

PROCEEDINGS

of the
**16th Green Chemistry Postgraduate
Summer School**

**30 June - 5 July 2024
Venice, Italy**



**Green Sciences For Sustainable
Development Foundation**

COLLECTION OF ABSTRACTS

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

GSSD Foundation ISBN: 978-88-945537-4-1



GREEN SCIENCES
FOR SUSTAINABLE
DEVELOPMENT
FOUNDATION



Ca' Foscari
University
of Venice

Department of Environmental
Sciences, Informatics and Statistics



GREEN CHEMISTRY POSTGRADUATE SUMMER SCHOOL

In memory of Professor Pietro Tundo

30th of June - 5th of July 2024

Venice, Italy

Organizers:

Francesco Trotta Chairman

Fabio Aricò

Aurelia Visa

Mirabbos Hojamberdiev

Graziana Gigliuto Secretary

Topics:

Benign synthesis routes

Green catalysis

Alternative solvents

Renewable and green raw materials

Green chemistry for energy

Clean processes

Green Chemistry education

Info:

www.greenchemistry.school

www.gssd-foundation.org

Contacts:

postmaster@pec.gssd-foundation.org

secretariat@gssd-foundation.org

16th Green Chemistry Postgraduate Summer School, 30 June - 5 July 2024, Venice, Italy

The Editors would like to thank Graziana Gigliuto for her outstanding support in the creation of Proceedings.

**PROCEEDINGS of the
16th Green Chemistry Postgraduate Summer School,
30 June - 5 July 2023, Venice, Italy**

**Published by Green Sciences for Sustainable Development Foundation
ISBN 978-88-945537-4-1 (e-book)**

All rights reserved:

No part of this work may be reproduced, stored in a retrieval system, or transmitted in any form or by any means, electronically, mechanical, photocopying, microfilming, recording, or otherwise, without written permission of the Publisher.

16th Green Chemistry Postgraduate Summer School, 30 June - 5 July 2024, Venice, Italy

Ideated and managed by



In collaboration with



Ca' Foscari
University
of Venice

Department of Environmental
Sciences, Informatics and Statistics



UNIVERSITÀ
DI TORINO

Endorsed by



Società
Chimica
Italiana



Consiglio Nazionale
delle Ricerche

Platinum Sponsors



Sponsors



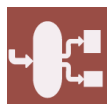
OPCW



SASOL



IUPAC



processes

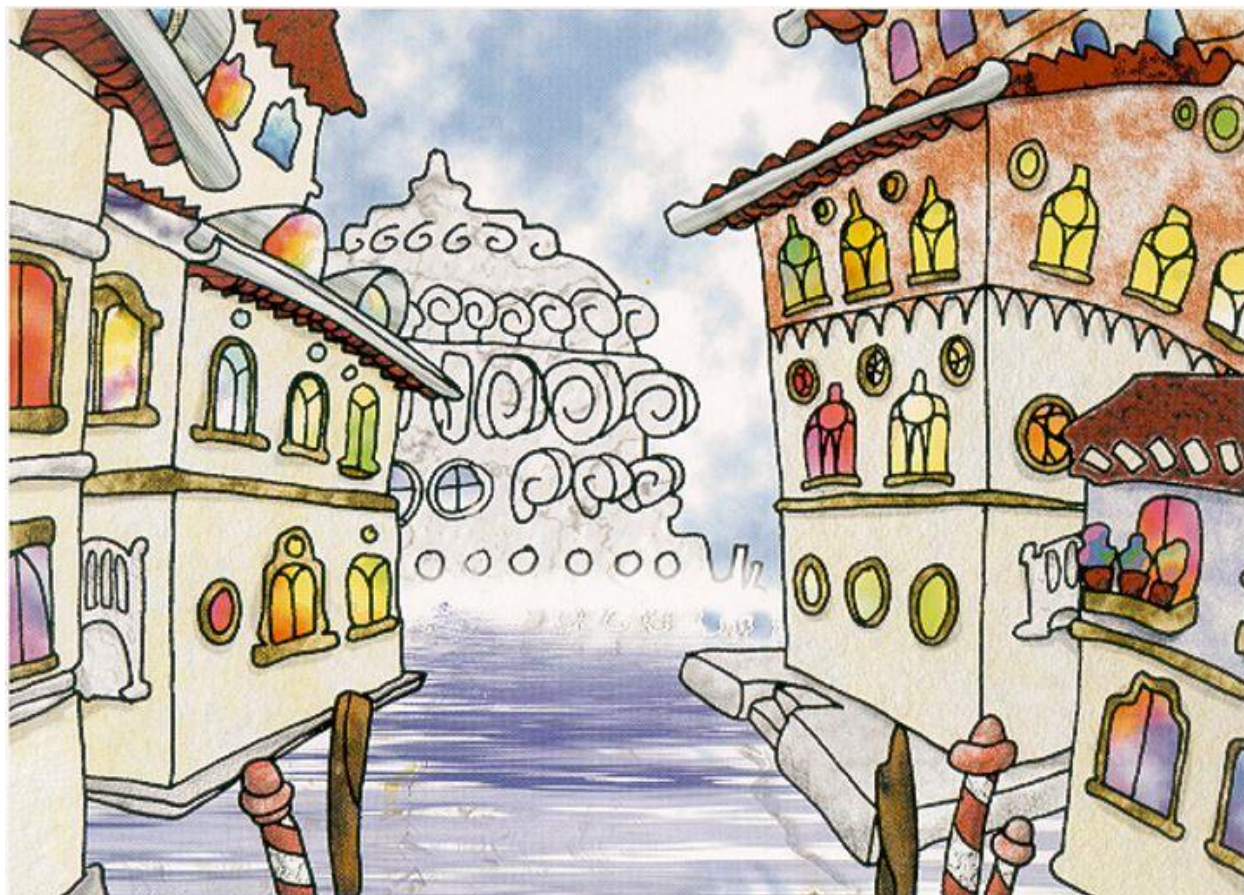
an Open Access Journal by MDPI



GREEN SCIENCES FOR SUSTAINABLE DEVELOPMENT FOUNDATION

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** (www.gssd-foundation.org), a non-profit Foundation established in February 2020 and based in Venice.*



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 achieving its goals.



PURPOSES

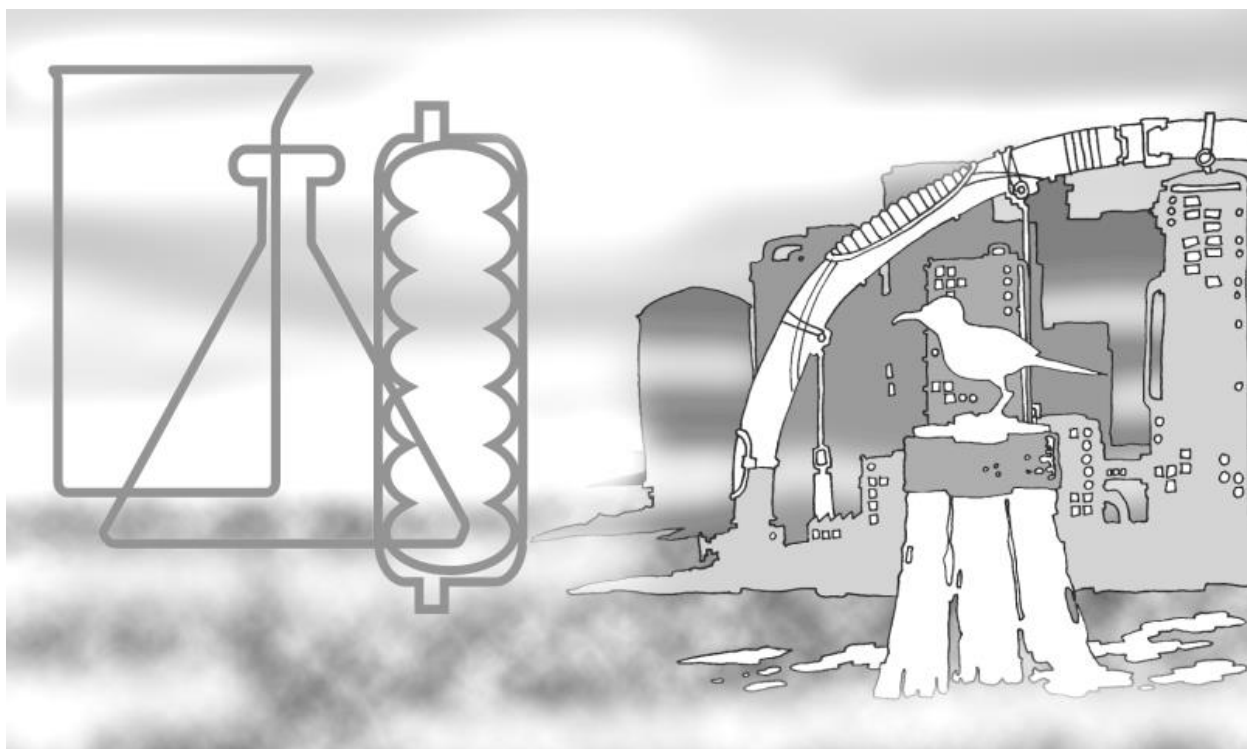
The main aims of the Foundation are:

- 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.



16th GREEN CHEMISTRY POSTGRADUATE SUMMER SCHOOL

30 June - 5 July 2024

BOOK OF ABSTRACTS

CONTENTS:

| | |
|--|-----|
| Welcome Message from the Chair of the Summer School..... | 10 |
| Foreword by the First Deputy CEO PJSC PhosAgro | 11 |
| Foreword by the Local Organizing Committee in Venice | 12 |
| Letters from IUPAC Representatives for Prof. Tundo's Memory | 13 |
| Summer School Committees..... | 15 |
| Lectures & Teachers (<i>alphabetical order of surnames</i>) | 16 |
| Timetable..... | 19 |
| Programme..... | 20 |
| In-person students Poster Programme | 25 |
| Teachers' Lecture Abstracts (<i>alphabetical order of surnames</i>)..... | 29 |
| Students' Abstracts (<i>alphabetical order of surnames</i>)..... | 59 |
| Photos (<i>in person and online</i>)..... | 118 |

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 **16th edition of the Green Chemistry Postgraduate Summer School (GCSS 2024)**.

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 2024 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 16th Green Chemistry Postgraduate Summer School 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.

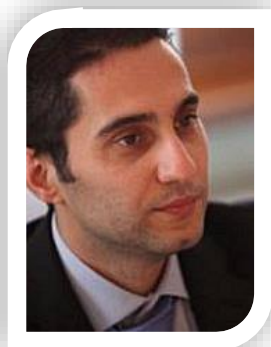
The Summer School on Green Chemistry is a key project for **PhosAgro** and **IUPAC**.

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 Green Chemistry Postgraduate Summer School 2024,

It is an honor for me to welcome you to this 16th 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 2024 edition of the Green Chemistry Postgraduate Summer School 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 (almost 100!) 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,
Organizing Committee of the
Green Chemistry Postgraduate Summer School 2024*

LETTERS FROM IUPAC REPRESENTATIVES FOR PROFESSOR TUNDO'S MEMORY



| | | |
|---|---|---|
| <i>President</i> Prof. Javier García Martínez (Spain) | <i>Vice President</i> Prof. Ehud Keinan (Israel) | <i>Secretary General</i> Prof. Richard Hartshorn (New Zealand) |
| <i>Past President</i> Prof. Christopher Brett (Portugal) | <i>Treasurer</i> Prof. Wolfram Koch (Germany) | <i>Executive Director</i> Dr. Lynn M. Soby (United States) |

Alicante, October 30th, 2023

Dear family and friends of Professor Pietro Tundo,

On behalf of the International Union of Pure and Applied Chemistry (IUPAC), I write to express my deepest condolences on the passing of Professor Pietro Tundo.

Professor Tundo was a distinguished scientist and a tireless advocate for a more rational use of chemistry. He made significant contributions to the fields of green chemistry and sustainable development, both through his research and his leadership. He was also a strong supporter of IUPAC and its mission to advance the chemical sciences. I would like to pay special tribute to him for organizing many editions of the IUPAC International Conferences on Green Chemistry and the Green Chemistry Summer School. His tireless efforts have shaped many of us and inspired generations of chemists.

Professor Tundo was particularly committed to the work of the IUPAC Interdivisional Committee on Green Chemistry for Sustainable Development, which he helped to establish and launch, and chaired from 2015 to 2022. Professor Tundo's contributions to IUPAC and to the field of green chemistry as a whole have been immense. He has been responsible for more than twenty IUPAC projects and served on the IUPAC Bureau from 2015 to 2019. In 2013 he contributed to the foundation of the Italian National Committee of CNR for IUPAC, of which he was President for four years. From 2007 to 2009, Prof. Tundo was President of IUPAC Division III (Organic and Biomolecular Chemistry). More recently, in 2020, Prof. Tundo founded the Green Sciences for Sustainable Development Foundation to promote the development of scientific education and the dissemination of green chemistry. He was the President of this organization since its inception.

For all of this, but especially for his friendship and willingness to help, IUPAC is grateful for Professor Tundo's service and dedication. He will be deeply missed by the IUPAC family and the entire green chemistry community.

Sincerely,

Professor Javier García-Martínez
President, International Union of Pure and Applied Chemistry



Interdivisional Committee on Green Chemistry for Sustainable Development(IGCSD)

October 31th, 2023

Dear family of Professor Pietro Tundo,

On behalf of the Interdivisional Committee on Green Chemistry for Sustainable Development (IGCSD of the International Union of Pure and Applied Chemistry (IUPAC), I write the letter condolences for the loss of Professor Pietro Tundo.

Professor Tundo was a world-leading scientist. He made great contributions to chemistry, especially green chemistry, through his excellent research and his leadership. He helped to establish and launch IGCSD, and he was the chair of the committee from 2015 to 2022. In 2020, Prof. Tundo founded the Green Sciences for Sustainable Development Foundation to promote green chemistry, and he has been the President of this organization since its establishment. He has organized many editions of the IUPAC International Conferences on Green Chemistry and the Green Chemistry Summer School. He helped establish the IUPAC-Zhejiang NHU International Awards for Advancement in Green Chemistry. In addition, he has been the chair of more than 20 IUPAC projects.

He always tried his best to help others, especially young scientists and students. His spirit to devote himself to science and technology has become a model for us, and we have learned a lot from him.

IGCSD thanks Professor Pietro Tundo very much for his significant contribution to the committee. The entire green chemistry community will very much miss him and remember him forever for both his great contribution to this important field and his friendship.

Sincerely,

A handwritten signature in black ink, which reads 'Buxing Han'. The signature is written in a cursive style with a long, sweeping underline.

Buxing Han

Chair of IGCSD, IUPAC

SUMMER SCHOOL COMMITTEES

CHAIR OF THE SUMMER SCHOOL

- **Francesco TROTTA**, *President of Green Sciences for Sustainable Development Foundation, Venice, Italy, and Professor at the Department of Chemistry, University of Turin, Italy*

LOCAL ORGANIZING COMMITTEE

- **Fabio ARICÒ**, *Professor of Organic Chemistry, Ca' Foscari University of Venice, Italy*
- **Aurelia VISA**, *Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry – Timisoara, Romania*
- **Mirabbos HOJAMBERDIEV**, *Technische Universität Berlin, Germany*
- **Graziana GIGLIUTO**, *Green Sciences for Sustainable Development Foundation, Italy*

INTERNATIONAL JURY FOR THE POSTER SESSIONS IN PRESENCE AND ONLINE FOR THE “Green Sciences for Sustainable Development Foundation Students Online Awards” AND “PhosAgro In Presence Students Award”

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*
- **Giancarlo Cravotto**, *Full Professor of Organic Chemistry, Department of Pharmaceutical Science and Technology University of Turin, Italy*
- **Chiara Samorì**, *Professor of Organic Chemistry Department of Chemistry ‘Giacomo Ciamician’, University of Bologna, Italy*
- **Banothile Makhubela**, *Professor at University of Johannesburg, Research Centre for Synthesis & Catalysis, South Africa*
- **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*
- **Giulia Licini**, *Professor of Organic Chemistry Department of Chemical Sciences, University of Padua, Italy*
- **Claudia Barolo**, *Professor at the Department of Chemistry, University of Turin, Italy*
- **Javier Garcia Martinez**, *Professor of Inorganic Chemistry at the University of Alicante, Spain*
- **Florent Allais**, *Full Professor in Chemistry at AgroParisTech (Paris, France) and the Director of the Chair ABI (Industrial Agro-Biotechnologies) in Reims (France)*

TEACHERS AND LECTURES

(alphabetical order of surnames)

FLORENT ALLAIS

URD ABI, CEBB, AgroParisTech, 3 rue des Rouges Terres, 51110 Pomacle, France

Valorizing Lignocellulosic Biomass Through the Combination of Green Chemistry, Biotechnologies and Downstream Processing

PAUL T. ANASTAS

Center for Green Chemistry and Green Engineering, Yale University, New Haven, CT 06520, United States

The Periodic Table of The Elements of Green and Sustainable Chemistry

FABIO ARICÒ

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

The Reactions of Dimethyl Carbonate and Its Derivatives

CARLO BARBANTE

University Ca' Foscari of Venice, Institute of Polar Sciences – National Research Council of Italy
Climate Changes: the Poles Matter

CLAUDIA BAROLO

Dipartimento di Chimica and Centro Interdipartimentale NIS, Centro di Riferimento INSTM, Università di Torino, Italy

Organic Functional Dyes: Key Elements for a Sustainable Energy Transition?

CHRISTOPHER BRETT

Department of Chemistry, University of Coimbra, Portugal

Deep Eutectic Solvents as a Greener Materials Approach and Electrochemical Applications

SAMORÌ CHIARA

Dipartimento di Chimica "Giacomo Ciamician", Alma Mater Studiorum, Università di Bologna, Italy

Microalgae as Cellular Factories: From Biofuels to High-Added Value Compounds

GIANCARLO CRAVOTTO

Dip.to di Scienza e Tecnologia del Farmaco, University of Turin, Italy

Enabling Technologies for Chemical Process Intensification, Scalability of Green Procedures

ALBERTO FIGOLI

Institute on Membrane Technology, National Research Council of Italy, Rende (CS) Italy

Toward a More Sustainable Membrane Fabrication

JONATHAN E. FORMAN

Science and Technology Advisor, Threat Prevention and Resilience Group, Pacific Northwest National Laboratory, 1100 Dexter Ave N, Suite 500, Seattle, WA 98109 USA

Chemicals of War and the Chemistry of Peace: Eliminating the World's Chemical Weapons Stockpiles and the Legacy Left Behind

JAVIER GARCÍA-MARTÍNEZ

Laboratorio de Nanotecnología Molecular, Dpto. Química Inorgánica, Universidad de Alicante, Ap. 99, E-03690 Alicante, Spain

Catalyzing the Green Revolution: Unlocking Previously Inaccessible Chemical Processes

GAETANO GUERRA

Dipartimento di Chimica e Biologia, Università di Salerno, Via Giovanni Paolo II 132, 84084 Fisciano (SA), Italy

Packaging Plastics in the Circular Economy

BUXING HAN

Institute of Chemistry, Chinese Academy of Sciences, 100190, Beijing, P.R. China

Conversion of CO₂, Biomass, and Waste Plastics into Chemicals and Fuels

MIRABBOS HOJAMBERDIEV

Institut für Chemie, Technische Universität Berlin, 10623 Berlin, Germany

Green Hydrogen Generation From Solar Water Splitting over Metal Oxynitrides

PHILIP JESSOP

Queen's University, Dept. of Chemistry, 90 Bader Lane, Kingston, Ontario, K7L 3N6, Canada

How Chemists Can Use Life Cycle Assessment to Guide Our Research

KLAUS KÜMMERER

Institute of Sustainable Chemistry, Faculty of Sustainability, Leuphana University, Universitätsallee 1, 21335 Lüneburg, Germany

Sustainable Chemistry as the Overarching Guiding Principle to Embed Chemistry into Sustainability

PETER LICENCE

School of Chemistry, University of Nottingham, United Kingdom

Ionic Liquids: The Good, The Bad and The Ugly

GIULIA LICINI

Dipartimento Scienze Chimiche, Università di Padova, via Marzolo, 1, 35131, Padova, Italy

Catalytic Aerobic Oxidations: From Simple Organic Reactions to Biomass Valorization

BANOTHILE C.E. MAKHUBELA

Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, Faculty of Science, University of Johannesburg, Auckland Park 2006, South Africa

Harnessing Renewable Carbon Sources: Catalytic Strategies for Biomass and Carbon Dioxide Conversion

KRZYSZTOF MATYJASZEWSKI

Carnegie Mellon University, Center for Macromolecular Engineering, Pittsburgh, PA, 15213, USA

