keywords: Hard carbon, Ultramicropores, Zinc salts, High plateau capacity

Platform Chemicals Obtained from Lignocellulosic Biomass by Fast Pyrolysis

Meile KRISTINE*, Dobele GALINA

Latvian State Institute of Wood Chemistry, Dzerbenes Str 27, LV-1006, Riga, Latvia *Corresponding author: kristine.meile@kki.lv

Lignocellulosic biomass is an abundant source of materials, fuels, and chemicals, and it can provide a sustainable alternative to the currently widely used fossil resources. However, the transition to a bioeconomy requires the development of new technologies to obtain green products in an economically feasible way. We propose thermochemical processing, namely, pyrolysis to obtain platform chemicals from biomass. The main constituents of biomass, such as wood, are cellulose, lignin, and hemicelluloses. Pyrolysis is considered to be a scalable process which can be integrated into a biorefinery to obtain a sequence of products from wood or other biomass. Acid pretreatment of wood produces monosaccharides, arising from the hydrolysis of hemicelluloses. Afterwards, the solid residue – lignocellulose – is subjected to pyrolysis. Pre-treatment with diluted sulfuric acid also optimizes the structure of the cellulose for pyrolysis, which is the source of anhydrosugars [1]. The decomposition of lignin gives rise to aromatic monomer products. Our aim is to investigate the formation of anhydrosugars from cellulose and adjust the process for maximum benefit. Currently, the most successful biomass-based anhydrosugar example is that of Cyrene [2], which is a green solvent obtained from the anhydrosugar levoglucosenone. Levoglucosan is also recognized as a potential platform chemical [3]. Our research has shown that the less known isomer of levoglucosan – 1,6-anhydro-β-D-glucofuranose – can also be collected from wood pyrolysis liquids [4]. Above all, it is necessary to strive for recovering as many valuable products from the pyrolysis process as reasonably possible – levoglucosan, 1,6-anhydro-β-D-glucofuranose, phenolic compounds, and to find an application for the solid by-product biochar. Increasing the yield of 1,6-anhydro-β-D-glucofuranose and developing a practical downstream processing method for the pyrolysis products can open new possibilities for the synthesis of green chemicals or solvents.

Keywords: Anhydrosugars, phenols, pyrolysis, wood.

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Bio-Hydroxyapatite and TamiSolve NxG Sustainable Solvent Integration for Green PES Mixed Matrix Membrane Development

Mouna MEKKI^{1,2,4}, Francesca Russo¹, Dorra Jellouli Ennigrou⁴, Raffaella Mancuso^{2,3}, Bartolo Gabriele^{2,3}, Alberto Figoli¹

¹Institute on Membrane Technology, National Research Council of Italy (CNR-ITM), Via P. Bucci 17/C, 87036 Rende, CS, Italy

Amid growing environmental concerns and tightening regulations on water pollution, the development of sustainable water treatment technologies has become more urgent than ever [1]. Membrane-based technology offers energy-efficient, low-chemical, and simple operating equipment, aligning well with green chemistry principles. Nevertheless, to completely fulfill sustainability requirements, membrane-based technology involves a green membrane manufacturing process in terms of additives and membrane materials, notably sustainable solvent [2].

This study presents an eco-friendly approach for the preparation of PES mixed matrix membranes (MMMs), using bio-derived hydroxyapatite (N-HAp) and TamiSolve NxG green solvent. The N-HAp, derived from waste fish bones, serves as a sustainable and effective additive to enhance the performance of the membrane. The MMMs were prepared using the non-solvent induced phase separation (NIPS) method and characterized in terms of morphology, porosity, pore size, thickness and contact angle.

The addition of N-HAp additive significantly improved the membrane hydrophilicity and water permeability of the membranes. This work highlights the potential of integrating green solvents and renewable biomaterials to produce high-performance membranes for wastewater treatment and environmental remediation.

Keywords: Membrane-based technology, TamiSolve NxG, Biomaterial hydroxyapatite.

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²Dipartimento di Chimica e Tecnologie Chimiche (CTC), Università della Calabria, , 87036 Rende, CS, Italy ³Laboratory of Industrial and Synthetic Organic Chemistry (LISOC), Department of Chemistry and Chemical Technologies, University of Calabria, 87036 Rende, CS, Italy

⁴ Faculty of Sciences of Tunis, University Campus El-Manar, 2092 El Manar, Tunisia

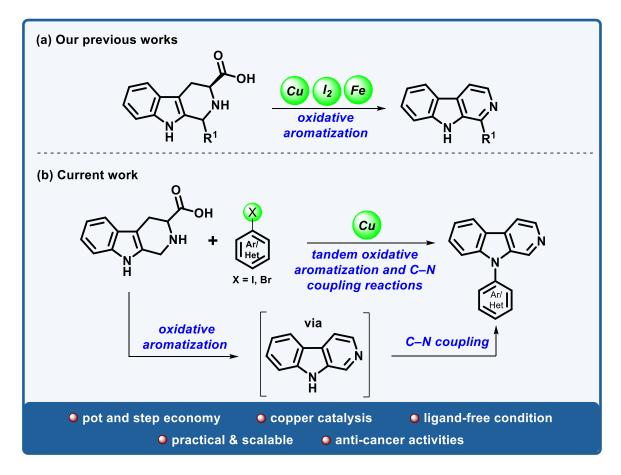
Copper-Catalyzed Synthesis of 9-Aryl-β-Carbolines through Tandem Oxidative Aromatization and Ullmann-Type C-N Cross-Coupling Reactions

Ahmad Saifuddin MOHAMAD ARSHAD1*, Nur Aziah Hanapi1, Mohd Nizam Mordi1

¹ Centre for Drug Research, Universiti Sains Malaysia, 11800 Minden, Penang, Malaysia *Corresponding author: saifudin pudin@yahoo.com

Pot and step economy synthesis are crucial strategies for addressing the challenges of efficiency and environmental sustainability in contemporary organic chemistry¹, often complementary to the twelve principles of green chemistry. To exemplify this strategy, we report a one-pot synthesis of 9-aryl- β -carbolines via a tandem oxidative aromatization and Ullmann-type C-N cross-coupling reactions. This strategy enables the direct conversion of tetrahydro- β -carbolines into the desired products by engaging aromatic β -carboline intermediates² with aryl halides under copper catalysis. Impressively, the cross-coupling reaction can be achieved under ligand-free conditions.

Keywords: Copper catalysis, oxidative aromatization, C–N cross-coupling, β-carbolines



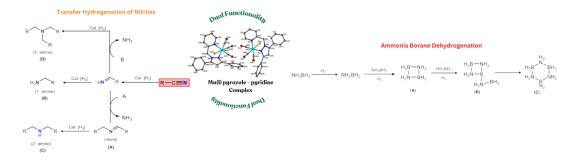
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Synthesis and Evaluation of Nitrogen-Chelated Mn(I) Complexes for (De)Hydrogenation Catalysis: Applications in Hydrogen Storage and Sustainable Chemistry

T. Molapo¹, A. Swarts^{1*}

¹Molecular Science Institute, University of Witwatersrand, South Africa

The catalytic dehydrogenation of amine boranes (ABs) to borazine, a vital precursor for advanced BN materials, continues to be primarily dominated by precious-metal systems, with Rh catalysts attaining yields of up to 95% under optimised conditions [1]. Manganese, a sustainable alternative, has shown promise in nitrile transfer hydrogenation (TH) (e.g., >99% conversion at 25°C using 1.3 AB equivalents [2]), yet its potential for AB dehydrogenation remains unexplored. This study aims to bridge this gap by designing Mn(I) pyrazole-pyridine complexes for dual functionality: (i) nitrile TH under mild conditions and (ii) AB dehydrogenation to borazine/polymers, to enhance the efficiency of Rh/Ru systems [1,2]. The Mn(I) complex catalyses nitrile reduction under mild conditions, reaching >99% conversion of aromatic, aliphatic, and heterocyclic substrates. Simultaneously, in situ NMR and FTIR studies reveal selective AB dehydrogenation to borazine. Mechanistic insights, informed by Rh systems [1], confirm hydride transfer from AB's B–H moiety as the TH driver, with ligand modifications suppressing competing H₂ evolution. Concurrently, controlled dehydrogenation yields borazine or processable BN polymers, reflecting Rh's selectivity [1], but without precious metals. This work establishes Mn's dual role in hydrogenation and dehydrogenation, valorising AB into amines and borazine within a single catalytic framework. The findings challenge the supremacy of noble metals in hydrogen storage and materials synthesis, providing a sustainable pathway to pharmaceuticals and BN/BCN materials.



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Lycopene Extraction from Tomato Waste using Sustainable Solvents

<u>Bryan Leonardo MORALES ESPINO</u>^{(a),(b)}, Cecilia Sepe^(b), Vanessa Spadavecchia^(b), Chiara Samorí^(b), Paola Galleti^(b)

(a) Erasmus Mundus Joint Master Degrees (EMJMD) in MSc. Chemical Innovation and Regulation (ChIR), (b) Dipartimento di Chimica "Giacomo Ciamician", Ravenna Campus, University of Bologna, Via Sant' Alberto 163, 48123 Ravenna, Italy.

The global production of fresh tomatoes exceeds 180 million tonnes annually, with around 40 million tonnes dedicated to processing, generating significant byproducts, mainly skins, seeds, and pulp residues. ^[1] Lycopene, which gives tomatoes their red color, has potent antioxidant properties and various health benefits, including cancer prevention and cardiovascular protection. ^[2] Conventional lycopene extraction methods often use toxic organic solvents. Sustainable alternatives like Deep Eutectic Solvents (DES) offer comparable efficiencies and are environmentally friendly. In this study, lycopene extraction from tomato peel waste using traditional and alternative solvents, including lipophilic DES, were investigated. The highest lycopene yield of 0.11 mg/g (considered as 100% benchmark) was achieved using 2-MeTHF. DES prepared with Menthol: Thymol at different molar ratios achieved extraction efficiencies up to 112%. Optimal conditions included 90°C, biomass ratio 1:10 (m/v), no light exposure, and constant stirring for 2 hours. DES methods proved more efficient than traditional and alternative solvents and offer an eco-friendly extraction approach.