Towards Green Atom Transfer Radical Polymerization

NATALIA TARASOVA

Mendeleev University of Chemical Technology, Institute of Chemistry and Problems of Sustainable Development, Miusskaya Sq., 9, 125047, Moscow, Russia

Green Chemistry within Planetary Boundaries

KONSTANTINOS TRIANTAFYLLIDIS

Aristotle University of Thessaloniki, Department of Chemistry, University Campus P.O. Box 116, 54124 Thessaloniki, Greece

Integrated Waste/Bio-Refineries to Fuels, Chemicals and Polymers

FRANCESCO TROTTA

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

Exploitation of Renewable Resources in Polymer Chemistry

LUIGI VACCARO

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

Novel Technologies for Green Synthesis and Catalysis

AURELIA VISA

Institute of Chemistry “Coriolan Dragulescu”, 24 M. Viteazul Ave, Timișoara - 300223, Romania,

Green and Environmentally Friendly Approaches for Metal-Organic Frameworks Synthesis and Applications

| CEST TIME (Central European Summer Time) | | MONDAY 1-July | | TUESDAY 2-July | | WEDNESDAY 3-July | | THURSDAY 4-July | | FRIDAY 5-July | |
|---|-------------|---------------|--|----------------|--|------------------|--|-----------------|---|---------------|--|
| | 9:00-10:00 | 9:00-10:00 | OPENING CEREMONY <i>Chair: F. Aricò</i> | 9:00-9:30 | Phosagro <i>Chair: F. Trotta</i> | 9:00-9:30 | Foundation <i>Chair: F. Aricò</i> | 9:00-9:30 | OPCW <i>Chair: F. Trotta</i> | 9:00-9:30 | IUPAC SCI- Gruppo interdivisionale Green Chemistry <i>Chair: F. Aricò</i> |
| | 10:00-11:00 | 10:00-11:00 | Klaus Kummerer <i>Chair: F. Aricò</i> | 9:30-10:30 | Krzysztof Matyjaszewski <i>Chair: G. Cravotto</i> | 9:30-10:30 | Gaetano Guerra <i>Chair: F. Trotta</i> | 9:30-10:30 | Philip Jessop <i>Chair: C. Samori</i> | 9:30-10:30 | Francesco Trotta <i>Chair: F. Aricò</i> |
| | 11:00-11:30 | 11:00-11:30 | Coffee Break | 10:30-11:15 | Alberto Figoli <i>Chair: G. Cravotto</i> | 10:30-11:15 | Chris Brett <i>Chair: F. Trotta</i> | 10:30-11:15 | Luigi Vaccaro <i>Chair: C. Samori</i> | 10:30-11:15 | Chiara Samorì <i>Chair: F. Aricò</i> |
| | 11:30-12:15 | 11:30-12:15 | Paul Anastas on line <i>Chair: F. Aricò</i> | 11:15-11:35 | Coffee Break | 11:15-11:35 | Coffee break | 11:15-11:35 | Coffee Break | 11:15-11:35 | Coffee Break |
| | 12:15-13:00 | 12:15-13:00 | Peter Licence <i>Chair: F. Aricò</i> | 11:35-12:20 | Giancarlo Cravotto <i>Chair: L. Vaccaro</i> | 11:35-12:30 | Buxing Han on line <i>Chair: G. Trapasso</i> | 11:35-12:20 | Florent Allais <i>Chair: C. Barolo</i> | 11:35-13:00 | CLOSING CEREMONY AND POSTER AWARDS |
| | 13:00-14:30 | 13:00-14:30 | Lunch | 12:20-13:05 | Kostas Triantafyllidis <i>Chair: L. Vaccaro</i> | 12:30-13:15 | Carlo Barbante <i>Chair: G. Trapasso</i> | 12:20-13:05 | Javier Garcia Martinez <i>Chair: C. Barolo</i> | | |
| | 14:30-15:15 | 14:30-15:15 | Fabio Aricò <i>Chair K. Triantafyllidis</i> | 13:05-14:30 | Lunch | 13:05-14:30 | Lunch | 13:05-14:30 | Lunch | | |
| | 15:15-16:00 | 15:15-16:00 | Aurelia Visa <i>Chair K. Triantafyllidis</i> | 14:30-15:15 | Claudia Barolo <i>Chair: A. Visa</i> | | | 14:30-15:15 | Giulia Licini <i>Chair: G. Trapasso</i> | | |
| | 16:00-16:30 | 16:00-16:30 | Coffee break | 15:15-16:00 | Banothile Makhubela <i>Chair: A. Visa</i> | | | 15:15-16:00 | Jonatan Forman <i>Chair: G. Trapasso</i> | | |
| | 16:30-17:00 | 16:30-17:00 | M. Hojamberdiev on line <i>Chair: A. Visa</i> | 16:00-17:30 | POSTER SESSION 1 ON SITE + Coffee break | 14:30-19:30 | Free Afternoon | 16:00-17:30 | POSTER SESSION 2 ON SITE + Coffee break | | |
| | 17:00-17:30 | 17:00-17:30 | Natalia Tarasova on line <i>Chair: A. Visa</i> | | | 19:30-21:00 | Social Dinner | | | | |
| | 17:00-19:00 | 17:00-19:00 | WELCOME TOGETHER | | | | | | | | |
| | | | SUNDAY 30-June | | | | | | | | |
| | 12:00-17:00 | | Check-in and Registration at Campus Santa Marta | | | | | | | | |



16th Edition of the Green Chemistry Postgraduate Summer School 2024

THE SUMMER SCHOOL 2024 PROGRAMME

MONDAY, 1 JULY 2024, MORNING

OPENING CEREMONY

PRESENTERS:

Francesco Trotta, Chairman of the Green Chemistry Summer Schools and President of the Green Sciences for Sustainable Development Foundation

Ferruccio Trifirò, Emeritus Professor, University of Bologna, Italy

Natalia Tarasova, Director, Institute of Chemistry and Problems of Sustainable Development, Mendeleev University of Chemical Technology of Russia, Past Ordinary Member of the ISC Governing Board 2018-2021, ISC Fellow

Siroj Loikov, First Deputy CEO of PJSC PhosAgro

Fabio Aricò, Delegate for Internationalization at DIAS Department, Ca' Foscari University of Venice, Italy

1st LECTURE SESSION:

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

Klaus Kümmeler, Professor of Sustainable Chemistry and Material Resources at the Institute for Sustainable Chemistry (INSC), Leuphana University Lüneburg and Bonn, Germany

Lecture title: Sustainable Chemistry as the Overarching Guiding Principle to Embed Chemistry into Sustainability

Paul Anastas, Teresa and H. John Heinz III Professor in the Practice of Chemistry for the Environment, Faculty Director, Yale University, USA

Lecture title: The Periodic Table of the Elements of Green and Sustainable Chemistry

Peter Licence, Full Professor of Chemistry and Director of The GlaxoSmithKline Carbon Neutral Laboratory, Faculty of Science, Nottingham, UK

Lecture title: Ionic Liquids: The Good, The Bad and The Ugly

MONDAY, 1 JULY 2024, AFTERNOON

2nd LECTURE SESSION:

Moderator: Konstantinos Triantafyllidis, Professor at the Department of Chemistry, Aristotle University of Thessaloniki, Greece

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

Lecture title: The reactions of dimethyl carbonate and its derivatives

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

Lecture title: Green and environmentally friendly approaches for Metal-Organic Frameworks synthesis and applications

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

Mirabbos Hojamberdiev, Technische Universität Berlin, Germany

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

Natalia Tarasova, Director, Institute of Chemistry and Problems of Sustainable Development, Mendeleev University of Chemical Technology of Russia

Lecture title: Green Chemistry within Planetary Boundaries

TUESDAY, 2 JULY 2024, MORNING

SPONSORS and INSTITUTIONS

PRESENTER:

Alexander Antonov, Director Department PJSC PhosAgro International Projects

3rd LECTURE SESSION:

Moderator: Giancarlo Cravotto, Full Professor of Organic Chemistry, Department of Pharmaceutical Science and Technology University of Turin, Italy

Krzysztof Matyjaszewski, Department of Chemistry Carnegie Mellon University, Pittsburgh, USA

Lecture title: Towards Green Atom Transfer Radical Polymerization

Alberto Figoli, Director of the Institute on Membrane Technology of the National Research Council of Italy, ITM-CNR

Lecture title: Toward a more Sustainable Membrane Fabrication

Moderator: Luigi Vaccaro, Full Professor of Organic Chemistry, Università degli Studi di Perugia, Italy

Giancarlo Cravotto, Full Professor of Organic Chemistry, Department of Pharmaceutical Science and Technology University of Turin, Italy

Lecture title: Enabling technologies for chemical process intensification, scalability of green procedures

Konstantinos Triantafyllidis, Professor at the Department of Chemistry, Aristotle University of Thessaloniki, Greece

Lecture title: Integrated Waste/Bio-Refineries to fuels, chemicals, and polymers

TUESDAY, 2 JULY 2024, AFTERNOON

4th LECTURE SESSION:

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

Claudia Barolo, Professor at the Department of Chemistry, University of Turin, Italy

Lecture title: Organic functional dyes: key elements for a sustainable energy transition?

Banothile Makhubela, Professor at University of Johannesburg, Research Centre for Synthesis & Catalysis, South Africa

Lecture title: Harnessing renewable carbon sources: Catalytic strategies for biomass and carbon dioxide conversion

1st IN-PERSON POSTER SESSION (22 POSTERS)

WEDNESDAY, 3 JULY 2024, MORNING

SPONSORS and INSTITUTIONS

PRESENTER:

Francesco Trotta, Green Sciences for Sustainable Development Foundation

5th LECTURE SESSION:

Moderator: Francesco Trotta, Full Professor of Industrial Chemistry, University of Turin, Italy

Gaetano Guerra, Full Professor of Macromolecular Chemistry at the Department of Chemistry and Biology 'A.Zambelli' at the University of Salerno, Italy

Lecture title: Packaging Plastics in the Circular Economy

Christopher Brett, Full Professor of chemistry, University of Coimbra, Portugal

Lecture title: Deep eutectic solvents as a greener materials approach and electrochemical applications

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

Buxing Han, Professor at Institute of Chemistry, Chinese Academy of Sciences, Director of Shanghai Key Laboratory of Green Chemistry and Chemical Processes – China

Lecture title: Conversion of CO₂, Biomass, and Waste Plastics into Chemicals and Fuels

Carlo Barbante, Full Professor of Analytical Chemistry, Director of the Institute of Polar Sciences – CNR, University Ca' Foscari Venice, Italy

Lecture title: Climate Changes: The Poles Matter

WEDNESDAY, 3 JULY 2024, AFTERNOON

FREE TIME

SOCIAL DINNER

THURSDAY, 4 JULY 2024, MORNING

SPONSORS and INSTITUTIONS

PRESENTER:

Jonathan FORMAN, Science and Technology Advisor in the Global Security Technology and Policy Group under the National Security Directorate of Pacific Northwest National (PNNL), USA

6th LECTURE SESSION:

Moderator: Chiara Samorì, Professor of Organic Chemistry Department of Chemistry 'Giacomo Ciamician', University of Bologna, Italy

Philip Jessop, Full Professor and Canada Research Chair of Green Chemistry at the Department of Chemistry, Queen's University in Kingston, Canada

Lecture title: How Chemists Can Use Life Cycle Assessment to Guide Our Research

Luigi Vaccaro, Full Professor of Organic Chemistry, Università degli Studi di Perugia, Italy

Lecture title: Novel Technologies for green synthesis and catalysis

Moderator: Claudia Barolo, Professor at the Department of Chemistry, University of Turin, Italy

Florent Allais, Full Professor in Chemistry at AgroParisTech (Paris, France) and the Director of the Chair ABI (Industrial Agro-Biotechnologies) in Reims, France

Lecture title: Valorizing lignocellulosic biomass through the combination of green chemistry, biotechnologies and downstream processing

Javier Garcia Martinez, Professor of Inorganic Chemistry at the University of Alicante, Spain

Lecture title: Catalyzing the Green Revolution: Unlocking Previously Inaccessible Chemical Processes

THURSDAY, 4 JULY 2024, AFTERNOON

7th LECTURE SESSION:

Giacomo Trapasso, Ca' Foscari University, Venice, Italy

Giulia Licini, Professor of Organic Chemistry Department of Chemical Sciences, University of Padua, Italy

Lecture title: Catalytic aerobic oxidations: from simple organic reactions to biomass valorization

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
Lecture title: Chemicals of War and the Chemistry of Peace: Eliminating the World's Chemical Weapons Stockpiles and the Legacy Left Behind

2nd IN-PERSON POSTER SESSION (21 POSTERS)

FRIDAY, 5 JULY 2024, MORNING

SPONSORS and INSTITUTIONS

PRESENTER:

Javier GARCÍA-MARTÍNEZ, International Union of Pure and Applied Chemistry (IUPAC)

8th LECTURE SESSION:

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

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

Lecture title: Exploitation of Renewable Resources in Polymer Chemistry

Chiara Samorì, Professor of Organic Chemistry Department of Chemistry 'Giacomo Ciamician', University of Bologna, Italy

Lecture title: Microalgae as cellular factories: from biofuels to high-added value compounds

CLOSING CEREMONY AND POSTER AWARDS

PRESENTERS:

Francesco Trotta, President of Green Sciences for Sustainable Development Foundation, Venice, Italy

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

Graziana Gigliuto, Ca' Foscari University, Venice, Italy

Mirabbos Hojamberdiev, Technische Universität Berlin, Germany

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

IN-PERSON POSTER PROGRAM

Poster session 1, Tuesday, 2nd July 2024, 16:00-17:30

| Poster number | Name | Affiliation and country | Title |
|---------------|--------------------------------------|---|--|
| 1 | Winifred Delali ANYOMIH | Department of Chemistry, University of Johannesburg, Kingsway Campus, Auckland Park, South Africa | Valorization of waste corn cobs into high yields of furfural using ionic liquids |
| 2 | Mariam AUDU | Nanostructured Interfaces and Surfaces (NIS), Centre of Excellence, Department of Chemistry, University of Torino, Italy | Benign synthesis routes for the production of biochar from artichoke biomass |
| 3 | Eugenia RODRIGUEZ RISTAU | Faculty of Chemical Sciences, UNC, Argentina | Search for photoactivated antimicrobial compounds from South American plant species |
| 4 | Bilal LOUMI | URD ABI, CEBB, AgroParisTech, 3 Rue des Rouges-Terres, 51110 Pomacle, France | Cellulose-Derived Mycosporine-Like Amino Acids Analogues as Novel UV Filters for Cosmetics |
| 5 | Ataollah NIYATI | <i>Department of Civil, Chemical, and Environmental Engineering - Università Di Genova, Via Opera Pia 15, I-16145, Genoa, Italy</i> | Investigating the Impact of Electrolyte Temperature on the Oxygen Evolution Reaction Efficiency of Ni-Co/NiFelt Nano Composite Electrode |
| 6 | Samira SULEYMANOVA | <i>Institute of Catalysis and Inorganic Chemistry, Baku, Azerbaijan</i> | Colloid-chemical features of an aqueous-phase catalytic system for the direct hydroxylation of phenol to dihydroxybenzenes with hydrogen peroxide by nano/micro-sized iron containing silica-gel |
| 7 | Gabriela Tuono Martins XAVIER | <i>Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Brazil</i> | Synthesis and characterization of a robust Ga-MOF catalyst for the epoxidation of <i>cis</i> -cyclooctene using H ₂ O ₂ as a green oxidant |
| 8 | Cecilia I. ETUKUDO | <i>Department of Chemistry, University of Uyo, Uyo, Nigeria</i> | Green Synthesis of Bio-inspired Nanocomposite using Kaolin Clay and Aloe Vera Extract for Column Treatment of Wastewater |
| 9 | Camila DIAS | <i>BasCat – UniCat BASF JointLab, Technische Universität Berlin, Berlin, Germany</i> | Synthesis of 1,6-Hexanediol through Catalytic Hydrodeoxygenation of 1,2,6-Hexanetriol in Continuous Flow System |
| 10 | Marcela IOSIVONI | <i>„Coriolan Dragulescu” Institute of Chemistry, 24 Mihai Viteazul Blv., 300223 Timisoara, Romania</i> | Metal-organic frameworks impregnated with ionic liquids as adsorbent materials for phenol and phenol derivatives |
| 11 | Ingrid MEZA | <i>Institute of Physics, Autonomous University of</i> | Green synthesis of nanohybrids as an alternative against cancer |

| | | | |
|----|---------------------------------|---|---|
| | | <i>San Luis Potosí, 78210 San Luis Potosí, SLP., México</i> | |
| 12 | Martina SILACO | <i>Università degli Studi di Palermo, Dipartimento STEBICEF, Palermo, Italy</i> | Efficient Conversion of L-Rhamnose into 5-methylfurfural combining performance of ionic liquids and zeolites |
| 13 | Giuseppe GRAVINA | <i>Dipartimento di Chimica e Biologia "Adolfo Zambelli", Università di Salerno, Fisciano (SA), Italy</i> | Novel Iron (II) complexes for efficient and versatile Ring Opening Polymerization of Bio-Based Lactones |
| 14 | Federica SANTULLI | <i>University of Salerno, Department of Chemistry and Biology "A. Zambelli", Fisciano, Salerno, Italy</i> | Chemical recycling of Polylactide promoted by Zinc-complexes |
| 15 | Jerome LIEW | <i>Centre of Ionics Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur, Malaysia</i> | The Evolution of MXene Synthesis: Towards Using Green Solvent |
| 16 | Francesco RABONI | <i>Università degli Studi di Genova, Dipartimento di Chimica e Chimica Industriale, via Dodecaneso 31, 16146, Genova, Italy</i> | Sustainable synthesis of functionalized glycerol oligoesters |
| 17 | Dmitrii KURNOSOV | <i>Università di Genova – Dipartimento di Chimica e Chimica Industriale, Via Dodecaneso, 31, 16146 Genova, Italy</i> | Enzymatic synthesis of amino acid-based surfactants |
| 18 | Irene PASERO | <i>Alma Mater Studiorum, University of Bologna, Italy</i> | Green Hydrogen production exploiting Capnophilic Lactic Fermentation pathway in the anaerobic hyperthermophilic bacterium <i>Thermotoga neapolitana</i> |
| 19 | Ana-Isabel QUILEZ-MOLINA | <i>Crystallography and Mineralogy Department, Faculty of Science, University of Valladolid, Spain</i> | Straightforward methods to design advanced materials using Melamine foams |
| 20 | Beatriz CHÍCHARO | <i>Department of Environmental Science, Informatics and Statistics, Ca'Foscari University, Venice, Italy</i> | A multi-gram synthesis to pure HMF and BHMF |
| 21 | Angelica MERO | <i>Department of Pharmacy, Via Bonanno 33, Pisa, Italy</i> | Sustainable valorization of cherry (<i>Prunus avium</i> L.) pomace waste via the combined use of (NA)DESs and bio-ILs |
| 22 | Claudio CECONE | <i>Department of Chemistry, University of Turin, NIS and INSTM Reference Centers, Via Giuria 7, 10125 Torino, Italy</i> | <i>In-situ</i> one-step production of gold nanoparticles supported on carbon sub-micrometric fibers from electrospun maltodextrin-based mats |