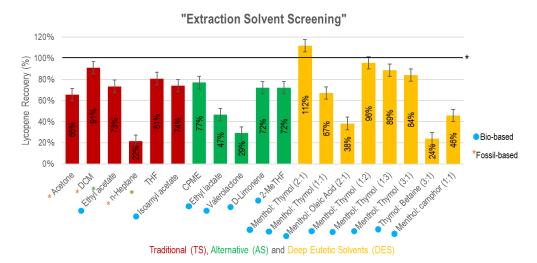


Figure 1. Extraction Solvent Screening using Traditional, Alternative, and Deep Eutectic Solvents. *A 100% Lycopene yield was obtained through solid-liquid extraction using 2-MeTHF until the solution residue became colorless.

Acknowledgments: Erasmus Mundus MSc in Chemical Innovation and Regulation (ChIR), grant agreement nr 619824-EMJMD and XVII International Postgraduate Summer School on Green Chemistry (GCSS 2025)

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Dual-Chemical Modification of Corn Starch using Dodecenyl Succinic and Acetic Anhydrides

Muhammad NASIF, Ayodeji Amobonye, Joana Bendoraitiene, Laura Peciulyte, Ramune Rutkaite

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu Rd. 19, 50254, Kaunas, Lithuania

*muhammad.nasif@ktu.edu

The dual chemical modification of starch has been shown to address numerous limitations associated with native and single modified starches, leading to materials with enhanced functionality. In this investigation, dual modification of corn starch utilizing dodecenyl succinic and acetic anhydrides was examined (see Fig. 1), alongside the effect of reaction temperature and duration on the degree of substitution. The initial modification was conducted with dodecenyl succinic anhydride under optimized conditions to obtain starch dodecenyl succinate of low degree of substitution (DS) of dodecenyl succinate groups, whereas the reaction parameters for acetylation were optimized using a central composite design. The succinvlation process yielded starch dodecenyl succinate with DS of succinate groups of 0.072, while the subsequent statistically optimized acetylation resulted into dual modified starches with DS of acetyl groups between 0.10 and 2.83. The quadratic model derived from the optimization reactions predicted optimal conditions encompassing a duration of 90 min, a temperature of 110 °C, a 3.69 acetic anhydride/starch mass ratio, and a 0.94 NaOH/starch molar ratio, to achieve a high degree of substitution of acetyl groups approximating 2.83. The model is considered statistically significant due to its high F-value (143.18), indicating strong overall regression significance. The high adequate precision ratio (40.512) shows a strong signal-to-noise ratio. Additionally, the R² (0.9923), adjusted R² (0.9854), and predicted R² (0.9487) values all suggest that the model fits the data very well and has strong predictive power. FTIR spectroscopy was employed to confirm alterations in the chemical structure of starch molecules during the modification and thermal properties of newly obtained starch derivatives were assessed. The findings from this study offer a theoretical framework for the dual-chemical modification of starches and providing insights into starch modification using a statistical approach and highlighting the functional properties of modified biopolymers for potential applications as biobased thermoplastics.

$$\begin{array}{c} \text{OH} \\ \text{OO} \\ \text{OO} \\ \text{OR} \\$$

Fig. 1. Reaction scheme of dual modification of starch: 1st step – dodecenyl succinylation; 2nd step – acetylation

Eco-Friendly Competitive Adsorption of Binary Dyes Using Moroccan Cactus Peel: A Green Approach to Wastewater Treatment

Safa NOUAA ¹, Rachid AZIAM ¹, Ridouan BENHITI ¹, Gabriela CARJA ², Fouad SINAN ¹, Mohamed CHIBAN ¹

¹Laboratoire de Chimie Appliquée et Environnement Département de ChimieDépartement De Chimie, Faculté des Sciences, BP. 8106, Hay Dakhla, Agadir, Maroc

*Corresponding author: safa.nouaa@edu.uiz.ac.ma

Wastewater contaminated with organic pollutants must be carefully treated before being discharged into the environment in order to reduce its negative effects on public health. Currently, much attention has been paid to the removal of dyes from industrial wastewater. The aim of this study is to investigate the removal of Acid Blue 113 (AB113) and Congo Red (CR) dyes by using Moroccan Prickly Pear Cactus Peel (MPPCP) from the binary system in a batch reactor. All the parameters influencing the adsorption of the dye in the binary system were studied namely the effect of mixture composition, contact time (20- 210 min), initial dye concentration (20-300 mg/L) and temperature (25-40 °C. The results showed that the uptake of both AB113 and CR dyes highly depends on initial dye concentration, solution composition dyes, and temperature. The kinetic study was performed by applying two kinetic models, the pseudo- first-order and the pseudo-second-order. The pseudo-second-order model better describes the adsorption of the dyes onto MPPCP adsorbent. The analysis of the obtained results shows that the correlation coefficients of the Freundlich model are higher which shows that the adsorption of AB113 and CR dyes in the binary mixture takes a multilayer form. The thermodynamic study showed that the adsorption of dyes in a binary system is spontaneous, physical, and exothermic. The obtained results in this work show that MPPCP can be considered a good material for the removal of anionic AB113 and CR dyes in the binary mixture and therefore used this material on an industrial scale.

Keywords: Adsorption, Moroccan prickly pear cactus peel, Wastewater Treatment.

²Laboratory of Materials Nanoarchitectonics, Faculty of Chemical Engineering and Environment Protection, Technical University of 'Gheorghe Asachi' of Iasi, Iasi, Romania.

Assessment of PFAS Contamination in Selected Consumable Liquids: Method Development, Validation, and Application to Market Basket Samples

Sochi Chinaemerem OSIGWE

Department of Chemistry, Orebro University, Sweden

Per- and polyfluoroalkyl substances (PFAS) are a group of highly persistent environmental contaminants widely used in industrial applications and consumer products. Their resistance to degradation and widespread occurrence raise growing concerns regarding environmental and human health. This study aimed to develop, validate, and optimize analytical methods for detecting and quantifying PFAS in consumable liquids, including drinking water, tea, apple juice, and coffee. Using advanced liquid chromatography—tandem mass spectrometry (LC-MS/MS), a broad range of both short- and long-chain PFAS compounds were analyzed. Method validation focused on assessing precision, accuracy, sensitivity, and specificity, confirming the method's reliability for measuring PFAS at environmentally relevant concentrations. Notably, low-level PFAS contamination was observed in blank samples, suggesting potential contamination during sample handling or processing. Overall, most PFAS compounds across the 18 tested samples were below the method detection limit. However, one apple juice sample showed detectable levels of 6:2 fluorotelomer sulfonic acid (6:2 FTSA). Since this compound was also present in the corresponding blank sample, cautious interpretation is required due to the likelihood of background contamination. These findings demonstrate the importance of rigorous analytical methods and contamination control in PFAS monitoring, particularly in food and beverage matrices.

Keywords: PFAS, Method Validation, Market Basket Monitoring

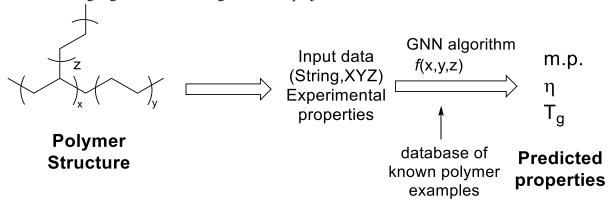
Enhancing Structural Representation and Inputs for Polymer Property Prediction

Ronan OZDURAL

School of Chemistry, the University of Nottingham, United Kingdom

The polymer structure is difficult to be represented completely in ML so polymers are often inputted by their monomeric counterpart. ¹ As the monomer is the small organic molecule from which the polymer is synthesised it lacks information regarding the bond connectivity along the polymer chain. This also discounts information on distributions present in the sample such as chemical composition, molar mass, and topology. Such simplification can overlook key structural features such as functional groups that link monomers. ² Improvements to the input for accurate structural representations will allow for more generalisable and explainable results. ^{1,3} To understand the current state of the art of the literature, a systematic literature review (SLR) was conducted that compiled a list of papers based off of keywords relevant to the topic. ⁴ The SLR aims to answer the following questions; what data representations have been used for polymers as inputs, what ML models have been utilized, what limitations were present in terms of the study, availability of data, and data representations, and how were structural features of the polymer accounted for.

Scheme 1: Highlights the ideal end-goal for this project.



Scheme 1: Proposed end-goal of product. 1. Polymer structure gets encoded into computer-readable inputs. Descriptors are extracted for the GNN and the model is trained on a known database of polymer examples. The final prediction of the properties are made and experimental and predicted values are compared⁵

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Plant Based Ionic Liquids as Sustainable Synergists in Insecticide Formulations

Ramana PYDI^a, Dr. Jennifer Bernard^b, Dr. Christoph Zutz^b, Dr. Patrick-Julian Mikuni*^a

^a Centre for Food Science and Veterinary Public Health, Clinical Department for Farm Animals and Food System Science, University of Veterinary Medicine Vienna, Veterinaerplatz 1, 1210 Vienna, Austria.
 ^bKwizda Agro GmbH, Universitätring 6, 1010 Vienna, Austria
 ^a Email: Ramana.Pydi@vetmeduni.ac.at

Synergists in insecticide formulations requiring safer, eco-friendly to enhance insecticide efficacy while reducing health risks and environmental impact. In this study, we explore secondary plant compounds, particularly pipernoylic acid derivatives, as innovative synergists for more eco-friendly formulations^[1] by using the Active Pharmaceutical Ingredient-Ionic Liquid (API-IL) concept^[2].

Methods: We synthesized 36 distinct piperonylic acid-based ionic liquids (PAILs) through a clean, one-pot reaction using green methods, utilizing 9 cations and 4 derivatives of piperonylic acid. Ecotoxicity was evaluated via antibacterial activity, a qPCR-based test and *in silico* biodegradability analysis of PAILs using the AquaBoxIL tool^[3–5]. Synergistic efficacy of PAILs was evaluated *in vitro* by determining their efficacy of inhibiting detoxification enzymes such as Glutathione-S-Transferase (GST) and Esterase from *Blattella germanica*^[6]. Further, as a proof-of-concept, PAILs efficacy as synergists was assessed by *in vivo* tests with insecticide (Pyrethroids) resistant *Blattella germanica* in comparison to a commercial synergist.