IN-PERSON POSTER PROGRAM

Poster session 2, Thursday, 4th July 2024, 16:30-17:30

| Poster number | Name | Affiliation and country | Title |
|---------------|---|---|--|
| 1 | Vanessa SPADAVECCHIA | <i>Dipartimento di chimica "Giacomo Ciamician", Università di Bologna, Via Pietro Gobetti 85, 40129 Bologna, Italy</i> | Multilayer packaging delamination process using CO ₂ -switchable surfactants |
| 2 | Valentina BENAZZI | <i>Dipartimento di Chimica Organica, Università degli Studi di Pavia (Via Torquato Taramelli 12, 27100 Pavia, Italia)</i> | Carbon dots as visible light biobased photocatalysts in organic synthesis |
| 3 | Khaoula HKIRI | | |
| 4 | Karen G. Duarte MAGALHÃES | <i>Federal University of Rio Grande do Norte, Natal/RN, Brazil</i> | Energy-saving electrochemical green hydrogen production coupled with active chlorine species valorization |
| 5 | Sulafa Abdalmageed Saadaldeen MOHAMMED | <i>Department of Energy, Aalborg University, 9220 Aalborg, Denmark</i> | Computational and experimental evaluation of triazolium and imidazolium-based ionic liquids as electrolyte for CO ₂ electrochemical reduction |
| 6 | Anara OMAROVA | <i>Center of Physical Chemical Methods of Research and Analysis, Faculty of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty, Kazakhstan</i> | Optimization of MOF-199-based solid-phase microextraction coatings synthesis for an efficient quantification of volatile organic compounds in air |
| 7 | Francesco CATALINI | <i>University of Perugia, Italy</i> | Sustainable activation of Pictet-Spengler Reaction by Brønsted Catalysts under Microwave Irradiation |
| 8 | Tian SANG | <i>Laboratory of Green SOC, Dipartimento di Chimica, Biologia e Biotecnologie Università degli Studi di Perugia Via Elce di Sotto, 8, 06124 Perugia, Italy</i> | Heterogeneous palladium-catalysed C(sp ³)-H α -arylation for the green synthesis of fused N-heterocycles |
| 9 | Anna SCETTRI | <i>Department of Industrial Engineering, University of Padova, Padova, Italy</i> | Valorisation of Coffee Silverskin through extractions and pyrolytic processes |
| 10 | Herbet LIMA OLIVEIRA | <i>Federal University of Rio Grande do Norte, Natal/RN, Brazil</i> | Reuse of Textile Effluents Treated by Electrooxidation with Green Hydrogen Cogeneration: A Sustainable Solution for the Textile Industry |
| 11 | Shadi MOHAMMADIAN | <i>Department of Chemistry, Institute for Advanced Studies in Basic Sciences</i> | Construction of Ru(II) Complexes Bearing Diphosphinoferrocene Ligands: |

| | | | |
|----|-------------------------------|--|--|
| | | <i>(IASBS), Zanjan, 45137-66731, Iran</i> | Electrochemical and Biological Investigations |
| 12 | Haroon AHMAD | <i>Department of Engineering and Applied Sciences and CSGI, University of Bergamo, Italy</i> | Innovative Application of Kolbe Reaction on the constituents of Plant Oils |
| 13 | Chiara FRATELLO | <i>Institute for the Study of Nanostructured Materials (ISMN), National Research Council (CNR), SP35d, 9, 00010 Montelibretti (Rome), Italy</i> | Sustainable corrosion inhibitors and carrier systems for the preservation of concrete heritage |
| 14 | S. Trastulli COLANGELI | <i>Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto, 8, 06123 – Perugia, Italy</i> | Sustainability in a can: upcycling aluminium scrap in the waste-minimized electrochemical synthesis of 2-oxazoline |
| 15 | Marta CIANI | <i>Laboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, 06123, Perugia, Italy</i> | Enhancing Sustainability in Cross-Coupling Reactions with Microwave irradiation: A Circular Approach |
| 16 | Alexander UNER | <i>School of Chemistry, University of Nottingham, UK</i> | Practical, Metal-Free Synthesis of Difluoroethylamines using Difluoroacetic Acid |
| 17 | Mikhail TRUKHAN | <i>University of Turin – Department of Science and Pharmaceutical Technology, via Pietro Giuria 9, 10125 Turin, Italy</i> | Copper-Catalyzed Transfer Hydrogenation in Flow Reactors: Advancing Green Aniline Production |
| 18 | Greta PALOMBELLA | <i>Department of Environmental Science Informatic and Statistics, Ca' Foscari University of Venice, Venezia Mestre, Italy</i> | 5,5'-[oxybis(methylene)]bis-2-furfural (OBMF) one-pot green synthesis from D-fructose |
| 19 | Giulio POTA | <i>Department of Chemical, Materials and Production Engineering, University of Naples Federico II, Italy</i> | Design of novel heterogeneous biocatalysts for the enantioselective synthesis of β -hydroxy acids |
| 20 | Ibrahim HUSSEIN | <i>University of Turin, Department of Chemistry, Italy</i> | Green synthesis of Cross-Linked Cyclodextrin for drug delivery applications |
| 21 | Giovanna RAIÀ | <i>Università degli Studi di Palermo, Dipartimento STEBICEF, Sezione di Chimica. Viale delle Scienze, Ed. 17 90128 Palermo, Italy</i> | Aminolysis of polycarbonate under us irradiation to obtain ionic liquids |

ABSTRACTS OF LECTURES

(alphabetical order of surnames)

Valorizing Lignocellulosic Biomass Through the Combination of Green Chemistry, Biotechnologies and Downstream Processing

FLORENT ALLAIS

URD ABI, CEBB, AgroParisTech, 3 rue des Rouges Terres, 51110 Pomacle, France

**Corresponding author: florent.allais@agroparistech.fr*

Abstract:

Located in the CEBB (European Center of Biotechnology and Bioeconomy, co-funded by the ERDF, the Grand Est Region, the Marne Department and the Urban Community of Grand Reims) at the heart of the Pomacle-Bazancourt biorefinery, the URD ABI (Industrial Agro-biotechnologies Research & Development Unit) is interested in the valorization of biomass.

Thanks to its expertise in chemistry, polymers/materials, microbiology/biochemistry/molecular biology, chemical engineering and separation process engineering, as well as in analytical chemistry, the URD ABI is able to carry out multi- and transdisciplinary fundamental and applied research projects with the ambition of developing and optimizing sustainable industrial processes and high value-added products from agro-resources and industrial by-products.

This talk will provide some illustrative examples on how lignocellulosic biomass can be efficiently transformed into flavors, antioxidants, UV filters, monomers, polymers etc... by combining biotechnologies, green chemistry and process engineering.

Keywords:

Biomass, byproducts, valorization, upcycling, green chemistry, biotechnologies, downstream process

Acknowledgments: The URD ABI acknowledges the following for their financial support: Grand Reims, Grand Est Region, ANR, European Union, ARC, NSF.

The Periodic Table of The Elements of Green and Sustainable Chemistry

PAUL T. ANASTAS

Center for Green Chemistry and Green Engineering, Yale University, New Haven, CT 06520, United States

Abstract:

The field of green chemistry has a more than twenty-five-year history of invention and innovation of creating new materials, new products, new manufacturing processes that perform better and cost less while being sustainable and safe for humans and the environment. The range of products invented and improved by green chemistry touches virtually every industry sector from agriculture to energy to medicine to plastics to electronics. While the scientific brilliance that enables these discoveries and innovations are essential and necessary, they are not sufficient. In order for green chemistry to make positive impact on a scale and with the urgency necessary to address the greatest challenges of our time as enumerated in the United Nations Sustainable Development Goals, there will need to be a supporting structure. This structure is outlined in the Periodic Table of the Elements of Green and Sustainable Chemistry using the metaphor of the original Periodic Table first introduced 150 years ago, to present the enabling conceptual frameworks, metrics, legal/economic/policy drivers to advance and empower the transition to a more sustainable world.

The Reactions of Dimethyl Carbonate and Its Derivatives

FABIO ARICÒ

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

*Corresponding author: Fabio.arico@unive.it

Abstract:

The involvement of basic sciences in pursuing sustainable development is one of the main goals of the current years, as highlighted by many international programs such as International Year of Basic Sciences for Sustainable Development and the United Nation Agenda 2030, 17 UNSDGs. Chemistry will play a pivotal role; in fact the use intrinsically innocuous reagents and products, minimization of energy and waste and recycling are just some of the major issues that are currently tackled by organic synthesis as well as being at the core of many International Organisations' actions such as Organisation for Economic Cooperation and Development (OECD), United Nation Environment Program (UNEP), International Union of Pure and Applied Chemistry (IUPAC), etc.



Discovering, developing, and applying new organic syntheses through the understanding of their reaction mechanisms constitute a fundamental research field.[1] In this view, due to its benign nature, interest in dimethyl carbonate (DMC) has enormously increased in the last few decades. Currently DMC is used in many chemical reactions as it can efficiently substitute chlorine-based chemicals. Green preparations via DMC chemistry of anti-inflammatory drugs, polymers, fragrances, and solvents have been extensively reported. Furthermore, dialkyl carbonates (DACs) have been exploited as fuel additive, solvent for lithium battery, and for the preparation of pharmaceuticals, pesticides, plastic (including membranes), paints and coatings, electronics and agrochemicals.

In this perspective, this lecture focuses on the use of DMC and more in general dialkyl carbonates (DACs) in the substitution of halogen-based compounds in alkylation, alkoxy-carbonylation and cyclization reactions. The similarities and differences between DACs and chlorine parent compounds will be highlighted in several examples. Halogen-based molecules are undoubtedly more reactive than organic carbonates; however, they usually do not allow selective or chemoselective reactions. Conversely, the less reactivity DACs often lead to alkylation with high selectivity. What is evident from the examples that will be discussed is that behind the apparent simplicity of organic carbonates hides a non-immediate and multifaceted chemistry because it combines the reactivity of a hard electrophilic site and a soft electrophilic site carbon [2].

Keywords: Green Chemistry, Organic carbonates, Halogen Free synthetic pathways, Alkylation, cyclization reaction

References:

[1] F. Aricò, P. Tundo, *ChemSusChem*, **2023**, *16*, e202300748.

[2] P. Tundo, M. Musolino, F. Aricò, *Green Chem.*, **2018**, *20*, 28.

Climate Changes: The Poles Matter

CARLO BARBANTE

*University Ca' Foscari of Venice
Institute of Polar Sciences – National Research Council of Italy
barbante@unive.it*

Abstract:

Polar regions, encompassing the Arctic and Antarctic, are vital components of Earth's complex climate system and hold significant ecological, geopolitical, and scientific importance. These regions, characterized by extreme conditions and unique environments, serve as critical indicators of global climate change. The melting of polar ice caps and glaciers is a stark manifestation of warming temperatures, contributing to rising sea levels and impacting global ocean currents and weather patterns. This speech explores the multifaceted significance of polar regions, emphasizing their role in climate regulation, biodiversity, and global security.

The polar regions act as Earth's natural refrigerators, reflecting sunlight and regulating the planet's temperature. The albedo effect, driven by the expansive ice cover, is essential for maintaining global thermal balance. However, diminishing ice due to climate change reduces this reflective capacity, accelerating global warming and creating feedback loops that exacerbate environmental changes worldwide. Polar regions are also biodiversity hotspots, home to unique flora and fauna adapted to extreme conditions. Species such as polar bears, penguins, seals, and various marine organisms depend on the icy habitat for survival. The intricate food webs and ecosystems in these regions are fragile and face unprecedented threats from climate change, pollution, and human activities, highlighting the urgent need for conservation efforts. Furthermore, the polar regions hold substantial geopolitical significance. The Arctic, rich in untapped natural resources like oil, gas, and minerals, is becoming a focal point for territorial claims and international disputes. The opening of new shipping routes due to melting ice also presents economic opportunities and challenges, necessitating robust international cooperation and governance to ensure sustainable and peaceful utilization of these areas.

Scientific research in polar regions provides invaluable insights into Earth's past, present, and future. Ice cores from glaciers and ice sheets offer records of atmospheric composition and climate conditions over millennia, aiding in the understanding of climate dynamics and human impact. The pristine environments also serve as natural laboratories for studying extreme life forms and potential analogs for extraterrestrial environments.

Organic Functional Dyes: Key Elements for a Sustainable Energy Transition?

NADIA BARBERO,^{a,b} IACOPO BENESPERI,^a MATTEO BONOMO,^a
FRANCESCA CARDANO,^a ANDREA FIN,^a SIMONE GALLIANO,^a PIERLUIGI
QUAGLIOTTO,^a CLAUDIA BAROLO,^{a,b,c}

^aDipartimento di Chimica and Centro Interdipartimentale NIS, Centro di Riferimento INSTM, Università di Torino, Via Pietro Giuria 7 and Via Quarellino 15a, Torino, Italia.

^bIstituto di Scienza Tecnologia e Sostenibilità dei Materiali Ceramici (ISSMC), CNR, Via Granarolo 64, Faenza, Italia.

^cCentro Interdipartimentale ICxT, Università di Torino, Lungo Dora 100, Torino, Italia.

*Corresponding author: claudia.barolo@unito.it

Abstract:

The transition to renewable energy sources and to more efficient energy-conversion devices is critical for addressing climate change and sustainable development. Nowadays most of the technologies for the transition are ready, but they still rely mostly on critical raw materials or on not completely sustainable production processes. For these reasons the mimicking of the light-matter interactions observed in Nature becomes an inspiration for interesting and fruitful research lines in science and technology to develop new sustainable “colored” materials.

In art and in everyday life, color is always inspiring and uplifting [1]. From the early ‘80s the term *Functional dyes* indicates dyes or pigments developed for purposes other than the classical coloration of substrates. The growth of this research, especially in the development of innovative molecules and materials for energy-related devices has been very fast and became the leitmotif of the research work of many groups [2].

This contribution will provide brief insights on the recently designed functional dyes with a specific emphasis on two different applications related to the energy transition:

- NIR dye-based dye-sensitized solar cells (NIR_DSSC) for transparent non-intrusive photovoltaic windows [3]
- sustainable bio-fluorophores in solid-state lighting [4]

Keywords:

Functional dyes, Renewable energy, DSSC, WHLED, photovoltaics

Acknowledgments:

The projects leading to these results have received funding from the European Union’s Horizon 2020 research and innovation program under grant agreement No 826013 (IMPRESSIVE) and No 863170 (ARTIBLED). This study is a result of the research project “nuovi Concetti, mAteriali e tecnologie per l’iNtegrazione del fotoVOLTaico negli edifici in uno scenario di generazione diffuSa” [CANVAS], funded by the Italian Ministry of the Environment and the Energy Security, through the Research Fund for the Italian Electrical System (type-A call, published on G.U.R.I. n. 192 on 18-08-2022) Authors acknowledge support from Project CH4.0 under the MUR program “Dipartimenti di Eccellenza 2023–2027” (CUP D13C22003520001).

References

- [1] P. Ball, *Bright Earth: The Invention of Colour*. 2011.
- [2] <https://www.moflabunito.com/>
- [3] F. Grifoni, M. Bonomo, W. Naim, N. Barbero, T. Alnasser, I. Dzeba, M. Giordano, A. Tsururyan, M. Urbani, T. Torres, C. Barolo, and F. Sauvage *Adv. En. Mater.* **2021**, *11*, 2101598; <https://impressive-h2020.eu/>
- [4] L. M. Cavinato, S. Wölfl, A. Pöthig, E. Fresta, C. Garino, J. Fernandez-Cestau, C. Barolo, and R. D. Costa *Adv. Mater.* **2022**, *34*, 2109228; <https://bfm.cs.tum.de/research/artibled/?lang=en>

Deep Eutectic Solvents as a Greener Materials Approach and Electrochemical Applications

CHRISTOPHER BRETT

Department of Chemistry, University of Coimbra, Portugal

Abstract:

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.

[1] D.J. Ramón, G. Guillena, (Eds.) *Deep eutectic solvents. Synthesis, properties and applications*. Wiley-VCH, Weinheim, 2020.

[2] C.M.A. Brett, *Curr. Opin. Electrochem.*, **2024**, *45*, 101465.

[3] X. Liang, Y. Zhou, J.M.S. Almeida, C.M.A. Brett, *J. Electroanal. Chem.*, **2023**, *936*, 117366.

[4] R.S. Zouleh, M. Rahimnejad, G. Najafpour-Darzi, D. Sabour, J.M.S. Almeida, C.M.A. Brett, *Microchem. J.*, **2023**, *195*, 109475.

Microalgae as Cellular Factories: From Biofuels to High-Added Value Compounds

SAMORÌ CHIARA

*Dipartimento di Chimica “Giacomo Ciamician”, Alma Mater Studiorum – Università di Bologna
chiara.samori3@unibo.it*

Abstract:

Today the main resources providing energy in the world are gas, coal and mineral oil. The use of these resources is continuously expanding to provide the growing populations and economies of the world with their increasing demands of energy. This is especially true for the global transport of goods and people. A new, sustainable energy supplier is needed, that can preferably be incorporated or linked to the existing energy infrastructure. Energy derived from purposely grown biomass potentially offers a (partial) solution to this challenge. An important role is foreseen for biofuels in the future supply of energy and transportation fuels (SET plan). In the past years, markets for so-called 1st generation (food-related) biofuels have been created in Europe (mainly biodiesel) and the USA (corn ethanol). Concerns about the side effects of these markets, e.g. influencing global food markets (by crop displacement) and increased prices are not unrealistic. If the scale of these markets would be expanded further, additional challenges arise, e.g. supply shortages in agricultural fertilizers (N and esp. P) and fresh water. A key indicator for biomass-derived energy carriers should therefore be the avoidance of any negative influence on food markets through land, crop, water or nutrient use.

Algae can be defined as unicellular, colonial or filamentous microorganisms, photosynthetic or heterotrophic, containing chlorophylls and other pigments. Depending on the species, their size can vary from a few micrometres to a few hundred micrometres. They are the fastest-growing organisms on earth, and distinctly different from higher plants as they lack stems, roots and leaves. Microalgae play a pivotal role in the oceanic food chains and in sustaining Earth's ecosystems. In addition to ecological and environmental benefits, many microalgal species are cellular factories that produce unique and high-added value bioproducts like photosynthetic pigments/proteins, carotenoids, polyunsaturated triacylglycerols, bioactive compounds, polysaccharides, and even biopolymers with plastic-like properties. These bioproducts are industrially exploited in “functional food” preparation, cosmetics, aquaculture, pharmaceuticals, or food technology. Moreover, after the recovery of highadded value compounds, algal biomass can be used as feedstock for producing energy or fertilizers, in a « zero-waste » framework. Although high in potential, when compared to 1st and 2nd generation biofuels, algae fuel technology still has several hurdles to overcome. Many aspects of industrial-scale microalgae cultivation have been proven technologically feasible by numerous research initiatives and (start-up-) companies, but no large-scale industrial initiative for fuels from microalgae exists at present. Most existing concepts are based on the limited lipid fraction of microalgae, supplemented by only a small added value from biogas, produced by co-digestion of algal debris (which represents up to 90 wt% of the algae biomass). When compared on revenue per energy output basis, oil-type products represent a fivefold higher value than biogas. However, other products from the non-lipid fraction, preferably more liquid fuels, are required to make algae cultivation economical and to reduce land use. Microalgae cultivation is a challenging process. Traditionally, microalgae are cultivated on a large scale in open ponds, thanks to reduced production costs but with the strong drawback of small productivity and, mostly, of being this cultivation process only partially controlled. Alternatively, the utilization of photobioreactors, i.e. closed systems allows accurate process control, reduces the risk of contamination and provides high volumetric productivity; however, these cultivation processes are characterized by very high operating costs.

Additionally, biomass collection and downstream treatment are challenging both at the technical, economic and environmental levels, thus claiming to develop new greener and innovative approaches. Most state-of-the-art processes rely on organic solvent extraction of the freeze-dried algal mass; however high energy input and environmental and safety concerns are associated with these technologies. Moreover, the purity requirements for products that are addressed to humans, require the development of new green technologies able to replace the traditional extraction methods.

Another drawback of many existing technologies based on microalgae is the “one target” approach: only a single product is obtained by exploiting a rigid technology. This contrasts with the integrated biorefinery strategy that is reputed as the only win-win strategy in the field of renewable sources. Finally, a lack of specific regulation to guarantee quality is also a barrier to the effective market development of microalgae-derived products: in fact, many microalgae products available in large amounts on the market are characterized by low quality (i.e. heavy metals, bacterial or animal contamination).

Keywords:

Microalgae, biodiesel, harvesting, carotenoids, green solvents, high-added value compounds

Enabling Technologies for Chemical Process Intensification, Scalability of Green Procedures

GIANCARLO CRAVOTTO

*Dip.to di Scienza e Tecnologia del Farmaco, University of Turin, via P. Giuria 9, 10125 Turin.
giancarlo.cravotto@unito.it*

Abstract:

Currently, the sustainability of chemical processes is driving innovation and industrialization in accordance with environmental friendliness, energy efficiency and scalability. Among emerging technologies, continuous-flow chemistry has become mainstream in the development of innovative, highly efficient catalytic syntheses of fine chemicals and active pharmaceutical ingredients (APIs) [1]. Unfortunately, the reproducibility and the claimed scalability reported in several papers are often proven wrong. Conventional conductive heating and mixing in batch reactors is no longer competitive with continuous-flow synthetic methods, and enabling technologies applied in flow mode can strongly promote reaction kinetics [2]. These advances are leading to faster and simplified downstream processes with easier workup, purification, and scaling-up. In the current Industry 4.0 revolution, new advances based on cyber-physical systems and artificial intelligence will be able to optimize and invigorate synthetic processes by combining cascade reactors with continuous inline monitoring and even predicting solutions in case of unforeseen events. Alternative energy sources such as dielectric [3,4] and ohmic heating [5], ultrasound [6], hydrodynamic cavitation [7], ball milling [8] reactive extruders [89] and plasma [10] have revolutionized standard processes. Also worth mentioning are the so-called hybrid or hyphenated techniques, where the combination of two different energy sources often produces synergistic effects. Relevant case studies at pilot and semi-industrial scale of continuous or semi-continuous extraction and synthetic processes under non-conventional techniques will be discussed.