Results: 24 PAILs (Out of 36 PAILs) were harmless to bacteria. In silico analysis using the AquaBoxIL tool predicted quaternary ammonium ILs are more biodegradable. Our *in vitro* assays revealed significant inhibitory activity of detoxification enzymes (GST, EST). On these insights, *in vivo* evaluations of 12 PAILs in *Blattella germanica* revealed efficacy of 12 PAILs (Out of 36 PAILs) comparable to a commercially available synergist.

Keywords: Synergists, Ionic Liquids, Ecotoxicity, AquaBoxIL, Detoxification Enzymes inhibition.

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A Greener Approach to 2,5-Furandicarboxylate Macrocycles and their Subsequent Ring Opening Polymerization

<u>Chaimaa SADRAOUI</u>, [a],* Giacomo Trapasso, [a] Feriel Abid, [b] Andreia F. Sousa, [b] Fabio Aricò [a]

[a] Ca' Foscari University of Venice, Department of Environmental Sciences, Informatics and Statistics,
Scientific Campus Via Torino 155, 30170, Venezia Mestre, Italy
[b] University of Aveiro, CICECO – Aveiro Institute of Materials, Department of Chemistry, University of
Aveiro, 3810-193 Aveiro, Portugal
*Corresponding author: chaimaa.sadraoui@unive.it

Thermoplastic polyesters (PEs) are widely used in industries such as packaging, textiles, electronics, and smart materials, demonstrating their versatility and importance. PEs like poly(ethylene terephthalate) (PET), and poly(butylene terephthalate) (PBT) are among the most used in everyday life. However, the production and consumption of fossil-derived PEs come with certain critical issues such as the depletion of crude oil resources and environmental concerns related to their frequent low levels of biodegradability. [1] The synthesis of PEF, as well as other similar 2,5-furandicarboxylic acid (FDCA) based polymers, is mainly based on bulk polycondensation. However, ring opening polymerization (ROP) represents a potential interesting alternative since it requires milder conditions and is intrinsically more atom economic since no by-products are formed. [2-5] From these premises, our recent work has been focused on developing an alternative synthetic strategy towards bio-based PEs via Ring Opening Polymerization (ROP) of macrocycles incorporating bio-based monomers, such as 2,5-furandicarboxylic acid dimethyl ester (FDME). The macrocycles were synthesized by reacting FDME with different diols such as tetraethylene glycol and hexaethylene glycol via pseudo-high dilution condensation (PHDC) [5]. Isolation of the pure macrocycles was achieved by simple crystallization from the reaction mixture. Subsequent ROP of pure macrocycles was also investigated as viable route to prepare the related PEs in mild reaction conditions.

Keywords

2,5-furandicarboxylic acid dimethyl ester • Macrocycles • Ring Opening Polymerization • Bio-based polyesters • Pseudo-high dilution

Acknowledgements

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Sustainable Green Chemistry Approach to Structure-Based Drug Discovery of Soursop (AnnonaMuricata) Bioactive Compounds: Anticancer Efficacy through Quantum Chemical Calculations, Molecular Docking, and ADMET Studies with 7SA9 and 4ZFI Proteins

H. S. SAMUEL^{1, 2*}; J. Dennis ²; D. Alahira³; B. Bako^{1, 2}; A. M. Abakpa²; E.E. Etim ^{1, 2} and J. P. Shinggu^{1, 2,}

The ongoing global fight against cancer, which remains a top mortality factor, requires the development of superior therapeutic agents. In this pursuit, researchers are increasingly turning to nature's pharmacy, examining plantderived compounds for their promising anticancer properties. This study focuses on the bioactive compounds Annonacin, Quercetin, Coreximine, and Kaempferol from Soursop (Annona muricata), and their potential anticancer efficacy. Utilizing a structure-based drug discovery approach, we employed molecular docking studies to predict the interactions and binding affinities of these compounds with cancer-related proteins Human MUC16 SEA5 Domain (7SA9) and Mouse Double Minute 2 (4ZFI). Additionally, density functional theory (DFT) with the B3LYP functional and the 6-311* (d, p) basis set was used to perform geometry optimization and frequency calculations, providing detailed insights into the electronic properties, stability, and reactivity of the compounds. ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) studies were conducted to evaluate the pharmacokinetic and safety profiles of the compounds. From the ADMET result, coreximine is safest and Annonacin has toxicity risks. Ouercetin and Kaempferol show intermediate potential but require optimization for solubility and toxicity mitigation. For the DFT result, Quercetin exhibits the strongest binding interactions (hydrogen bonds, π -stacking, and electrostatic contacts), followed by Coreximine's high-affinity but hydrophobicdriven binding to 4ZFI, whereas Annonacin and Kaempferol show weaker, less-specific interactions. The finding identifies bioactive compounds from Annona muricata as a compound for developing new cancer drugs. The structure-based drug discovery framework can be applied to other medicinal plants, accelerating the identification of new natural product-based drugs.