Keywords:

Non-conventional energy sources; Process intensification; Scaling up; Sustainable protocols; Continuous-flow chemistry; Pilot and semi-industrial scale reactors.

References:

- [1] M. Comito, R. Monguzzi, S. Tagliapietra, A. Maspero, G. Palmisano, G. Cravotto, *Pharmaceutics*, **2023**, *15*, 1322.
- [2] G. Grillo, P. Cintas, M. Colia, E. Calcio Gaudino, G. Cravotto, *Front. Chem. Eng.* **2022**, *4*, 966451.
- [3] K. Martina, G. Cravotto, R.S. Varma, *J. Org. Chem.* **2021**, *86*, 13857-13872.
- [4] M. Salgado-Ramos, S. Tabasso, E. Calcio Gaudino, G. Cravotto, *Ind. Eng. Chem. Res.* **2024**, *63*, 7507.
- [5] V.L.M. Silva, L.M. Santos, A.M.S. Silva, *Chem. Eur. J.* **2017**, *23*, 7853.
- [6] R.F. Martínez, G. Cravotto, P. Cintas, *J. Org. Chem.* **2021**, *86*, 13833.
- [7] Z. Wu, S. Tagliapietra, A. Giraud, K. Martina, G. Cravotto, *Ultrason. Sonochem.* **2019**, *52*, 530-546.
- [8] L. Jicsinszky, F. Rossi, R. Solarino, G. Cravotto, *Molecules* **2023**, *28*, 467.
- [9] E. Calcio Gaudino, G. Grillo, M. Manzoli, S. Tabasso, S. Maccagnan, G. Cravotto, *Molecules* **2022**, *27*, 449
- [10] F. Verdini, E. Canova, R. Solarino, E. Calcio Gaudino, G. Cravotto, *Environ. Pollut.* **2024**, *342*, 123041.

Toward a More Sustainable Membrane Fabrication

ALBERTO FIGOLI, FRANCESCA RUSSO, FRANCESCO GALIANO

Institute on Membrane Technology, National Research Council of Italy,

Via P. Bucci 17c, Rende (CS) Italy

**Corresponding author: alberto.figoli@cnr.it*

Abstract:

Environmental protection and climate change are current issues at the heart of global economic growth. The awareness of the real risks connected with industrial membrane production sector has been the push towards the search of new, more sustainable, solvents and raw materials [1]. The 5th principle of Green Chemistry encourages the use of safer solvents and auxiliaries [2]. Solvents are the most common example of auxiliary substances for membrane preparation *via* phase inversion. They are needed for dissolving the selected polymer and their chemical-physical properties strongly influence the membrane formation too. Among the most widely used solvents, N,N-dimethyl formamide (DMF), N,N-dimethyl acetamide (DMAc) and N-methyl pyrrolidone (NMP), represent an excellent choice for dissolving polyvinylidene fluoride (PVDF) and sulfones polymers. However, since they are classified as highly reprotoxic and developmental harmful, their use should be avoided whenever possible. In this context, the use of alternative, less-toxic, diluents for making polymeric membranes open new perspectives for the sustainable membrane fabrication. Herein, the main techniques and properties of solvents to be used in membrane fabrication, and case studies on membrane production via Non-solvent- coupled with Vapor-Induced Phase Inversion using different innovative non-toxic solvents, such as, dimethyl isosorbide (DMI) [3] and CyreneTM (dihydrolevoglucosenone) [4] and dimethyl isosorbide (DMI), will be discussed in details. These solvents are completely miscible with water and alcohols; their high boiling point make them a favorable alternative for dissolving polysulfones, as PES or PSU, as well as fluoropolymers, such as PVDF, sulfones, by using different coagulation bath. The possibility of tuning the morphology and pore size of the polymeric membranes produced by using these polymers will be reported too. Finally, the new frontier toward the fabrication of membranes completely greener, substituting also traditional polymers as PVDF and PSU with biopolymers, will be also discussed.

Keywords:

Polymeric membranes, Membrane preparation, Green solvents, Biopolymers,

Acknowledgments:

The authors acknowledge the project FOE-FUTURAW – CUP B53C23008390005

References:

- [1] A. Figoli, T. Marino, S. Simone, E. Dinicolò, X.-M. Li, T. He, S. Tornaghi, E. Drioli, Towards non-toxic solvents for membrane preparation: a review, *Green Chemistry*, **2014**, 16, 4034-4059;
- [2] P. T. Anastas et al., *Green Chemistry: Theory and Practice*, Oxford Univ. Press New York, **1998**;
- [3] F. Russo, F. Galiano, F. Pedace, F. Aricò, A. Figoli, Dimethyl Isosorbide As a Green Solvent for Sustainable Ultrafiltration and Microfiltration Membrane Preparation, *ACS Sustain. Chem. Eng.*, **2020**, 8, 659–668;
- [4] P. Tomietto, F. Russo, F. Galiano, P. Loulergue, S. Salerno, L. Paugam, J.-L. Audic, L. De Bartolo, A. Figoli, Sustainable fabrication and pervaporation application of bio-based membranes: Combining a polyhydroxyalkanoate (PHA) as biopolymer and CyreneTM as green solvent, **2022**, 643, 120061.

Chemicals of War and the Chemistry of Peace: Eliminating the World's Chemical Weapons Stockpiles and the Legacy Left Behind

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*

Abstract:

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

Catalyzing the Green Revolution: Unlocking Previously Inaccessible Chemical Processes

JAVIER GARCÍA-MARTÍNEZ

Laboratorio de Nanotecnología Molecular, Dpto. Química Inorgánica, Universidad de Alicante, Ap. 99, E-03690 Alicante, Spain

Abstract:

The development of intracrystalline mesoporosity within zeolites has been a long-standing goal in catalysis as it greatly contributes to alleviating the diffusion limitations of these widely used microporous materials. During my presentation, I will discuss the main techniques that have been developed during the last years to produce zeolites with controlled mesoarchitectures comparing the different methods, their advantages and limitations. Among the different techniques used to characterize the composition, porosity and structure of these materials, I will present unprecedented insights on the formation of intracrystalline mesoporosity in zeolites obtained by *in situ* synchrotron X-ray diffraction, Atomic Force Microscopy (AFM), and Liquid Cell Transmission Electron Microscopy (Liq-TEM). By combining experimental results and theoretical calculations, the presence of intracrystalline mesoporosity was recently confirmed. Moreover, through the direct observation of individual zeolite crystals by *in situ* AFM and Liq-TEM, we have been able to provide the first time-resolved visualization of the formation of mesoporosity in zeolites.

During the presentation, I will describe a new strategy for the synthesis of superior hierarchical catalysts, which lack long-range order but at local scale contain zeolite building units. [1,2] In fact, they are made out of fragments of one or even various zeolite structures and display improved accessibility, strong acidity, and excellent stability. Because of these features, they effectively catalyze reactions involving very bulky molecules, which currently are produced using highly corrosive homogenous catalysts (Fig. 1). To achieve this goal, we built on a well-known technique, namely the interconversion of zeolites, which we interrupted at different times to yield the desired amounts of building units of the zeolites involved. The addition of quaternary ammonium surfactants during their preparation allows the development of well-defined mesoporosity and large surface areas. Using this simple procedure, we were able to produce families of materials with controlled amounts of different zeolitic building units and, consequently, optimize their catalytic performance for various reactions including Friedel-Crafts alkylations and Claisen-Schmidt condensations, and the cracking of 1,3,5-triisopropylbenzene.

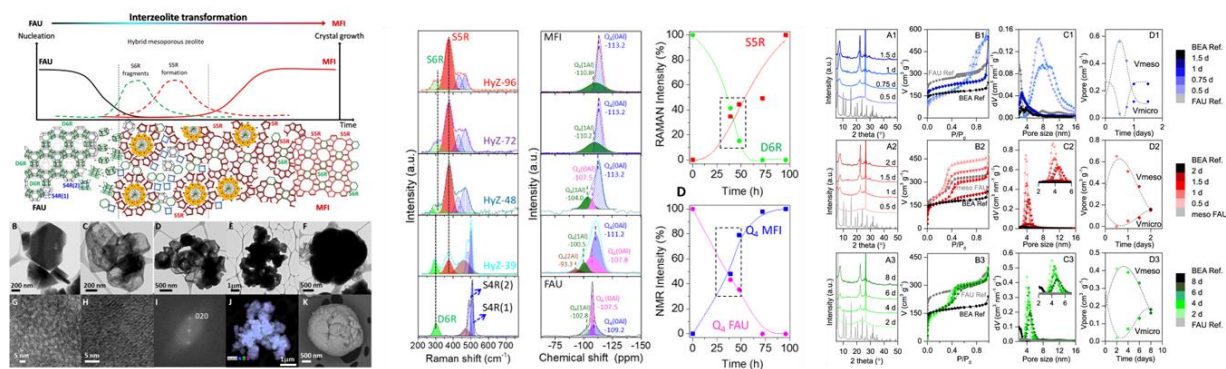


Figure 1. Textural, structural, and morphological characterization of some intermediates of the interconversion of zeolite FAU into MFI and BEA structures.

An important advantage of this strategy is that the physicochemical properties and, therefore the catalytic performance, of the hierarchical catalysts can be finely tuned by simply stopping the interzeolite transformation at different times. This creates countless opportunities for the development of hierarchical catalysts [3] with optimized properties and superior catalytic performance for those reactions in which zeolites present significant

diffusion limitations (Fig. 1). This paves the way for the fabrication of hybrid hierarchical catalysts with optimized properties for those processes in which the combined use of different zeolites yields improved performance.

The presence of this mesoporosity was further evidenced through *ex situ* gas adsorption, which also confirmed the preservation of most of the microporosity of the zeolites. All these new insights, obtained by combining a number of time-resolved techniques, are an example of the enormous potential of current *in situ* characterization methods for the rational design of hierarchical zeolites with superior properties and optimal catalytic performance as it has been proved at lab, pilot plant, and industrial scale.

In several operations in a number of refineries, a steady increase in LPG olfinicity was observed when replacing the incumbent FCC catalyst with another containing our mesostructured Y zeolite. Commercial data confirmed what we observed in equilibrium catalysts, i.e. a gradual increase in the LPG olefinicity, as the concentration of the FCC catalyst containing mesostructured Y zeolite in the circulating inventory steadily increased. Furthermore, a very valuable increase in gasoline octane is typically observed due to a higher concentration of olefins in the lighter gasoline fraction.

The commercialization of hierarchical zeolites, first through the MIT spin-off Rive Technology and now by Shell and GRACE, as superior refining catalysts is an example of academic entrepreneurship, which is expected to foster the development of new hierarchical zeolites and their use in both existing processes and new opportunities. Finally, I cover other applications of hierarchical zeolites in catalysis, including biomass valorization and fine chemistry, ending with a personal view of the new directions, and opportunities in this field.

Keywords:

Catalysis, Green Chemistry, Zeolites, Mesoporous Solids, Hybrid Materials, Advanced Characterization Techniques, and Entrepreneurship

Acknowledgements:

The author would like to acknowledge the support provided by the European Union's Horizon 2020 research and innovation program under grant agreement No 872102 and the Generalitat Valenciana for the project GRISOLIAP/2020/165.

References:

- [1] M. Mendoza-Castro, Z. Qie, N. Linares, J. García-Martínez, *Nat. Comm.*, DOI: 10.1038/s41467-023-36502-3
- [2] M. Mendoza-Castro, E. De Oliveira-Jardim, N.T Ramírez-Márquez, C. A. Trujillo, N. Linares, J. García-Martínez, *J. Am. Chem. Soc.* **2022**, 144, 11, 5163–5171.
- [3] A. Sachse, J. García-Martínez, *J. Chem. Mater.* **2017**, 29 (9), 3827– 3853.

Packaging Plastics in the Circular Economy

GAETANO GUERRA

*Università di Salerno, Dipartimento di Chimica e Biologia, Via Giovanni Paolo II 132, 84084 Fisciano (SA),
gguerra@unisa.it*

Abstract:

The contribution is mainly based on the report of the European Academies Science Advisory Council (EASAC) on "Plastics & Circular Economy" of March 2020,¹ update on February 2024.²

EASAC is a body that provides scientific advice for the benefit of Europe and involves the National Scientific Academies of the EU states and Norway and Switzerland (for Italy, the Accademia Nazionale dei Lincei).

Emphasis will be given above all to the suggestions of the EASAC report to improve the technical and economic feasibility of recycling, starting from the concept of **design aimed at recycling** ('design for recycling'). In this short summary, only the most relevant EASAC tips are indicated: - Limitation in the use of multi-material packaging

- Limitation in the use of dark colors, which make separation by optical techniques (NIR) difficult.
- Limitation in the types of polymers to be used for specific applications.
- Use of pure polymers (avoiding "blends" and special products, for large volume applications)

Different methods of chemical recycling will be shortly compared:

Depolymerization: re-obtaining monomers from pre-sorted polymers

Pyrolysis: thermal decomposition in the absence of air

Gasification: thermal decomposition in the presence of air

Some emphasis will be also given to **polymer upgrading** processes, i.e. processes that increase (rather than reduce) the molecular mass (chain length) of post-consumer polymers. Upgrading is expected to be particularly helpful for a true circular economy, because it allows recycling in the same application that generated the waste.

References:

1. <https://easac.eu/publications/details/packaging-plastics-in-the-circular-economy>
2. <https://easac.eu/publications/details/update-on-the-easac-plastics-report-towards-a-plastics-tre-aty>

Conversion of CO₂, Biomass, and Waste Plastics into Chemicals and Fuels

BUXING HAN

*Institute of Chemistry, Chinese Academy of Sciences, 100190, Beijing, China
Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular
Engineering, East China Normal University, Shanghai 200062, China
Email: hanbx@iccas.ac.cn*

Abstract:

Carbon dioxide (CO₂) is the main greenhouse gas, and it is also a renewable, abundant, and cheap C₁ feedstock. Biomass is abundant renewable carbon resource. Use of biomass and CO₂, and waste plastics as carbon sources to produce fuels and value-added chemicals is of great importance for the sustainable development of our society. In recent years, we are very interested in catalytic conversion CO₂, biomass, and waste plastics. In this lecture, I would like to discuss green chemistry, and some of the recent results in our group on design of green solvent-catalyst systems and their application in conversion of CO₂, biomass, and waste plastics into valuable chemicals and fuels.

Keywords:

Transformation, Carbon dioxide, Biomass, Waste plastics, Chemical, Fuel

Green Hydrogen Generation from Solar Water Splitting over Metal Oxynitrides

MIRABBOS HOJAMBERDIEV

Institut für Chemie, Technische Universität Berlin, 10623 Berlin, Germany

**Corresponding author: hmirabbos@gmail.com*

Abstract:

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

Acknowledgements:

This project received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement no. 793882.

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*

Abstract:

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, metrics, research strategy

Sustainable Chemistry as the Overarching Guiding Principle to Embed Chemistry into Sustainability

KLAUS KÜMMERER

Institute of Sustainable Chemistry, Faculty of Sustainability, Leuphana University, Universitätsallee 1, 21335 Lüneburg, Germany
Klaus.Kuemmerer@leuphana.de

Abstract:

Chemistry is indispensable for a high standard of living and health. For long time chemistry came along with heavy environmental pollution by toxic waste, exhausts, and effluents from production. In the 1980ies and early 1990ies several approaches were developed by many individuals and organizations and manifested as legislation [1] and summarized in the 12 principles of Green Chemistry (GC) [2]. These are important for a greener synthesis and less hazardous chemicals. However, several shortcomings of GC become obvious when a broader systems view is applied [3-5]. This includes among other that total substance flows, total resource needs, limitations of renewables, the need to use metals which are non-renewable, circular economy (CE) and sustainability are not addressed by GC.

Recently, 12 principles of circular chemistry (CC) were introduced [6]. Half of them is very similar to some of the principles of GC. Others address CE issues and call for application of the ladder of circularity. CC promises a waste free chemical industry. While GC and CC are indispensable for a greener future, they are not sufficient. Not every process or product which is greener or more circular is necessarily more sustainable. Both, circulation and recycling come a long with certain severe and insurmountable limitations, which are rooted in thermodynamics [7]: There is neither up-cycling, nor is energy endlessly available, there are always losses of energy and materials. There is no waste free circulation, neither recycling and industry and consumption. To minimise these unavoidable losses, products must be designed for circulation and recycling from the very beginning (Benign by Design) [8]. In addition, it is obvious that substance, material, and products flows must be reduced in size, dynamics and complexity with respect to composition, size, space and time [5,7-11]. On top of this, many products cannot be recycled, e.g. personal care products, pharmaceuticals, pesticides, disinfectants, detergents, abrasions from surfactants, additives released during use from plastics, and many others as they enter the environment unavoidably due to their use or at the end of their life. Such products must be designed for complete and fast mineralization in the environment at the end of their life (Principle #10 of GC, design for degradation (Benign by Design) [12-15]. To allow for a sustainable contribution of chemistry to Sustainable Development [16] a new radical understanding of chemistry is needed, which is Sustainable Chemistry (SC) [5,17]. It enables chemistry to contribute in a sustainable manner to sustainability. To do so the very first question has to ask for service and function needed and whether non-chemical alternatives (e.g. different design, behaviour, construction, alternative business model) could provide the service or if a chemical only can provide it. If a chemical product is needed its end of life has to be identified first based on whether it will be used within CE or whether it cannot be circulated or recycled and will enter the environment. In both cases products have to be designed even before synthesis accordingly from the atomic to the molecular, material building bloc and product level for circulation and recycling or fast and full environmental mineralisation. The final step, only, then is of synthesis of individual chemicals according to the 12 principles of GC. SC Includes systems thinking and all stakeholders along the whole life cycle of products and services. Ethical considerations and social aspects are important parts of it, too. This holds for research, education and industrial practice [18-20] to allow chemistry of the future to contribute to sustainability in a sustainable manner.

Keywords:

Green chemistry, circular chemistry, sustainable chemistry, circular economy, benign by design, sustainable development goals, planetary boundaries

References:

- [1] <https://eur-lex.europa.eu/legal-content/EN/TXT/PDF/?uri=CELEX:31996L0061>
- [2] <https://www.epa.gov/greenchemistry/basics-green-chemistry#definition>
- [3] Mahaffy, P.G. Matlin, S.A. Holme, T.A. MacKellar, J. *Nature Sustainability* **2019**, 2, 362–370
- [4] Constable, J. C. Jiménez-González, C. Matlin, S.A. *Journal of Chemical Education*, **2019**, 96, 2689-2699
- [5] K. Kümmerer, *Angewandte. Chemie. International Edition* **2017**, 56, 16420-16420
- [6] Keijer, T. Bakker, V. Slootweg, J.C. *Nature Chemistry* **2019**, 190-195
- [7] Lehmann, H. Hinske, C. de Margerie V., Slaveikova Nikolova A. (Eds.) *The Impossibilities of the Circular Economy Separating Aspirations from Reality* **2023**, Routledge
- [8] Kümmerer, K. Zuin V.G, Clark J.H. *Science* **2020**, 367, 369-370
- [9] Zuin, V.G. Kümmerer, K., *Nature Reviews Chemistry* **2021**, 5, 76–77
- [10] Zuin, V.G. Kümmerer, K. *Nature Reviews Materials* **2022**, 7, 76–78
- [11] Persson, L. Carney Almroth, B.-M., Collins C.D., Cornell, S. de Wit C.A., Diamond M.L., Fantke, P., Hassellöv, M. MacLeod, M. Ryberg, M.W. Søggaard Jørgensen, P. Villarrubia-Gómez P. Zhanyun, W. Zwicky Hauschild, M. *Environmental Science and Technology*, **2022**, 56, 1510–1521
- [12] Kümmerer K., *Green Chemistry*, **2007**, 9, 899-907
- [13] Kümmerer, K. Dionysiou, D.D. Olsson, O. Fatta-Kassions, D. *Science* **2018**, 361, 222-224
- [14] Leder C. Suk, M. Lorenz, S. Rastogi, T. Pfeifer, C. Kietzmann, M. Jonas, D. Buck, M. Pahl, A. Kümmerer, K. *ACS Sustainable Chemistry and Engineering*, **2021**, 9, 9358–9368
- [15] Suk, M. Kümmerer, K. *Green Chemitry*, **2023**, 25, 365-374
- [16] <https://sdgs.un.org/goals>
- [17] Kümmerer, K., Amsel, A.-K. Bartkowiak, D. Bazzanella, A. Blum, C. Cinquemani C. *Key Characteristics of Sustainable Chemistry. Towards a Common Understanding of Sustainable Chemistry*. Dialogue Paper by the International Sustainable Chemistry Collaborative Centre (ISC3), 2021, https://www.isc3.org/cms/wpcontent/uploads/2022/06/ISC3_Sustainable_Chemistry_key_characteristics_20210113.pdf
- [18] Wissinger, J. E. Visa, A. Saha, B. B. Matlin, S. A. Mahaffy, P. G., Kümmerer, K. Cornell, S., *Journal of Chemical Education*, **2021**, 98, 1061-1063
- [19] E.g. <https://www.leuphana.de/en/professional-school/masters-studies/sustainable-chemistry.html>, <https://www.leuphana.de/en/professional-school/masters-studies/sustainable-chemistry-management.html>

Ionic Liquids: The Good, The Bad and The Ugly

PETER LICENCE

School of Chemistry, University of Nottingham, United Kingdom

Abstract:

Room Temperature Ionic Liquids are sterically hindered organic salts that exhibit melting points below the boiling point of water. Because they are composed entirely of ions, ionic liquids have almost zero vapour pressures and do not evaporate even under a vacuum! This feature set alongside the large liquid-ranges observed for many ionic liquids has led to them being characterised as Green Solvents. Furthermore, structural diversity in the ionic components that can be brought together to form simple binary salts and mixtures, each with a unique set of physical and chemical properties, has led to them becoming known as designer solvents which could, in principle, be designed or engineered with a specific reaction or process in mind. This lecture will give an overview of the basic physical chemistry that underpins the field of ionic liquid based chemistry, I will challenge the perception that these liquid solvents are indeed green and attempt to give examples where ionic liquid based technologies deliver advantages that may not be achieved using more traditional solvent systems. I will explore opportunities to control chemistry via systematic ion choice and demonstrate the designer nature of simple systems to control physical parameters. I will close with a brief overview of the impacts of science-based research across multiple scales, including a whole laboratory scenario.