Keywords: Sustainability, Molecular-Docking; Cancer; Soursop (*Annona muricata*); DFT; Pharmacokinetics; Green Chemistry

¹Computational Astrochemistry and Bio-Simulation Research Group, Federal University Wukari, Wukari, Taraba State, Nigeria.

²Department of Chemical Sciences, Federal University Wukari, Wukari, Taraba State, Nigeria.

³Department of Food Science and Technology, Federal University Wukari, Wukari, Taraba State, Nigeria.

⁴Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC, 29208 United States

Corresponding Author Email: humphreysedeke@gmail.com

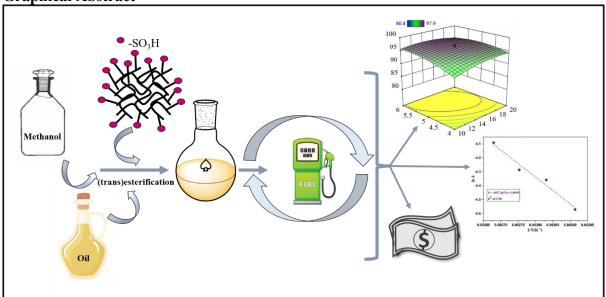
Catalytic Performance Optimization of Agro-waste Derived Solid Acids Using Statistical Approach

Ankita SARKAR¹, Amrit Puzari¹, Bappi Paul²

¹Department of Chemistry, National Institute of Technology Nagaland, Nagaland 797103, India ²School of Engineering and Technology, National forensic Sciences University, Sector-09, Gandhinagar 382007, India Email: ankitasarka40@gmail.com

The sustainability of the biodiesel industry, which acts as a feasible alternative to traditional fossil fuels within the transportation sector, is significantly influenced by the costs associated with the production process. The designing of efficient cost-effective catalysts can facilitate biodiesel production under ambient conditions, consequently leading to a potential decrease in overall expenditures. In this investigation, a sustainable and economically feasible surface-functionalized solid acid catalyst was synthesized from agro-industrial waste (Litchi waste) via a one-step hydrothermal carbonization and sulfonation procedure. The concentration of the -SO₃H group was adjusted by modifying the ratios of the sulfonating agent to the dehydrated biomass. The resultant catalyst underwent comprehensive characterization to elucidate its surface, morphological, and functional attributes. Its efficacy was evaluated in the catalytic transesterification of Jatropha curcas oil. The Central Composite Design (CCD) of Response Surface Methodology (RSM) was employed to evaluate the influence of reaction parameters on the yield of biodiesel. Under optimized conditions of catalyst loading at 4.25 wt.%, a Methanol to Oil molar ratio (MOMR) of 20:1, a temperature of 110 °C, and a reaction time of 3.9 hours, a maximum biodiesel yield of 97.8% was attained. The produced biodiesel was characterized utilizing ¹H-NMR and GC-MS techniques. The activation energy (Ea) for the reaction was determined to be 16.026 kJ mol⁻¹. The Life Cycle Cost Analysis (LCCA) demonstrated that both the catalyst utilized and the biodiesel production process are economically sustainable. Additionally, the fuel properties of the product biodiesel were determined to conform the specifications of both ASTM D6751 and EN 14214 standards.





Four Pillars of Environmentally Friendly Cement

Sophie SHEARLAW^{123*}; Simon Woodward¹, Darren Lee²

¹GSK Carbon Neutral Laboratories for Sustainable Chemistry, Nottingham, United Kingdom
²Nottingham Trent University, Nottingham, England
*E-mail: sophie.shearlaw@nottingham.ac.uk

Cement is the source of nearly 8% of all global CO₂ emissions accounting for approximately 4 billion tons per year. To adhere with the Paris Climate agreement, annual emissions must fall by 16% by 2030, this translates to roughly 650 million tons every year. Efficient alternatives are needed to combat emissions on such scales with government regulations also tightening on the cement sector to reach the 2030 goal. Demand for cement is a driver for these large emissions. By 2050 it is projected that global cement use will be 12-23% above 2020 levels. The cement industry are taking multiple steps to improve their practices and reduce their large levels of CO₂ emissions such as; alternative fuels for the kiln heating process, carbon capture within cement plants, alternative cement clinker materials and the application of additives to reduce water consumption and improve workability. These proposed practices are compared in terms of their sustainability and longevity for making a positive impact on current cement emissions.

Keywords: Cement, Carbon Dioxide Utilisation, Additives

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Sustainable Polymer Modifications for Microplastic Replacement

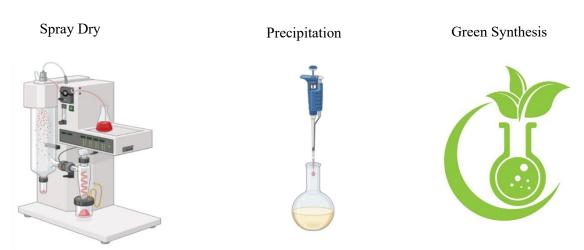
<u>G. SINESI</u>^{1,2}, M. Giustra², G. Distefano³, S. Sangiorgio³, C. Pirovano³, N. Galotto Galotto³, P. Valsesia³, D. Prosperi², M. Colombo²

¹Department of Earth and Environmental Sciences DISAT, University of Milano-Bicocca, Milan, Italy ²Department of Biotechnology and Biosciences, University of Milano-Bicocca, Milan, Italy ³INTERCOS S.p.A., Agrate Brianza (MB), Italy

Most cosmetic products contain substances whose interaction with the environment is the subject of ongoing research and reassessment. Plastics and microplastics (MPs) are one of the principal materials in cosmetic products that are toxic for the environment. Companies are trying to replace them with biobased or natural materials which are not harmful for our planet. The aim of this project is to synthesize or modify materials derived from bio-based polymers, in order to replicate the functional properties of microplastics without their environmental drawbacks.

Biodegradable polymers as alternatives to MPs

Sustainable approaches³



CONCLUSIONS

Through these innovative methods:

- ✓ Sustainable protocols are designed
- ✓ High yield
- ✓ Morphology changement

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Direct Symmetric Synthesis of Triarylamines Via Acceptorless Dehydrogenative Coupling from Phenol-derived Compounds

Antonio VELLA 1*, Giulia Brufani 1,2, Anastasiia M. Afanasenko 2, Chao-Jun Li 2 and Luigi Vaccaro 1

Lignin provides a renewable way to produce phenols and building blocks like anilines and triarylamines, offering a sustainable alternative to petrochemical sources. Following this idea, we herein report a novel methodology for the synthesis of triarylamines from cyclohexanone and aniline. Triarylamines are useful in optoelectronics for OLEDs, organic solar cells, and photocatalysis, as well as in the pharmaceutical field for APIs and carrier synthesis, as EDA complexes. These compounds are commonly synthesized through a two-step procedure involving the formation of diarylamines, then coupled with iodoarenes via Ullmann-type or Buchwald–Hartwig reactions. These methodologies rely on haloarenes and inevitably generate metal-halide byproducts. K. Yamaguchi et al. reported a sequential synthesis from anilines and cyclohexanones to diarylamines, which were then transformed into triarylamines. In this work, we present a one-pot Pd/C catalyzed strategy for synthesizing symmetric triarylamines via acceptorless dehydrogenative aromatization.

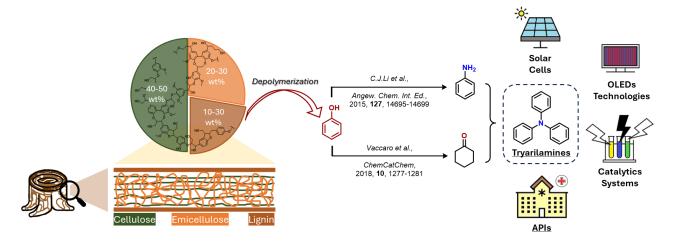


Figure 1. Valorization of phenols from lignin for triarylamines synthesis.

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¹Laboratory of Green S.O.C. – Dipartimento di Chimica, biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, Perugia 06123, Italy

²Department of Chemistry, and FQRNT Centre for Green Chemistry and Catalysis – McGill University, 801, Sherbrooke Street West, Montreal, QC H3A0B8, Canada *Corresponding author: antonio.vella@dottorandi.unipg.it

Direct and Indirect Utilization of CO₂ for the Production of Sustainable Aviation Fuel in the Fischer Tropsch and Mixed Alcohol Synthesis

Imanuel WUSTINGER^{1,2,*}, Matthias Kuba^{1,2,3}, Gerald Weber¹

¹BEST – Bioenergy and Sustainable Technology, Inffeldgasse 21b, 8010 Graz, Austria ²TU Wien, Institute of Chemical, Environmental & Bioscience Engineering, Getreidemarkt 9/166, 1060 Vienna, Austria

³Institute of Chemical and Energy Engineering, BOKU University, Muthgasse 107/I, Vienna, A-1190, Austria *Corresponding author: imanuel-wustinger@best-research.eu

The shift in the view of CO₂ away from a disruptive by-product of our industrialized society that contributes to climate change and towards a valuable material as a source of carbon in a sustainable economic system is reflected worldwide in a large number of research projects and technology directions under consideration. Of particular relevance is the development of processes for the production of Sustainable Aviation Fuel (SAF), as the extensive electrification of air traffic, in contrast to other forms of mobility, will not be technically feasible in the medium term. In this context, Fischer Tropsch synthesis (FTS) and mixed alcohol synthesis (MAS) are promising processes. Therefore, a comprehensive analysis of the direct and indirect utilization of CO₂ in these two processes shall be conducted. [1 - 3]

For the experimental investigation of the FTS, a lab scale plant is available at the Syngas Platform Vienna of the company BEST – Bioenergy and Sustainable Technology, whereas a lab scale plant for MAS needs to be planned and constructed. The MAS plant, visualized by its process flow diagram in Figure 2, shall have a syngas input capacity of 7 Nm³/h, a maximum operating temperature of 300°C and a maximum operating pressure of 200 barg. To allow for experiments close to industrial reality, the plant is equipped with a tail gas recycle system. In order to accommodate for different experimental setups and catalysts, a flexible reactor system consisting of three tubular fixed bed reactors that can be interconnected by valves in a multitude of ways (in series, in parallel, using only one tube, etc.) is planned. In order to gain values for the ideal geometrical formation of the reactors, multiphysics simulations shall be conducted using the software COMSOL Multiphysics.