References:

- K. R. J. Lovelock, I. J. Villar-Garcia, F. Maier, H.-P. Steinrück and P. Licence, *Chem. Rev.*, 2010, 110, 5158-5190.
- I. J. Villar-Garcia, E. F. Smith, A. W. Taylor, F. Qiu, K. R. J. Lovelock, R. G. Jones and P. Licence, *Phys. Chem. Chem. Phys.*, 2011, 13, 2797-2808.
- I. J. Villar-Garcia, K. R. J. Lovelock, S. Men and P. Licence, *Chem. Sci.*, 2014, 5, 2573-2579.

Catalytic Aerobic Oxidations: From Simple Organic Reactions to Biomass Valorization

GIULIA LICINI

Dipartimento Scienze Chimiche, Università di Padova, via Marzolo, 1, 35131, Padova Italy

*giulia.licini@unipd.it

Abstract:

Oxidative carbon-carbon bond cleavage of vicinal diols yielding carbonyl compounds is a fundamental reaction in organic synthesis [1] as well as in lignin-cellulose valorization and the general context of renewable feedstock transformation. [2] The design of more efficient and environmentally benign aerobic catalytic processes for the C-C bond cleavage of diols is still a topic of key importance and it will be a topic of the present lesson. Starting from the stoichiometric processes (high-valent inorganic oxidants, like periodates, [3] or lead tetracarboxylates.[4]) we will describe more recent examples dealing with catalytic aerobic oxidative reactions using different catalysts (manganese [5], cerium[6], silver [7], etc.) and we will describe the results obtained in our lab relative to the use of vanadium aminotriphenolate complexes [(V)-TPAs] as aerobic redox-catalysts in organic solvents [8] and micellar medium [9] at high temperatures and also photocatalytic conditions. Optimization and applications of the catalytic system to a series of substrates of increasing complexity together with reaction mechanism studies (kinetic studies, isotope effect, DFT calculations) will be presented (Figure 1).

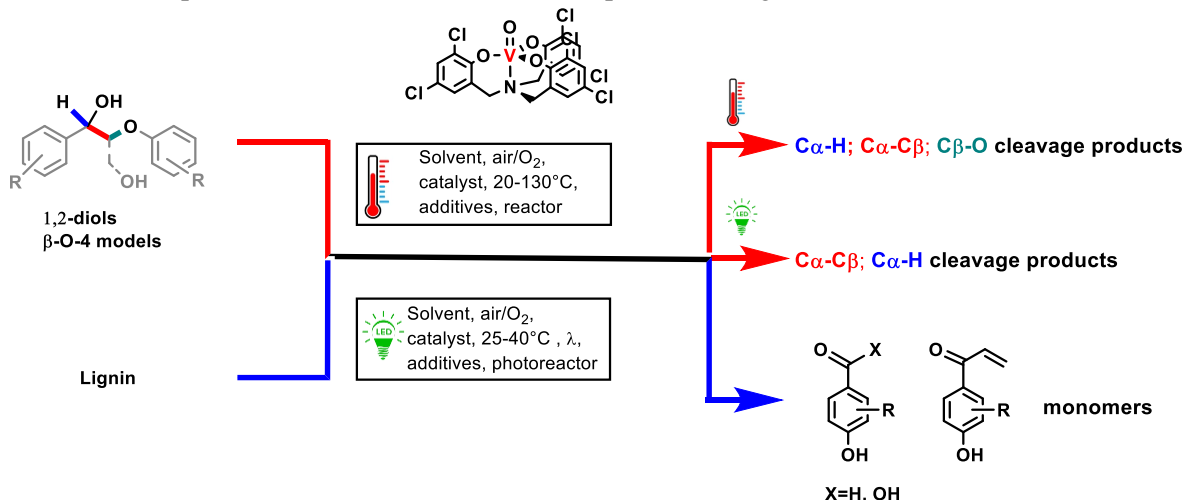


Figure 1. (V)-TPAs aerobic oxidation of 1,2-diols, lignin models and lignin under thermo and photocatalytic conditions.

Keywords:

aerobic oxidation, 1,2-diols, C-C bond cleavage, catalysis, vanadium, aminotriphenolates

Acknowledgements:

This study was carried out within the MICS (Made in Italy- Circular and Sustainable) Extended Partnership and received funding from Next-Generation EU (Italian PNRR - M4 C2, Invest 1.3 - D.D. 1551.11-10-2022, PE00000004).

References:

- [1] A. H. Haines, *Methods for the Oxidation of Organic Compounds: Alcohols, Alcohols Derivatives, Nitroalkanes, Alkyl Azides, Carbonyl Compounds, Hydroxyarenes and Aminoarenes*, Academic Press, London, **1988**, pp 277–304.
- [2] M. D. Karkas, B. S. Matsuura, T. M. Monos, G. Magallanes, C. R. J. Stephenson, *Org. Biomol. Chem.* **2016**, *14*, 1853–1914; and references therein.

- [3] A. Sudalai, A. Khenkin, R. Neumann, *Org. Biomol. Chem.* **2015**, *13*, 4374–4394;
- [4] E. Baer, J. M. Grosheintz, H. O. L. Fischer, *J. Am. Chem. Soc.* **1939**, *61*, 2607–2609;
- [5] V. Escande, C.H. Lam, C. Grison, P.T. Anastas, *ACS Sustainable Chem. Eng.* **2017**, *5*, 3214–3222; V. Escande, C.H. Lam, P. Coish, P.T. Anastas, P. T. *Angew. Chem., Int. Ed.* **2017**, *56*, 9561–9565.
- [6] Schwarz, J.; König, B. *Chem. Commun.* **2019**, *55*, 486–48866
- [7] Zhou, Z.; Liu, M.; Lv, L.; Li, C.-J. *Angew. Chem., Int. Ed.* **2018**, *130*, 2646–2650.
- [8] Amadio, E.; González-Fabra, J.; Carraro, D.; Denis, W.; Gjoka, B.; Zonta, C.; Bartik, K.; Cavani, F.; Solmi, S.; Bo, C.; Licini, G. *Adv. Synth. Catal.* **2018**, *360*, 3286–3296;
- [9] Carpentier, R. Denis, W. Sanz Azcona, F., Carraro, D., Grauwels, G. Orlandi, M., Zonta, C., Licini, G., Bartik *ACS Sustainable Chem. Eng.* **2023**, *11*, 8633–8641.

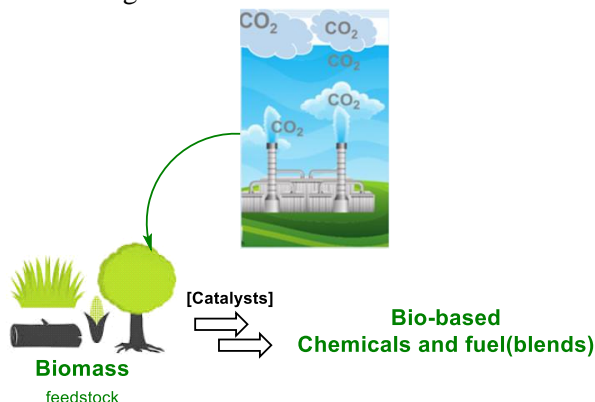
Harnessing Renewable Carbon Sources: Catalytic Strategies for Biomass and Carbon Dioxide Conversion

BANOTHILE C.E. MAKHUBELA

Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, Faculty of Science, University of Johannesburg, Auckland Park 2006, South Africa. email: bmakhubela@uj.ac.za

Abstract:

Carbon dioxide (CO₂) is the primary greenhouse gas, but it also serves as a renewable, abundant, and inexpensive single-carbon feedstock. Similarly, biomass is an abundant and renewable carbon resource. The transformation of biomass into versatile platform chemical products has garnered significant interest in industry and academia. This focus aligns with global efforts to increase the use of renewable chemicals and fuels, thereby reducing reliance on fossil-derived products. Utilizing CO₂ and biomass as carbon sources to produce fuels and value-added chemicals is essential for the development of a sustainable future and for achieving carbon neutrality. In recent years, our research has focused on the catalytic conversion of CO₂ and biomass. In this presentation, I will discuss some of our recent results, particularly the design of green solvents, homogeneous and heterogenized homogeneous catalysts, and their application in converting CO₂ and biomass into valuable chemicals and fuels.



Acknowledgements:

Funding by the National Research Foundation of South Africa is acknowledged.

References:

1. Centi G. and van Santen, R.A., *Catalysis for Renewables: From Feedstock to Energy Production*, 2007, Wiley-VCH Verlag GmbH and Co. KgaA, pp 1-46.
2. Chheda, J.N. and Dumesic, J.A., *Catalysis Today*, 2007, **123**, 59.
3. H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S.B. Choi, E. Choi, A.Ö. Yazaydin, R. Q. Snurr, M. O’Keeffe, J. Kim, O.M. Yaghi. *Science*. 2010, **329**, 424.
4. Makhubela, B.C.E. and Darkwa J., *Johnson Matthey Technol. Rev.*, 2018, **62**, 4.
5. Amenuvor, G.; Makhubela, B. C. E.; Darkwa, J., *Catal. Sci. Technol.*, 2018,,**8**, 2370.
6. P. Tshuma, B.C.E. Makhubela, N. Bingwa, G. Mehlana. *Inorg.Chem.*, 2020, **59**, 6717-6728.
7. Matsheku, A.C.; Maumela, M.C. Makhubela B.C.E., *RSC Sustainability*, 2023, **1**, 1471.
8. M. Gumbo, E. Ocansey, B.C.E. Makhubela, F.M. Amombo Noa, L. Ohrström, O.S. Mudrajid, G. Mehlana. *Sustainable Energy Fuels*, 2024, **8**, 777.

Towards Green Atom Transfer Radical Polymerization

KRZYSZTOF MATYJASZEWSKI

Carnegie Mellon University, Center for Macromolecular Engineering, Pittsburgh, PA, 15213, USA
matyjaszewski@cmu.edu

Abstract:

Fundamentals of copper-catalyzed ATRP (atom transfer radical polymerization) will be presented. Recently, by applying new initiating/catalytic systems, the Cu level in ATRP was reduced to a few ppm. To combat unavoidable radical termination, several techniques for the regeneration of the catalytic systems have been developed. They include various benign chemical reagents such as ascorbic acid or sugars but also external stimuli: electrical current, light, mechanical forces and ultrasound. ATRP was carried out without organic solvents, in bulk and in aqueous media under homogeneous conditions or in dispersed media. Reducing agents and enzymes permit the reaction without deoxygenation in the flasks open to the air.

The range of monomers for ATRP has been expanded to (meth)acrylates and acrylamides made from renewable resources. They have been used for the synthesis of well-defined polymers with precisely controlled molecular architecture with designed shape, composition, and functionality. Block, graft, star, hyperbranched, gradient and periodic copolymers, molecular brushes, and various hybrid materials or bioconjugates were prepared. Some examples of nanostructured multifunctional hybrid materials for applications related to environment, energy, and biomedicine will be presented.

References:

- (1) Moini Jazani, A.; Rawls, C.; Matyjaszewski, K., Photo-RDRP for everyone: Smartphone light-induced oxygen-tolerant reversible deactivation radical polymerization, *European Polymer Journal* **2024**, *202*, 112631. <http://dx.doi.org/https://doi.org/10.1016/j.eurpolymj.2023.112631>.
- (2) Hu, X.; Szczepaniak, G.; Lewandowska-Andralojc, A.; Jeong, J.; Li, B.; Murata, H.; Yin, R.; Jazani, A. M.; Das, S. R.; Matyjaszewski, K., Red-Light-Driven Atom Transfer Radical Polymerization for High-Throughput Polymer Synthesis in Open Air, *Journal of the American Chemical Society* **2023**, *145*, 24315-24327. <http://dx.doi.org/10.1021/jacs.3c09181>.
- (3) Cvek, M.; Jazani, A. M.; Sobieski, J.; Jamatia, T.; Matyjaszewski, K., Comparison of Mechano- and PhotoATRP with ZnO Nanocrystals, *Macromolecules* **2023**, *56*, 5101-5110. <http://dx.doi.org/10.1021/acs.macromol.3c00250>.
- (4) De Bon, F.; Fonseca, R. G.; Lorandi, F.; Serra, A. C.; Isse, A. A.; Matyjaszewski, K.; Coelho, J. F. J., The scale-up of electrochemically mediated ATRP without deoxygenation, *Chem. Eng. J.* **2022**, *445*, 136690. <http://dx.doi.org/10.1016/j.cej.2022.136690>.
- (5) Dworakowska, S.; Lorandi, F.; Gorczyński, A.; Matyjaszewski, K., Toward Green Atom Transfer Radical Polymerization: Current Status and Future Challenges, *Advanced Science* **2022**, *9*, 2106076. <http://dx.doi.org/10.1002/advs.202106076>.

Green Chemistry within Planetary Boundaries

NATALIA TARASOVA*

Mendeleev University of Chemical Technology, Institute of Chemistry and Problems of Sustainable Development, Miusskaya Sq., 9, 125047, Moscow, Russia

**Corresponding author: tarasova.n.p@muctr.ru*

Abstract:

Green chemistry may become an efficient tool for overcoming chemophobia and agrochemophobia as a variant of it. It is not a new, earlier unknown, trend. It is rather a compact formulation of thinking principles for well-trained and socially responsible chemists–scientists or technologists. The latter thesis is confirmed by the active practical application of green chemistry approaches in industry including in Russia. However, not only the business community, but also top-level politicians have begun to try to follow this way of thinking. The United Nations has pointed out that green chemistry is a key science development trend.

When increasing the productivity of crops, protecting them from pests, manufacturing new materials and products, developing transport, and creating medicines, humanity has caused unintended harm to the planet. In this connection, scientific papers devoted to the exhaustion of natural resources and the negative effect of human activity on the environment began to appear in the 1960s–1970s. According to some nonprofit organizations, such as the Global Footprint Network and the World Wildlife Fund, the consumption of natural resources for more than 40 years beginning from 1970 has exceeded the capability of our planet for their reproduction. This has led to a deficit in biocapacity, which is the capability of Earth’s ecosystems to reproduce certain biomaterials and utilize the wastes of anthropogenic activity. According to the estimates of ecologists, in 2018, the needs of humanity exceeded the capabilities of nature by 1.5 times. In 2024, the Earth’s annual resources will be exhausted on August 1st. Upon continuation of this trend, three planets like the Earth would be required to satisfy the needs of humanity by the year 2050.

A logical continuation of scientific knowledge accumulation is the concept of sustainable development, according to which economic and social development must be combined with the preservation of nature, i.e., the protection of the structure, functions, and diversity of the Earth’s natural systems. The notion “planetary boundaries” has come into common use [1]. This field has actively been under development for the past 15 years. Nine planetary boundaries, including climate change, loss of biodiversity, and change in terrestrial ecosystems have been described [2]. Numerical values were established for most boundaries. However, all the attempts to give quantitative estimates for the limits of the chemical pollution have not yet given any results [3]. It has not been possible to calculate what amount of contaminants can lead to irreversible changes in the biosphere. This uncertainty, in our opinion, may be considered as one of the reasons for the rise of chemophobia.

Chemophobia, as well as any other phobia, cannot favor sustainable development. A cure for this disease is total chemical literacy formed beginning with one’s school days and the responsible handling of chemicals, including their household use. The principles of green chemistry should become a code of conduct for specialists in chemistry who have graduated from institutions of higher education [4,5].

Keywords:

planetary boundaries, chemophobia, green chemistry, chemical literacy

References:

- [1] J. Rockström, W. Steffen, K. Noone, et al., *Ecol. Soc.*, **2009**, *14* (2) .
<http://www.ecologyandsociety.org/vol14/iss2/art32/>
- [2] J. Rockström, W. Steffen, K. Noone, et al., *Nature*, **2009**, *461*, 472–475.
- [3] N. P. Tarasova, A. S. Makarova, *Russ. Chem. Bull.*, **2016**, *65*, 1383–1394.
- [4] N.P.Tarasova, A.S.Makarova, *Herald of the Russian Academy of Sciences*, **2020**, *90*, 245–250.
- [5] N.Tarasova, A. Dodonova, A. Zanin, *ACS Symposium Series*, **2020**, *1345*, 137 - 145.

Integrated Waste/Bio-Refineries to Fuels, Chemicals and Polymers

KONSTANTINOS TRIANTAFYLLIDIS

¹ Aristotle University of Thessaloniki, Department of Chemistry, University Campus P.O. Box 116, 54124 Thessaloniki, Greece

² Aristotle University of Thessaloniki, Center for Interdisciplinary Research and Innovation (CIRI), Balkan Center, 10th km Thessaloniki-Thermi Rd, P.O. Box 8318, 57001 Thessaloniki, Greece

*Corresponding author: ktrianta@chem.auth.gr

Abstract:

The utilization of alternative feedstocks for fuels, chemicals and polymers is of paramount importance. Biomass derived waste, such as forest and agricultural pruning, sawdust, kernels and other byproducts from food/agricultural crops processing, etc., represent an abundant renewable source, supporting the concept of “Biorefining”. Constant availability and logistics (collection, transport, storage) of biomass waste is an issue and approaches towards “Integrated Biorefineries” aiming to “whole-biomass” valorization as well as “co-processing” of biomass-derived streams with petroleum fractions appear more feasible in the near future, at least for the refining/fuel sector.

On the other hand, plastic waste originating from every-day consumer products (i.e. plastic bottles, bags, etc) or more specialized industrial materials (i.e. used turbine blades, circuit boards, etc.) represent an even more abundant and accessible source due to the increasing recycling awareness and adoption of Circular Economy strategies.

However, both biomass and plastic waste utilization will be beneficial for the environment and society, only if efficient and benign conversion technologies will be developed and optimized to meet the specific needs of these diverse feedstocks. To this end, thermochemical pretreatment/fractionation methods and heterogenous catalytic processes will play a significant role towards the economically feasible and sustainable production of fuels, chemicals and polymers.

In this presentation, we will discuss tailored methods for lignocellulosic biomass fractionation to hemicellulose, cellulose and lignin, down-stream conversion to chemicals (i.e. sugar alcohols, furanics, phenolics, and BTX aromatics) via catalytic pyrolysis, hydrogenation and other related processes, and follow-up upgrading to fuels or polymers/composites. Furthermore, the chemical recycling/upcycling of polymers and plastic wastes via (catalytic) pyrolysis will be also discussed.

Acknowledgements:

The support of European Union’s Horizon Europe Research and Innovation Programme under Grant Agreement No. 101058412 (ELECTRO project) is gratefully acknowledged. KST would also like to acknowledge the support of European Union H2020, Greek National funds (ESPA 2014-2020) as well as internal funds.

Exploitation of Renewable Resources in Polymer Chemistry

FRANCESCO TROTTA

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

Abstract:

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 dextrans 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.

References:

[1] Janet L. Scott¹, Antoine Buchard. *Managing Global Warming*, 2019, Academic Press, 503-525

[2] Krabicová, I., Appleton, S.L., Tannous, M., Hoti, G., Caldera, F., Pedrazzo, A.R., Cecone, C., Cavalli, R., Trotta, F. *History of Cyclodextrin Nanosponges*, *Polymers*, 2020, 12, 1122; doi:10.3390/polym12051122

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

Abstract:

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 Skłodowska-Curie entitled STiBNite (N_ 956923), PRIN-PNRR 2022 project "P2022XKWH7 – CircularWaste.

References

[1] Some recent examples L. Vaccaro et al: *Chem. Sci.* **2024**, *15*, 3831-3871; *Green Chem.* **2024**, *26*, 4871-4879; *Green Chem.* **2024**, in press, DOI: 10.1039/D4GC00830H, hot article; *Green Chem.* **2024**, in press DOI:10.1039/D4GC00699B, hot article and invited front cover; *Green Chem.* **2024**, *26*, 6625–6633, DOI: 10.1039/D4GC00930D; *ACS Sus Chem. Eng.* **2024**, in press, doi.org/10.1021/acssuschemeng.4c02486.

Green and Environmentally Friendly Approaches for Metal-Organic Frameworks Synthesis and Applications

AURELIA VISA

*Institute of Chemistry “Coriolan Dragulescu”, 24 M. Viteazul Ave, Timișoara - 300223,
Romania, apascariu@yahoo.com*

Abstract:

The twelve principles lead green chemistry research [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), a well-studied class of complex structured porous materials, are composed of different central metal nodes bridged by organic linkers. These fascinating materials have been extensively studied for a variety of environmental applications. The complexity and diversity of architectural structures of MOFs provide unique properties such as high thermal, chemical, and mechanical stability, which direct these materials for applications in numerous areas looking at remediation pollution issues, such as heavy metal contaminants in water, the treatment of textile and dye industry effluents, catalysis, gas storage, solar energy conversion, and drug delivery. An emerging focus in MOF research is the development of novel synthetic routes that use non-hazardous reagents under mild synthetic conditions, leading to less waste as well as a lower environmental impact than conventional approaches, which frequently involve harsh conditions and hazardous solvents. Some alternative green methods are energy-efficient methods, solvent-free synthesis, solvent minimization or using water as a solvent, the use of renewable and biodegradable solvents, and green precursors.

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) [2-7].

Acknowledgment:

This work was partially supported by a grant of the Ministry of Research, Innovation and Digitization, CNCS - UEFISCDI, project number PN-III-P4-PCE-2021-0089, within PNCDI III.

References:

- [1] H.S. Cho, H. Deng, K. Miyasaka, Z. Dong, M. Cho, J.K. Kang, O.M. Yaghi, O. Terasaki, *Nature*, **2015**, 527, 503
- [2] P. Anastas, J. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, New York, **1998**
- [3] L. Lupa, N. Tolea, M. Iosivoni, B. Maranescu, N. Plesu, A. Visa, *RSC Adv.* **2024**, 14, 4759
- [4] T.Y. Gu, M. Dai, D.J. Young, Z.G. Ren, J.P. Lang, *Inorg. Chem.*, **2017**, 56, 4668
- [5] B. Maranescu, A. Visa, *Int. J. Mol. Sci.* **2022**, 23(8), 4458
- [6] B. Maranescu, L. Lupa, A. Visa, *Appl. Surf. Sci.*, **2019**, 481, 83
- [7] Á. Vílchez-Cózar, E. Armakola, M. Gjika, A. Visa, M. Bazaga-García, P. Olivera-Pastor, D. Choquesillo-Lazarte, D. Marrero-López, A. Cabeza, R.M. P. Colodrero, K.D. Demadis *ACS Appl. Mater. Interfaces* **2022**, 14, 11273–11287

ABSTRACTS OF STUDENTS

(alphabetical order of surnames)

Innovative Application of Kolbe Reaction on the Constituents of Plant Oils

Haroon AHMAD^{1,*}, Benedetta BERTOLOTTI¹, Isabella NATALI SORA¹

¹*Department of Engineering and Applied Sciences and CSGI, University of Bergamo, Italy*

**Corresponding author: haroon.ahmad@unibg.it*

Biomass has a complex structure and is very challenging to convert directly into valuable chemical products. The conversion of biomass into defined chemical products is a multi-step process. In the first step the biomass is converted into defined intermediates, which are then converted into fine chemical products. In recent years, organic electrosynthesis has attracted great interest, especially in terms of sustainability, as an inherently green method of replacing hazardous chemicals with electrons for oxidation and reduction. This method can be used to produce chemicals from agricultural waste and in the chemical industries to access fine chemicals more efficiently and sustainably. A common challenge for biomass electrochemical conversion is their minimum solubility especially in the environmentally friendly solvents. Further, for enabling efficient reactant conversion, it is important to ensure the contact between substrate and electrode. There are many approaches for the production of biofuels. The most common and conventional method is the transesterification method [1]. Different electrochemistry reactions like anodic/cathodic decarboxylation also called Kolbe electrolysis [2].

This work represents an innovative approach for the synthesis of aliphatic long chain hydrocarbons starting from bio-oils through Kolbe electrolysis in combination with biological conversion. In particular, Kolbe electrolysis enables to upgrade the mixture of fatty acids, obtained from commercial oils after transesterification/hydrolysis. In detail, this work presents the conversion of single and mixture of fatty acids (1:1) into defined chemical products using an electrolysis technique. Lauric acid and palmitic acid are used as substrates as both acids are principal constituents of different vegetable oils like coconut oil and palm oil. The impact of operating parameters such as current intensity (10 mA–100 mA), amount of KOH (0.4–1.7 eq.), electrolysis time (2–18 h), and different solvent environments on the process performance has been investigated in terms of chemicals production, especially focusing on the dimers yield. The achieved results show 65% and 23% of the dimers yield from the electrolysis of lauric acid and palmitic acid respectively, with nearly full dissociation of substrate acids, at 70 mA current intensity with alternate polarity of 30 minutes, 1.5 eq. of KOH, 6 h of electrolysis time in EtOH:MeOH:H₂O solvent system. Whereas, using the same experimental conditions, the mixture of both acids (1:1) shows 45% of the dimers including *n*-docosane and *n*-triacontane as homocoupling and *n*-hexacosane as hetero-coupling, with nearly fully dissociation of acid substrate. All the electrochemical experiments were conducted using ElectraSyn 2.0 which is commercially available, easy to use and makes the reaction easily repeatable and the analysis of products were investigated using GC/MS.

References

- [1] Mansir, N., Taufiq-Yap, Y. H., Rashid, U., & Lokman, I. M, *Energy Conversion and Management* (2017), 141, 171–182.
- [2] Hegner, R., Neubert, K., Rosa, L. F. M., & Harnisch, F, *ChemElectroChem* (2019), 6(14), 3731–3735.

Using “Young of the Year” Fish as Bio-monitors for Pollution in Selected Aquatic Environments in Lagos State

Senami ANKO^{1*}, Abdulrafiu MAJOLAGBE², Adeniyi ADEJARE³

¹*Department of Chemistry, Lagos State University, Ojo, Nigeria*

²*Department of Chemistry, Lagos State University, Ojo, Nigeria,*

³*Department of Chemistry, Lagos State University, Ojo, Nigeria*

**Corresponding author: senamianko@gmail.com*

Potentially toxic metals remain a serious environmental pollutant due to their toxicity and persistence in the environment. Water bodies are usually polluted by oil spills, industrial waste, sewage and waste water, mining activities, burning of fossil fuels, chemical pesticides and fertilizer residues. This leads to the reproductive change, migration and death of fish, which poses a big problem to artisanal fishermen as well. Therefore, while aquatic organisms (fish) have been reportedly used as a bio-monitor in many studies, there is scarcity of data on the use of very young fish in the capacity to monitor pollution in the environment. This study was designed to use "young of the year" fish (YOY) - used to describe fish that is not sexually mature - to indicate metals present in aquatic environments in Lagos, Nigeria. Fish, water and sediment samples were collected from Langbasa, Tumaro (Liverpool market), and Badagry, and digested using mineral acid digestion. The digested samples were analysed for six metals (Cu, Fe, Zn, Pb, Ni, and Cd), with the use of a Flame Atomic Absorption Spectrometer. The trace metal values in water samples ranged between 0.02-0.12, Cu; 0.36-16.21, Fe; 0.28-3.12, Zn; 0.05-1.97, Pb; 0.52-3.01, Ni; and 0.02-0.09, Cd(mg/l). The mean concentrations for metals in the young of Catfish and Tilapia, ranged between 0.23-0.57, Cu; 0.16-4.79, Fe; 8.15-12.30, Zn; 0.00-0.64, Pb; 1.07-1.19, Ni; and 0.00-0.04, Cd(mg/l) for all three locations. The results revealed that YOY can be effectively used as bio-monitors of trace metals in water, as they are sensitive, and show early signs of contamination in their systems.

Keywords: Young of the year fish, Bio-monitor, Trace metals, Aquatic environments.

References

- [1] R.B. Baird, L.S. Clesceri, A.D. Eaton, et al., eds, Standard Methods for the Examination of Water and Wastewater (22nd ed.). (2012). Washington, DC: American Public Health Association. ISBN 978-0875530130.
- [2] D.K. Williams, How does water pollution affect fish? (2018). Sciencing.com

Valorization of Waste Corn Cobs into High Yields of Furfural Using Ionic Liquids

Winifred Delali ANYOMIH¹, Banothile MAKHUBELA^{2*}, Paseka MOSHAPO³

^{1,2,3} Department of Chemistry, University of Johannesburg, Kingsway Campus, Auckland Park, South Africa
*Corresponding author: bmakhubela@uj.ac.za

Climate change is a major global issue that is brought on by the combustion of fossil fuels, which emits toxic gases into the atmosphere. Therefore, it is imperative to find more environmentally friendly and sustainable sources of fuels and chemicals to counteract this.[1] Lignocellulosic biomass, an alternative carbon source, comprises polymers of carbohydrates that can be transformed into various compounds including, but not limited to furfural, which can then be further processed into fine chemicals and biofuels. [2] Because ionic liquids (ILs) have certain advantages over mineral acids in industrial use, the ILs have drawn interest in the conversion of biomass.[3]

It has been shown that employing metal halides as co-catalyst and anchoring sulfonyl groups to the cation of the ionic liquids can increase their catalytic activity.[4] The literature reports fewer cases of using raw biomass directly, and the reported yields are lower than those obtained from using pure xylose as a substrate for the production of furfural. This study reports on the synthesis and characterization costeffective ionic liquids with sulfonyl groups attached to their cation with the presence of both Bronsted and Lewis acidic sites. These ionic liquids have been investigated as catalysts for the highly efficient conversion of raw waste biomass (corn cobs) into furfural in a one-pot reaction system. The synthesized ionic liquids were selective in converting only the hemicellulosic content of the biomass.

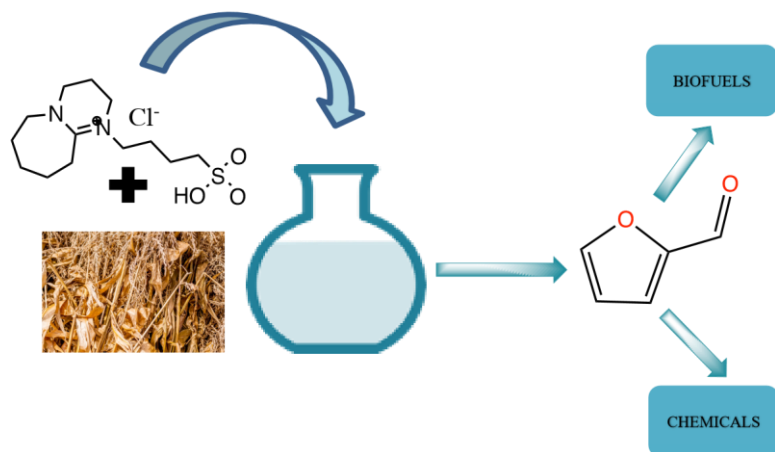


Figure 1. Conversion of biomass with ionic liquids into useful compounds. [5]

References

- [1] O. Ibraheem and B. K. Ndimba, *Int. J. Biol. Sci.*, 2013, 9, 598–612
- [2] A. Mittal, S. K. Black and D. K. Johnson, *ACS Sustain. Chem. Eng.*, 2017, 5, 5694–5701.
- [3] S. M. Zakaria, A. Idris, and Y. Alias, *Ind. Crops Prod.*, 2020, 157, 1–10.
- [4] S. Liu, K. Wang, H. Yu, B. Li and S. Yu, *Sci. Rep.*, 2019, 9, 1–9.
- [5] <http://clipart-library.com/clipart/433816.htm>

Benign Synthesis Routes for The Production Of Biochar From Artichoke Biomass

Mariam AUDU^{1*}, Eya, Ben KHALIFAH,¹ Giuliana MAGNACCA,¹ Gloria BERLIER¹

Nanostructured Interfaces and Surfaces (NIS), Centre of Excellence, Department of Chemistry, University of Torino, Italy

*Corresponding Author: mariamfadeke.audu@unito.it

Biochar, a carbonaceous material obtained by pyrolysis of biomass, has attracted significant attention in various fields such as environmental remediation, catalysis, and soil amendment due to its unique surface chemistry and physicochemical properties [1]. Its properties are mainly dependent on precursor used and preparation method. The utilization of biomass from agricultural and urban wastes as biochar precursor is an effective route to a sustainable waste management and enhances large scale biochar production globally [2].

In this study, artichoke bracts were employed as a cost effective source to prepare biochars. Thermogravimetric analysis (TGA) was employed to determine the best pyrolysis conditions: a single step activation at 550 °C with solid K_2CO_3 in nitrogen atmosphere. The influence of activator/precursor weight ratio (1:1 and 1:0.5) on the physicochemical properties of biochars was investigated. Fourier transform infrared spectroscopy (FT-IR) indicates a very limited presence of oxygenated functional groups. pH of zero charge indicated that biochars are negatively charged above around pH 4. Nitrogen adsorption–desorption isotherms indicated that both materials possess high surface area and are microporous. The surface area and porosity are compared with those of artichoke bracts biochar prepared by H_3PO_4 activation.

KEYWORDS: Biochar, Biomass, Single step activation.

References

- [1] P. Danesh, P. Niaparast, P. Ghorbannezhad, I. Ali, *Fuel* **2023**, 337, 1-8.
- [2] C. Zhang, Y. Ji, C. Li, Y. Zhang, S. Sun, Y. Xu, L. Jiang, C. Wu, *Industrial and Engineering Chemistry Research* **2023**, 62, 17168–17181.

Carbon Dots as Visible Light Bio-based Photocatalysts in Organic Synthesis

Valentina BENAZZI^{1*}, Arianna BINI¹, Carlotta CAMPALANI², Mariangela NOVELLO¹, Maurizio SELVA², Alvis PEROSA², Stefano PROTTI¹

¹ Dipartimento di Chimica Organica, Università degli Studi di Pavia, Via Torquato Taramelli 12, 27100 Pavia, Italy

² Dipartimento di Scienze Molecolari e Nanosistemi, Università Cà Foscari di Venezia (Via Torino 155 edificio alpha, 30170 Venezia Mestre, Italy

*valentina.benazzi01@universitadeglistudidipavia.it

This project is based on the valorization of agri-food waste from Rigoni di Asiago, extracting the nutraceutical molecules from waste, converting the residual into Carbon dots through hydrothermal treatments and use them as photocatalyst in organic reactions. Carbon-dots (CDs) are highly emissive nanomaterials characterized by solubility in water, good stability and low toxicity that can be prepared through hydrothermal or pyrolytic bottom-up approaches from organic and bio-organic sources. The proprieties of CDs (dimension, shape, emission, quantum yield) depend on starting precursors and reaction conditions. The first part of this work was focused on demonstrating the effectiveness of CDs as photocatalysts, investigating the photophysics and photochemical behavior of different types of CDs. Initially, we tested amorphous CDs doped with nitrogen, prepared with a hydrothermal treatment from citric acid and diethylenetriamine (DETA), in visible light photocatalyzed 1,2-difunctionalization reactions of olefins via Atom-Transfer Radical Addition (ATRA) processes. Subsequently we compared different types of CDs synthesized from different precursors (glucose, citric acid and bass scales) as photocatalyst in the photoreduction of triaryl sulfones. The second part of this project will be focused more on the use of CDs synthesized starting from the company's actual waste. The reducing power of carbon dots in the excited state makes them efficient photocatalysts, then considering their low cost and the possibility of being able to synthesize them starting from bio-based waste, makes them potentially very interesting both in the field of photocatalysis and in the field of the circular economy.

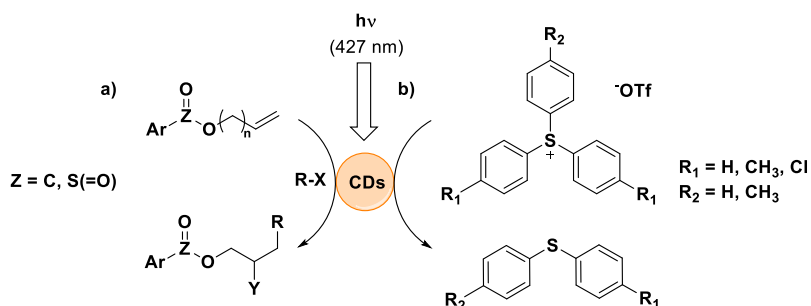


Figure 1. CDs as photocatalyst in ATRA processes (a) and photoreductions of triaryl sulfones (b)

Acknowledgements. We gratefully acknowledge the support from Fondazione Cariplo (Photo and Mechano-Chemistry for the Upgrading of Agro- and Sea-food Waste to advanced polymers and nanocarbon materials, CUBWAM, project 2021–0751).

References

- [1] S. Cailotto, R. Mazzaro, F. Enrichi, A. Voimero, M. Selva, E. Cattaruzza, D. Cristofori, E. Amadio, A. Perosa *ACS Appl. Mater. Interfaces*, **2018**, 10, 40560-40567.
- [2] A. Hamadamin, V. Benazzi, C. Campalani, L. Quattri, D. Ravelli, F. Hussain, A. Perosa, M. Selva, S. Protti *ChetCatChem*, **2023**, e202300708
- [3] J. W. Knapczyk, W. E. McEwen, *J. Org. Chem.* **1970**, 35, 2539-2543.

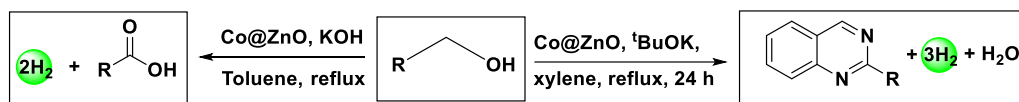
Cobalt Doped ZnO Nanostructured Material as a Multifunctional Catalyst for Oxidant-free Alcohol Dehydrogenation and Dehydrogenative Coupling reaction

Krisangi BORDOLOI¹, Pankaj DAS^{1,*}

¹Department of Chemistry, Dibrugarh University, Dibrugarh, Assam-786004, India

*Corresponding author: pankajdas@dibru.ac.in

Oxidation of alcohols in an oxidant-free condition commonly known as the acceptorless dehydrogenation (AD) reaction has recently emerged as one of the widely used process in synthetic organic chemistry that can be considered as atom economical, sustainable alternative strategy to the historical method. The reaction produces molecular hydrogen as the by product, thereby serving as an energy vector. Alcohol acts as one of the fundamental feedstock that can be used as an excellent chemical precursor to produces a variety of dehydrogenated value-added products such as carbonyls, acids, and several coupling products *via* acceptorless pathway. As a continuation of our previous work^{1,2} we have developed a low cost, easily available transition metal based heterogeneous catalytic system by doping ZnO with Co (Co@ZnO) *via* simple wet chemical method. The material was then characterized with various analytical techniques such as TEM-HRTEM, SEM-EDS, XPS, and PXRD etc. The as-synthesized material was used as a multifunction catalyst towards AD reaction of alcohol to produce dehydrogenated products like carboxylic acid, quinazoline. We have explored the material as a catalyst for synthesis of carboxylic acid from primary alcohols *via* AD pathway and quinazoline *via* AD coupling reaction of 2-aminobenzylamine and benzyl alcohol. This low cost, easy accessible metal containing heterogeneous catalytic system can give access to a number of dehydrogenated products and acts as a multifunctional catalyst thereby making it one of the exceptional catalytic system for AD reaction.