Using this plant as well as the FTS plant, which is designed similarly, the direct utilization of CO₂ is to be investigated. In the course of this, parameter variation studies including parameters like pressure, temperature and syngas flow rates and compositions will be conducted, leading to values for ideal operating windows. Such, a data basis for direct CO₂ utilization is gained.

In order to also obtain a data basis for the indirect utilization of CO₂, literature research is conducted and partner inputs are gathered. Thereby, technology employing the reverse water gas shift reaction shall be investigated. The combined foundation of data regarding the direct and indirect utilization of CO₂ in FTS and MAS will then be used to design multiple process configurations. By simulating these configurations in the open source chemical process simulation software DWSIM, their techno-economical evaluation becomes feasible. The aim of this is a comparison of the different configurations, identifying the optimal variants. Finally, detailed flow diagrams will be created for the selected variants.

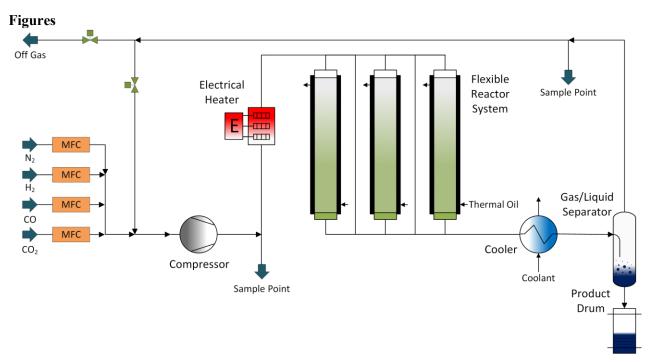


Figure 2: Process Flow Diagram of the Alcohol Synthesis Plant.

Keywords

Fischer Tropsch Synthesis, Mixed Alcohol Synthesis, Methanol Synthesis, Carbon Capture and Utilization (CCU), Power-to-X (PtX)

Acknowledgements

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POSTER WINNERS AWARDS

The scientific quality of the posters presented at the XVII Postgraduate Summer School on Green Chemistry has significantly improved compared to previous editions. This enhancement reflects the increasing availability of high-level scientific instrumentation in underdeveloped regions and the growing focus on green chemistry research.

A total of 46 posters were presented, with 14 from online students and 32 from in-person attendees. Students showcased their research during the poster sessions held on Tuesday, July 8th, and Thursday, July 10th. Additionally, the posters from online students were made available for ongoing consultation on the website https://www.greenchemistry.school/poster-sessions/.

The Poster Sessions are a highlight of the Summer School, notable for the originality and diverse scientific contributions. The sessions featured a significant number of young researchers sharing their work, generating considerable interest among participants. During the poster awarding ceremony, five participants were recognized for their outstanding posters and were given the opportunity to present their work orally during the Closing Ceremony.

There were 5 Awards: 2 for online poster presenters, and 3 for in-person presenters.

The 2 In-Person Poster Award Winners of the XVII International Postgraduate Summer School on Green Chemistry were:

Joy Salome Dotse from the Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, South Africa, on "Interaction of cellulose with a new phosphonium salt-lactic acid deep eutectic solvent: Amorphization vs. Functionalization"

Vinícius de Paula from CICECO – Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Portugal, on "Mild-condition dissolution-based recycling of ABS with renewable solvents"

The 2 Online Poster Award Winners of the XVII International Postgraduate Summer School on Green Chemistry were:

Bryle Matthew F. Bacatan from Chulalongkorn University, Thailand, on "Upcycling PET waste into Bimetallic Metal Organic Framework"

Maria-Iuliana Chirica from the National Institute of Materials Physics and Faculty of Physics, University of Bucharest, Romania, on "Acid modified MXenes for catalytic PET depolymerization"

The 1 Special Poster Award Winner of the XVII International Postgraduate Summer School on Green Chemistry was:

Beatriz Nunes Zambujal Chicharo from Ca' Foscari University of Venice, Italy and URD-ABI AgroParisTech, France, on "Sustainable Bio-Based Epoxy Thermosets from 2,5-Furan Dicarboxylic Acid Derivates with Tunable Chain Length"

The In-Person Poster Awards consisted of a cash price (250 EUR each), and one Special Poster Award is a honorable mention has been a gadget of Ca' Foscari University. The Awards have been handed over to the Winners during the Closing Ceremony. The Online Poster Award Winners consist of two scholarships for in-person attendance in the next edition of the Summer School in 2026 from 6th July to 10th July in Venice, Italy. The Poster Winners presented their research work during the Closing Ceremony on the last day.

PHOTOS



Prof. Francesco Trotta, Chair of Summer School



Members of The Organizing Committee



Teachers and Students of the Summer School





In-person poster award winners: Vinícius de Paula (left) and Joy Salome Dotse (right)





In-person poster award winners: Maria-Iuliana Chirica (left) and Bryle Matthew F. Bacatan (right)



Special poster award winner: Beatriz Nunes Zambujal Chicharo

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