Scheme 1. Acceptorless dehydrogenation reaction of alcohol over multifunctional Co doped ZnO nanocatalyst

References

- [1] K. Bordoloi, G. D. Kalita, P. Das, *ACS Appl. Nano Mater.* **2023**, 6, 14786–14797.
 [2] K. Bordoloi, G. D. Kalita, P. Das, *Dalton Trans.* **2022**, 51, 9922-9934.

Innovative Bio-Stimulants for Plants Obtained by Slaughter Waste Treatment

Alba CAO¹, Tiziana PIVETTA¹, Paola CASTI², Costantino PALMAS²

¹ *Chemical and Geological Sciences Department, University of Cagliari, Italy*

² *Concimi Biologici Srl*

This study is the topic of my PhD project, carried out in collaboration with the company Concimi Biologici Srl sited in Macchiareddu-Grogastu Zone, SU, Sardinia Italy and the Chemical and Geological Sciences Department of the University of Cagliari, Italy.

Concimi Biologici S.r.l. produces organic fertilizers from category 3 animal by-products (SOA3), with a transformation process involving an innovative approach with radio frequencies (Italian patent no. 1425494 dated 03/11/2016, international patent no. WO2016/012986 A1 dated 28/01/2016, US patent US 2017/0210676 dated 27/07/2017).

The resulting product was proven to be effective in enhancing soil fertility and promoting the growth of various crops, including wheat (Mulè et al., 2020, Plants). The company is currently focusing on protein hydrolysates from the application of the patented process to slaughterhouse wastes. These hydrolysates, resulting from thermal hydrolysis with microwaves, are hypothesized to contain molecules capable of directly affecting plants, thus qualifying as biostimulants under the new EU regulation 1009/2019 on fertilizers. In 2013 the EBIC (The European Biostimulants Industry Council) released its definition of biostimulants: "Biostimulants are substances and/or microorganisms which, when applied to the plant or rhizosphere, stimulate natural processes that improve the efficiency of absorption and assimilation of nutrients, tolerance to stress abiotic and product quality. Biostimulants have no direct effects on parasites and pathogens and therefore do not fall into the category of pesticides."

The aim of this study is the chemical characterization of fatty acids in slaughter wastes before and after treatment with microwaves (MW). Amino acids and proteins will be also studied. Gas chromatography coupled with mass spectrometry was used for the identification and quantitation of the analytes.

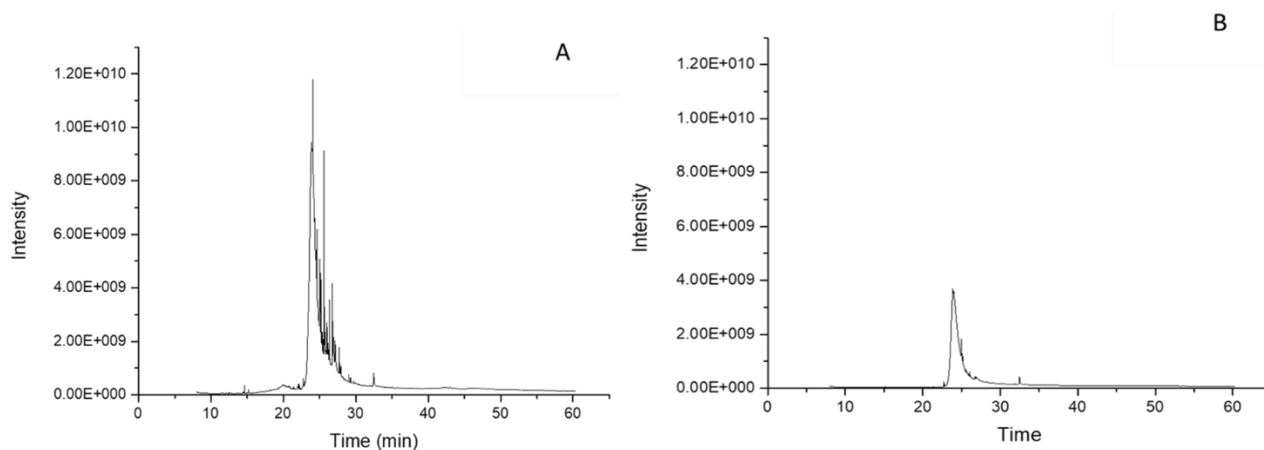


Figure 1. Chromatogram of untreated sample (A) and MW treated sample (B).

References

[1] M. Loi, C. Paciolla, A.F. Logrieco, G. Mulè, *Frontiers in Microbiology* **2020**, volume 11, article 243, 16.

Sustainable Activation of Pictet-Spengler Reaction by Brønsted Catalysts under Microwave Irradiation

Francesco CATALINI^{1*}, Dario GENTILI², Cristina CIMARELLI², Gabriele LUPIDI², Serena GABRIELLI², Enrico MARCANTONI²

¹PhD student DIN Catalysis of University of Perugia; hosting institution: University of Camerino

²Organic Chemistry Division, School of Science and Technologies, CHIP Building Center, University of Camerino, via Madonna delle Carceri, 62032 Camerino, Italy

*francesco.catalini@dottorandi.unipg.it

Heterogeneous Catalysis in synthetic chemistry allows to lower the waste production, to improve selectivity, but also to agree with environmental and economic points of view, ensuring an interesting alternative to conventional synthetic processes.¹ The use of solid state catalysts can ease its recovery and reuse, in order to help separation steps, improving its recycling and reduce the production costs and waste generation.² In this work, the Heterogeneous Catalysis is applied to improve the Pictet-Spengler Reaction based synthesis of important biological active compounds. Pictet-Spengler Reaction (PSR) is well-known more than a century and it represents one of the most successful strategies for the synthesis of N-heterocycles, e.g. isoquinolines and indole-based alkaloids.³ The reaction is generally performed through a Brønsted or Lewis acid catalysed cyclization between β -arylethylamines, like tryptamines/phenylethylamines, and carbonyl compounds, such as aldehydes and ketones.⁴ More sustainable synthetic processes are needed to optimize PSR-based synthesis of important molecules, not only to perform products formation, but especially for ensuring the application of a green chemistry approach. Indeed, our work takes advantages from Heterogeneous Catalysis combined with Microwave Irradiation, well-known for its advantages, especially in agreement with green chemistry principles.⁵ We utilized safe and environmental friendly Brønsted acids like Graphene Oxide and Amberlyst-15®, avoiding the employment of common mineral acids, usually used in this type of reaction.⁶ This double combination allows us to develop a two steps-one pot protocol in which we can afford intermediate and the final products in chemo-selectivity pathway.

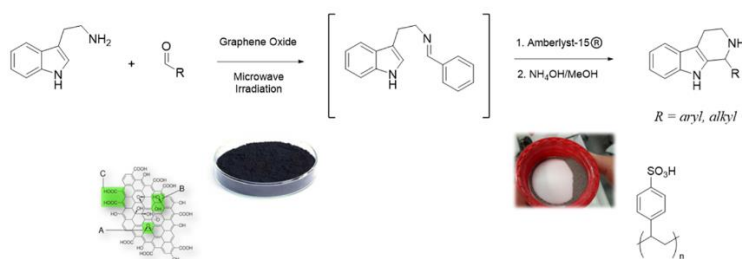


Figure 1 Brønsted acids catalyzed PSR-based synthesis of tetrahydro- β -carbolines.

References

- [1] G. Sartori, R. Ballini, F. Bigi, G. Bosica, R. Maggi, P. Righi, *Chem. Rev.* **2004**, 104, 1, 199–250
- [2] M. Miceli, P. Frontera, A. Macario, A. Malara 1, *Catalysts* **2021**, 11, 591
- [3] J. Stöckigt, A. P. Antonchick, F. Wu, H. Waldmann, *Angew. Chem. Int. Ed.* **2011**, 50, 8538 – 8564.
- [4] R. N. Rao, B. Maiti, K. Chanda, *ACS Comb. Sci.* **2017**, 19, 199–228
- [5] A. de la Hoz, A. Díaz-Ortiz, A. Moreno, *Chem. Soc. Rev.* **2005**, 34, 164 – 178.
- [6] A. Calcaterra, L. Mangiardi, G. Delle Monache, D. Quaglio, S. Balducci, S. Berardozzi, A. Iazzetti, R. Franzini, B. Botta, F. Ghirga, *Molecules* **2020**, 25, 414.

***In-situ* One-Step Production of Gold Nanoparticles Supported on Carbon Sub-Micrometric Fibers From Electrospun Maltodextrin-Based Mats**

Claudio CECONE,^{1*} Andrea JOUVE,¹ Sara MORANDI,¹ Maela MANZOLI,² Francesco TROTTA,¹ Marco ZANETTI,¹ Pierangiola BRACCO¹

¹*Department of Chemistry, University of Turin, NIS and INSTM Reference Centers, Via Giuria 7, 10125 Torino, Italy*

²*Department of Drug Science and Technology, University of Turin, NIS and INSTM Reference Centers, Via Giuria 9, 10125 Torino, Italy*

**Corresponding author: claudio.cecone@unito.it*

Thanks to the low price, water solubility, and bioderived nature, starch-derived maltodextrins have been exploited to obtain polysaccharide-based fibers via electrospinning technique. The addition of citric acid with maltodextrins has also proven to allow cross-linked fibrous materials by taking advantage of post-processing curing treatments at mild temperatures. Furthermore, when subjected to a high-temperature pyrolysis process, the same spun mats behaved as carbon precursors, giving well-defined sub-micrometric porous carbon fibers as the product [1,2].

During the last decades, nanotechnology has gained significant interest in scientific and industrial realities, with nanoparticles being considered a bridge between homogeneous and heterogeneous catalysis. In this context, gold nanoparticles have attracted growing attention due to their unique features. However, their catalytic activity strongly depends on their size and shape, making controlled syntheses a vital step. After their formation, nanoparticles are commonly immobilized on a support that plays a key role in heterogeneous catalysis, by providing e.g. acidic/base sites or metal-support interactions. In this regard, carbonaceous materials represent an ideal choice [3-4].

In the present work, a commercial maltodextrin has been electrospun from water solutions previously added with chloroauric acid as a gold precursor. Subsequently, the dry fibers were subjected to pyrolysis treatments, obtaining sub-micrometric carbon fibers. In parallel, the formation of the carbon products induced the reduction of chloroauric acid to gold nanoparticles. The yield in carbon as well as the size and number of nanoparticles, resulted dependent on the pyrolysis temperature and quantity of chloroauric acid added to the maltodextrins solution, respectively. The reported approach represents a novel and unique one-step in-situ strategy to obtain gold nanoparticles supported on porous carbon sub-micrometric fibers, produced from sustainable materials, avoiding the use of organic solvents or toxic compounds.

References

- [1] C. Cecone, G. Hoti, M. Zanetti, F. Trotta, P. Bracco, *RSC Adv.*, 2022, 12, 762-771
- [2] C. Cecone, G. Hoti, F. Caldera, M. Zanetti, F. Trotta, P. Bracco, *Polym. Degrad. Stab.*, 2022, 202, 110040
- [3] A.M. Echavarren, A.S.K. Hashmi, F.D. Toste, *Adv. Synth. Catal.*, 2016, 358, 1347-1347
- [4] A. Jouve, M. Stucchi, I. Barlocco, C. Evangelisti, F. Sodomio, Alberto Villa, L. Prati, *Top Catal.*, 2018, 61, 1928-1938.

Enhancing Sustainability in Cross-Coupling Reactions with Microwave Irradiation: A Circular Approach

Marta CIANI¹, Giulia BRUFANI¹, Luigi VACCARO¹

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
marta.ciani@dottorandi.unipg.it

Cross-coupling reactions have revolutionized the synthesis of complex molecules. In particular, Suzuki-Miyaura (SM) and Buchwald-Hartwig (BH) reactions are widely applied across various sectors of chemistry, especially in the production of active pharmaceutical ingredients (APIs)¹. In industry, it is essential to implement circular processes that incorporate the recovery and reuse of heterogeneous Pd catalysts, minimizing metal leaching. A careful selection of the reaction medium allows for waste production reduction and improvement in process sustainability. With the aim of developing alternative and low-impact synthetic pathways, we present here the simultaneous use of different tools to enhance the overall sustainability of SM and BH cross-coupling processes with a circular economy approach. We have combined the use of heterogeneous Pd-based catalysts with reaction media derived from biomass such as γ -valerolactone (GVL) and 2-Me THF², demonstrating that it is possible to obtain an optimized protocol suitable for various substrates. Microwave irradiation technology has significantly improved energy efficiency, enabling the synthesis of various biphenyls and arylamines while reducing reaction times. Furthermore, the high efficiency and selectivity of both couplings have led to further optimization of the work-up procedure, minimizing waste generation and associated E-factor values³.

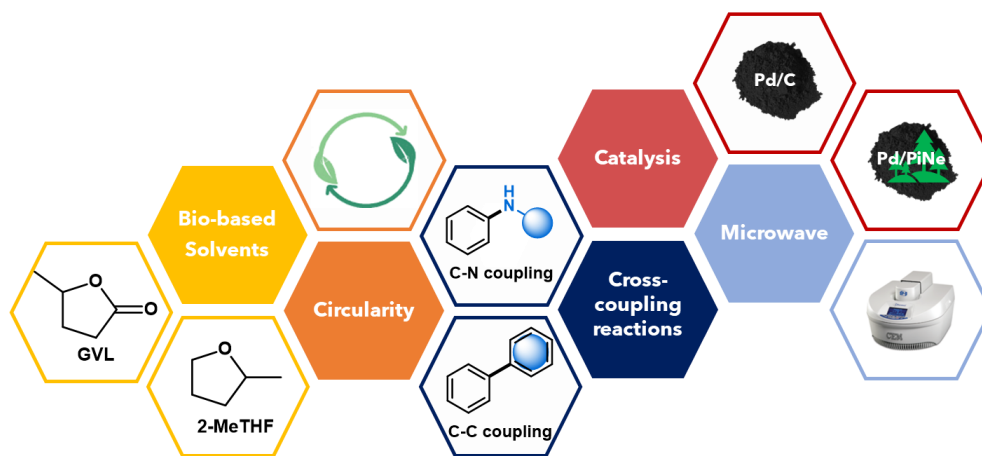


Figure 1. Illustrative scheme of our work.

References

- [1] B.S. Takale, F.-Y. Kong, R.R. Thakore, *Organics* **2022**, 3, 1-21.
- [2] F. Valentini, G. Brufani, B. Di Erasmo, L. Vaccaro, *Current Opinion in Green and Sustainable Chemistry* **2022**, 36:100634; V. Pace, P. Hoyos, L. Castoldi, P. Domínguez de María, A.R. Alcántara, *ChemSusChem*. **2012**, 5, 1369-1379.
- [3] F. Valentini, B. Di Erasmo, M. Ciani, S. Chen, Y. Gu, L. Vaccaro *Green Chem.* **2024**, 26, 4871-4879.

Sustainability in a Can: Upcycling Aluminium Scrap in the Waste-Minimized Electrochemical Synthesis of 2-oxazoline

S. Trastulli COLANGELI^a, F. FERLIN^a, L. VACCARO^a

^aLaboratory of Green S.O.C. – Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto, 8, 06123 – Perugia - Italy
E-mail: simone.trastullicolangeli@studenti.unipg.it
trastullicolangelis@gmail.com

To achieve net-zero carbon dioxide emissions, the decarbonization of the chemical industry is of particular importance as it is responsible for 15% of global industrial greenhouse gas (GHG) emissions.¹ In this context, electrochemical production based on the use of electricity from renewable sources is becoming a promising alternative to reduce the carbon footprint of chemicals.² To succeed in the challenging application of electrochemistry in industrial chemical synthesis, researchers are focusing their efforts on optimizing key process parameters such as energy efficiency, product selectivity, productivity per time unit, and electrocatalyst efficiency.³ The consumption of electrodes represents a key aspect influencing the efficiency and sustainability of electrosynthesis. When electrodes are based on metals, their cost and preparation are critical.⁴ While research on finding durable and stable electrodes is extensive, more emphasis should be placed on using electrodes made from waste materials.⁵ This can be even more crucial considering the availability of metallic materials compared to polymers. Aluminium, while being widely used in electrochemistry, is currently included in the list of critical raw materials and is classified as “primary” or “secondary”. Primary aluminium is derived directly from bauxite, while secondary aluminium is derived from the recycling of primary aluminium. The production of secondary aluminium is a more sustainable access route to this metal as its energy cost is only 5% of that of the primary production, and in addition, it includes the advantage of reducing the waste and the consumption of bauxite.⁶ For this purpose, the aim of this project was the development of a novel electro-synthetic approach toward the obtainment of 2-oxazolines by employing electrodes made of spent aluminium scraps.

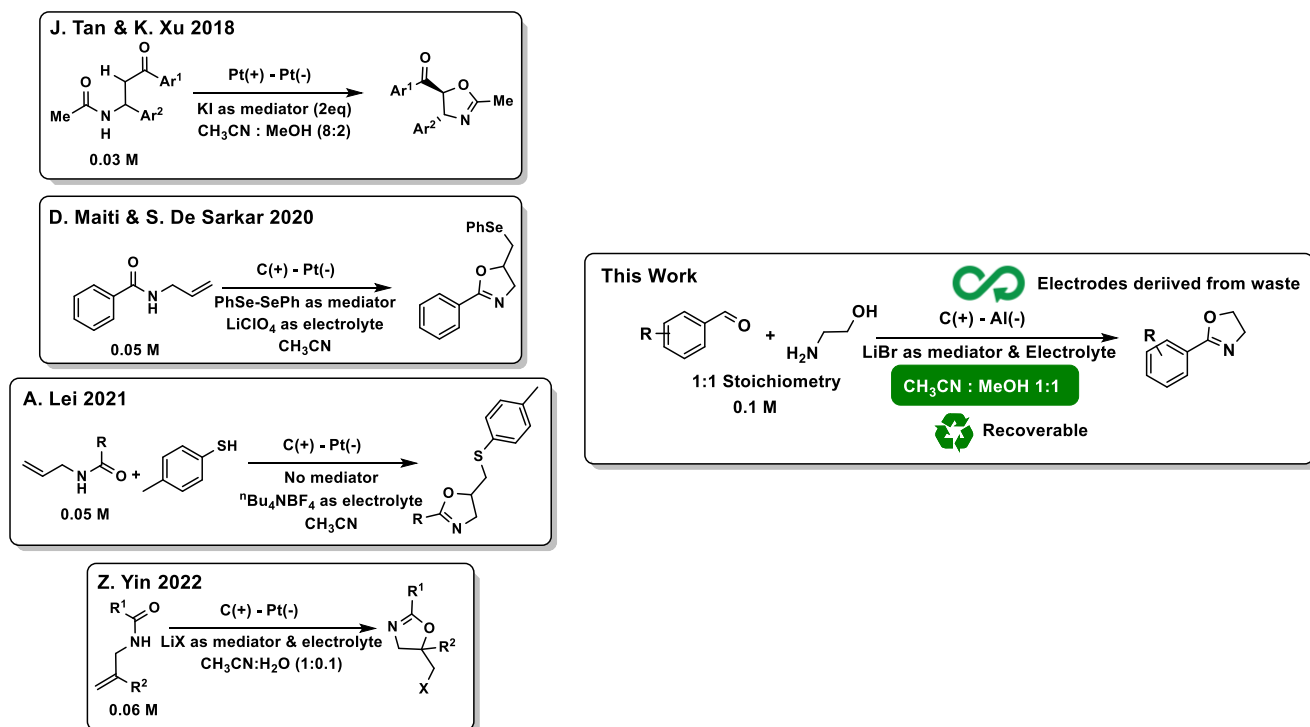


Figure 1: Electrochemical synthesis of 2-oxazolines employing upcycled aluminium electrodes.

References

1. M. H. Barecka and J. W. Ager, *Energy Adv.*, 2023, **2**, 268–279.
2. R. Xia, S. Overa and F. Jiao, *JACS Au*, 2022, **2**, 1054-1070.
3. N. Tanbouza, T. Ollevier and K. Lam, *iScience*, 2020, **23**, 101720.
4. M. Moradi, Y. Vasseghian, A. Khataee, M. Kobya, H. Arabzade and E.-N. Dragoi, *J. Ind. Eng. Chem.*, 2020, **87**, 18–39.
5. N. Idusuyi, O. O. Ajide, R. Abu, O. A. Okewole and O. O. Ibiyemi, *Mater. Today Proc.*, 2022, **56**, 1712–1716.
6. https://rmis.jrc.ec.europa.eu/uploads/CRM_2020_Factsheets_critical_Final.pdf

Synthesis of 1,6-Hexanediol through Catalytic Hydrodeoxygenation of 1,2,6-Hexanetriol in Continuous Flow System

Camila DIAS^{1,*}, Matthias DRIEB^{1,2}, Majd AL-NAJI¹, Helena I. S. NOGUEIRA³, Frank ROSOWSKI^{1,4}

¹BasCat – UniCat BASF JointLab, Technische Universität Berlin, Berlin, Germany

²Metal Organics and Inorganic Materials, Technische Universität Berlin, Berlin, Germany

³Chemistry Department, University of Aveiro, Aveiro, Portugal

⁴BASF SE, Catalysis Research, Ludwigshafen, Germany

*Corresponding author: camila.dias@campus.tu-berlin.de

1,6-hexanediol (1,6-HDO) is an important monomer, used in the synthesis of polyesters and polyurethane, derived from fossil fuels [1]. However, the existence of an alternative route within the biorefinery context is possible, as 1,6-HDO can be produced from C6 sugars, deriving from renewable resources such as lignocellulosic biomass. These sugars can be converted in 1,2,6-hexanetriol (1,2,6HTO), and through catalytic hydrodeoxygenation, into the desired diol [2]. This study focuses on the development of bifunctional catalysts for this process in continuous flow process.

1 wt.% and 5 wt.% Pt catalysts supported on β Zeolite were prepared through incipient wetness impregnation. The 3.5 wt.% Co catalyst supported on heteroatom-doped carbon was prepared as described by Liu *et al.*, 2018 [3]. The catalysts were characterized through N₂-sorption, XRD, and NH₃TPD. They were tested in a continuous flow fixed-bed reactor. All the Pt catalysts achieved complete conversion at specific conditions (175 °C – 250 °C). For all catalysts and in all temperatures tested, the main product obtained was tetrahydropyran-2-methanol (THP-2-M), a well-known intermediate for the studied reaction. The selectivities and yields obtained by the bifunctional catalysts produced can be observed on Figure 1.

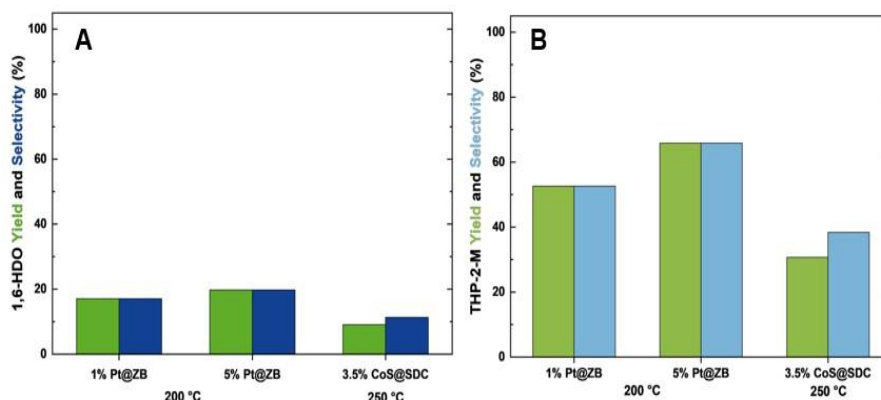


Figure 1.- A - Yield and selectivity 1,6-HDO; B - Yield and selectivity THP-2-M; reaction conditions: C_{1,2,6-HTO} = 1 wt.%, T = 150 °C - 250°C, Q_{educt} = 0.3 mL/min, Q_{H₂} = 30 mL/min, and P = 7.0 MPa.

Temperature was a fundamental condition for the conversion of 1,2,6-HTO, and the selectivity towards the desired compound. Improvements are needed in the Pt catalyst, to improve the hydrolysis of THP2-M to 1,6-HDO. The Co catalyst results suggest potential for studies at higher temperatures.

References

- [1] J. He, S.P. Burt, M. Ball, D. Zhao, I. Hermans, J.A. Dumesic, G.W. Huber, *Faraday Discuss.* **2017**, 202, 247-267.
- [2] T. Buntara, S. Noel, P.H. Phua, I.M. Cabrera, J.G. De Vries, H.J. Heeres, *Top Catal.* **2012**, 55, 612619.
- [3] S. Liu, A.P. van Myuden, L. Bai, X. Cui, Z. Fei, X. Li, X. Hu, P.J. Dyson, *ChemSusChem.* **2019**, 12, 3271-3277.

Cost-Effective Valorization of Factory Tea Waste: Enhancing Circular Economy Practices

Prangan DUARAH^{1*}, Mihir Kumar PURKAIT²

¹*Centre for the Environment, Indian Institute of Technology Guwahati, Assam-781039, India*

²*Department of Chemical Engineering, Indian Institute of Technology Guwahati, Assam-781039, India*

**Corresponding author: dprangan@iitg.ac.in*

This study delineates a sustainable strategy for the extraction of antioxidant-rich polyphenols from the byproducts of tea manufacturing, which are often disregarded and disposed of, thereby contributing to environmental waste. Centred on principles of the circular economy and sustainable development, the investigation introduces a green chemistry framework utilizing aqueous solvents for the extraction of polyphenols under rigorously optimized operational conditions. A comprehensive evaluation of various extraction methodologies was conducted to identify the most effective and economically viable approach, thereby enhancing the polyphenolic yield and ensuring the preservation of their antioxidative properties. Process optimization was achieved through a systematic adjustment of parameters, significantly increasing the efficiency of polyphenol recovery. The analytical characterization of tea waste-derived polyphenols was performed using Liquid Chromatography-Mass Spectrometry/Mass Spectrometry (LC-MS/MS), providing insights into the compositional diversity and potential bioactivity of the extracts. This study not only demonstrates the viability of repurposing tea industry byproducts into high-value applications across nutraceutical, food preservation, and cosmetic sectors but also contributes to the reduction of industrial waste. Through innovative recycling strategies and the advancement of green chemistry techniques, this work underscores the pivotal role of sustainable waste management practices in environmental remediation and the promotion of a circular economy.

Keywords: Factory tea waste; Polyphenols; Catechins; Phytochemicals; Waste utilization

From Fruit Residues to Leather Enhancement: Pomegranate Tannins as Eco-Friendly Collagen Crosslinkers

Sara EL MOUJAHED^{1,2,*}, Rodica Mihaela DINICA², Hicham ABOU OUALID, Fouad OUAZZANI CHAHDI¹, Faouzi ERRACHIDI⁴

¹ *Laboratory of Applied Organic Chemistry, Faculty of Sciences and Technologies, Sidi Mohamed Ben Abdellah University, Imouzzar street, B.P. 2202, Fez, Morocco*

² *Laboratory of Organic Chemistry, Faculty of Sciences and Environment, Dunarea de Jos University of Galati, 111 Domneasca Street, 800201 Galati, Romania*

³ *Green Energy Park, IRESEN-UM6P, Benguerir, Morocco*

⁴ *Laboratory of Functional Ecology and Engineering Environment, Faculty of Sciences and Technologies, Sidi Mohamed Ben Abdellah University, Imouzzar street, B.P. 2202, Fez, Morocco*

*Corresponding author: sara.elmoujahed@usmba.ac.ma

Chrome tanning, the prevailing method for leather production, has raised environmental and health concerns. In response, researchers have sought alternatives, with the circular economy proposing the use of biomasses to reduce waste. In Morocco, fruit waste generated by juice processing industries remains an untapped source of tannins. To address this, a new eco-friendly tanning method based on vegetable biomass has been developed. The study focuses on extracts from six Moroccan pomegranate by-products (PR) varieties, investigating their crosslinking behavior with insoluble collagen (IC) extracted from sheep hide under industrial tanning conditions. Herein, molecular distributions of crosslinkers extracts were carried out using gel exclusion chromatography to follow polymerization degree and crosslinking kinetics during tanning process. Key findings include distinct behaviors of tannins and phenolics during crosslinking, intermolecular interactions, as well as the influence of crosslinkers on the collagen triple helix structure, which was observed via Fourier Transform Infrared Spectroscopy and X-Ray Diffraction analysis. Scanning Electron Microscopy observations shows the fibrial size variations of crosslinked collagenous structure by varying the extract variety. Additionally, the thermal stabilities followed by Differential Scanning Calorimetry and thermogravimetric measurements of crosslinked collagen vary based on the origin of the extracts while enhancing thermal stability. Theoretical studies using Gaussian was used as a complementally tool to compare the reactivity and the stability of the major molecules that contributes in the crosslinking process. The crosslinking ability of extracts was found to be controlled by catechic tannins. Using an ecological and simple extraction process, pomegranate by-products used can produce rich extracts in terms of tannins yields with a large variation in molecular weight distributions. The study underscores the potential of these extracts, produced ecologically, as promising candidates for sustainable leather production

Keywords: Pomegranate by-products, vegetable biomass, tannins, molecular weight, crosslinking, leather enhancement, eco-friendly tanning.

Green Synthesis of Bio-inspired Nanocomposite using Kaolin Clay and Aloe Vera Extract for Column Treatment of Wastewater

Cecilia I. ETUKUDO^{1,2}, Solomon E. SHAIBU^{1,2} and Edu J. INAM^{1,2*}

¹*Department of Chemistry, University of Uyo, Uyo, Nigeria*

²*International Centre for Energy and Environmental Sustainability Research (ICEESR), University of Uyo, Uyo, Nigeria*

**Corresponding author: eduinam@uniuyo.edu.ng*

Portable water remains a challenge for many households in Nigeria, especially the rural communities. In this study, bio-inspired nanocomposite using kaolin clay was synthesized using aqueous extracts from fresh leaves of Aloe vera as a bio-reducing agent and evaluated for use in the removal of Lead and Cadmium from simulated wastewater. The properties of the bio-inspired nanocomposite were investigated using transmission electron microscopy (TEM), scanning electron microscopy (SEM), x-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), energy dispersive x-ray (EDX) spectroscopy, Brauner-Emmett-Teller (BET) and ultraviolet-visible (UV-Vis) spectrophotometry with average particle size ranging from 45 to 60 nm. The bio-inspired nanocomposites (Ag-Kaolin and Fe-Kaolin) were loaded into a bamboo column 20cm in length and 1cm in diameter alongside a bed of activated carbon and sand for the filtration of simulated contaminated water. On observation of the retention time, the result showed that the rate of adsorption followed the order Fe-clay > Ag-Clay > Clay > Activated carbon > sand.

Keywords: Wastewater, Bio-inspired nanocomposite, and Green synthesis

Sustainable Corrosion Inhibitors and Carrier Systems for the Preservation of Concrete Heritage

Chiara FRATELLO^{1,2,*}, Elena MESSINA², Francesca BOCCACCINI¹, Cristina RICCUCCI¹, Marianna PASCUCCI¹, Gabriella DI CARLO

¹ Institute for the Study of Nanostructured Materials (ISMN), National Research Council (CNR), SP35d, 9, 00010 Montelibretti (Rome)

² Department of Chemical Engineering Materials Environment, Sapienza University of Rome, Via Eudossiana, 18, 00184 Rome

*Corresponding author: chiara.fratello@uniroma1.it

One of the major problems affecting the stability of reinforced concrete is the corrosion of the steel rebar. This is caused by the loss of the passivating oxide layer that occurs as carbonation proceeds and the pH in concrete matrix decreases, but can be also worsened by atmospheric and environmental factors such as the presence of chlorides. The resulting structural damage indirectly affects both safety and economics¹. Often corrosion, if in an advanced state, may even require invasive restoration interventions but, when dealing with concrete heritage, this is obviously not advisable and it is, therefore, even more important to preserve the integrity of the steel rebars to ensure the preservation of the cultural asset over time².

To date some organic and inorganic corrosion inhibitors exist that provide good protection, but they are not always effective and able to migrate into the concrete porosity up to rebars. Among them, there are amines, usually volatile, and heterocyclic compounds (i.e. BTA), harmful to operators and toxic to the environment. This research aims to seek increasingly *green* solutions that are not only effective but also safe to use, by identifying new inhibitors for steel in concrete.

In addition, as the inhibitor can only be applied on the surface, the chosen product has to be able to migrate into the innermost layers until it reaches the rebars. Part of this research is, therefore, also focused on the synthesis and validation of carrier systems that can deliver these inhibitors through the cement matrix and release them in a controlled mode upon environmental stimuli (pH change, presence of chlorides) such as layered double hydroxides³.

The current research began with the validation of some corrosion inhibitors 5 years after their application, a particularly relevant analysis as these tests are usually conducted only over shorter timescales. To evaluate their efficacy, a multianalytical approach was chosen by means of optical and metallographic microscopy, as well as FTIR and SEM analysis of corrosion products present on the surface. At the same time, the synthesis of carriers that can contain the inhibitor is being carried out.

The results of this ongoing research are promising: some of the inhibitors have been shown to provide good protection even over long timescales.

Acknowledgements:

This activity is carried out within the MUR PRIN2022 ECOforCONCRETE project (2022M4KCKP) which is kindly acknowledged for financial support.

References

- [1] Poursaee, A.; Hansson, C. M. Potential Pitfalls in Assessing Chloride-Induced Corrosion of Steel in Concrete. *Cement and Concrete Research* **2009**, *39* (5), 391–400.
- [2] Bertolini, L.; Carsana, M.; Gastaldi, M.; Lollini, F.; Redaelli, E. Corrosion Assessment and Restoration Strategies of Reinforced Concrete Buildings of the Cultural Heritage. *Materials & Corrosion* **2011**, *62* (2), 146–154. <https://doi.org/10.1002/maco.201005773>.
- [3] Giuliani, C.; Messina, E.; Staccioli, M. P.; Pascucci, M.; Riccucci, C.; Liotta, L. F.; Tortora, L.; Ingo, G. M.; Di Carlo, G. On-Demand Release of Protective Agents Triggered by Environmental Stimuli. *Front. Chem.* **2020**, *8*, 304.

Sargassum Hydrochar for the Removal of Cadmium and Lead in Aqueous Solutions: A New Perspective for Environmental Remediation

Lázaro Adrián GONZÁLEZ FERNÁNDEZ^{1,2}, Nahum Andrés MEDELLÍN CASTILLO^{1,3}, Amado Enrique NAVARRO FRÓMETA⁴, Candy Carranza ÁLVAREZ¹, Rogelio FLORES RAMÍREZ¹, Manuel SÁNCHEZ POLO², Ventura CASTILLO RAMOS², Francisco CARRASCO MARÍN²

¹*Programa Multidisciplinario de Posgrados en Ciencias Ambientales, Universidad Autónoma de San Luis Potosí, México.*

²*Facultad de Ciencias, Universidad de Granada, España.*

³*Centro de Investigación y Estudios de Posgrado, Facultad de Ingeniería, Universidad Autónoma de San Luis Potosí, México.*

⁴*Universidad Tecnológica de Izúcar de Matamoros, Puebla.*

*Corresponding author: lazaroadrian1995@gmail.com; lazaroadrian@correo.ugr.es

Environmental contamination with heavy metals poses a significant threat to ecosystems and human health. This study explores a novel approach to remediate cadmium and lead contaminated water using hydrochar derived from brown algae Sargassum. Sargassum is an abundant biomass resource in coastal regions and presents a sustainable solution for heavy metal removal. The main objective of this research is to evaluate the adsorption potential of Sargassum-derived hydrochar for the removal of Cd and Pb from aqueous solutions. The influence of pH on the adsorption efficiency is investigated and information on the underlying mechanisms is provided. Experiments were performed using static adsorbers to evaluate single and multicomponent adsorption systems. This approach allows us to examine the competitive adsorption behavior of Cd and Pb when present together in water, providing valuable insights into real-world scenarios. Our findings reveal that Sargassum-derived hydrochar exhibits remarkable adsorption capacity for both Cd and Pb (141 and 333 mg g⁻¹, respectively).

The Radke-Prausnitz isotherm model fits the experimental data well, suggesting both monolayer and multilayer adsorption. It was observed that the presence of lead is antagonistic to cadmium removal, reducing its adsorption efficiency. However, this antagonistic effect is not observed in the reverse scenario, as previously reported for unmodified Sargassum. Sargassum-derived hydrochar demonstrates great potential as an effective adsorbent for the removal of Cd and Pb from polluted waters. This sustainable and readily available material offers a promising solution for environmental remediation.

Novel Iron (II) complexes for efficient and versatile Ring-Opening Polymerization of Bio-Based Lactones

Giuseppe GRAVINA, Alessia LIPORACE, Claudio PELLECCIA*

Dipartimento di Chimica e Biologia "Adolfo Zambelli", Università di Salerno, Fisciano (SA), Italy

**Corresponding author: cpellecchia@unisa.it*

Aliphatic polyesters have garnered significant attention for a sustainable polymer industry, primarily owing to their bio-based origins, biodegradability, and recyclability. Their versatility and eco-friendly attributes make them prime candidates for a wide range of applications, from packaging materials to biomedical devices. The most effective synthetic method for producing this class of polymers, also utilized in industrial processes, is the Ring Opening Polymerization (ROP) of cyclic esters (lactones), which are often derived from renewable sources

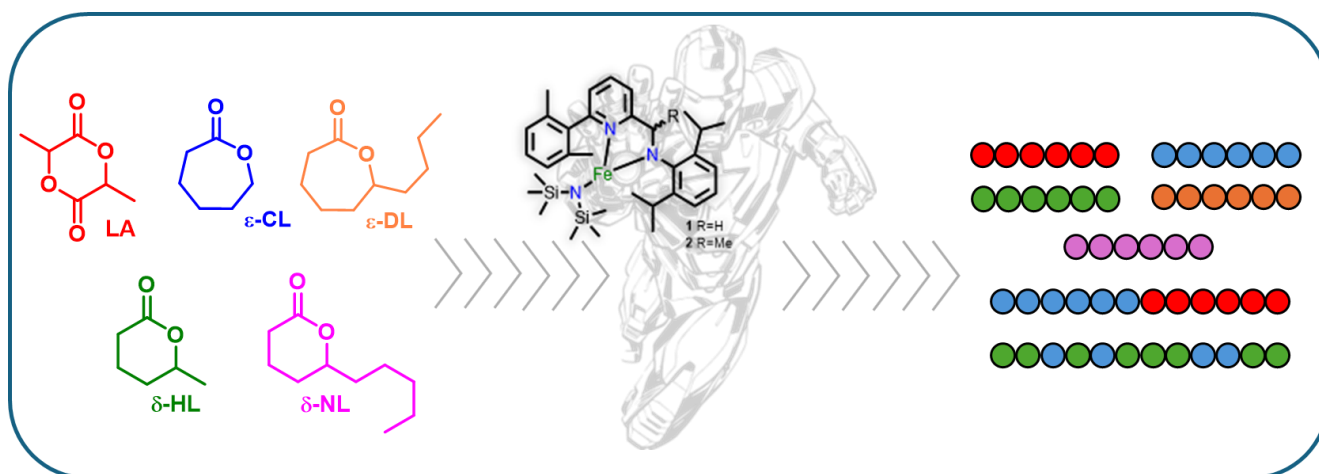


Figure 1. Polymerization of cyclic esters

In this contribution, we present novel 3-coordinated pyridylamido iron (II) complexes that serve as highly active catalysts for the ROP of L-lactide, the most industrially significant cyclic ester. [2] Notably, our catalysts demonstrate versatility by efficiently promoting the polymerization and copolymerization of various bio-based lactones, including the less reactive δ -lactones. The catalysts also exhibit living behavior, enabling the one-pot sequential addition of monomers to produce multiblock copolymers. This broad substrate scope and the living character opens avenues for the synthesis of diverse polymer architectures with tailored properties, addressing to specific application requirements.

References

- [1] X. Zhang, M.Fevre, G.O. Jones, R. Waymouth, *Chem.Rev.* **2018**, 188, 839-885
 [2] G.Gravina, G.Pierri, C.Pellecchia, *Molecular Catalysis* **2024**, 555, 113891

Green synthesis of Cross-Linked Cyclodextrin for drug delivery applications

Ibrahim HUSSEIN, Fabrizio CALDERA, Gjylje HOTI

*University of Turin, Department of Chemistry, Italy
(ibrahim.mahussein@unito.it)*

Cyclodextrin nanosponges (CD-NS) are an innovative class of nanostructured, crosslinked polymers derived from cyclodextrins (CD), which are safe, low-cost, and biodegradable polysaccharide derivatives¹. CD-NS consist of a nanosized three-dimensional network formed through the crosslinking of cyclodextrins with bi- or multifunctional chemicals such as dianhydrides, diisocyanates, diepoxides, and dicarboxylic acids².

The standard synthetic pathway involves dissolving cyclodextrins and an appropriate crosslinker in organic polar aprotic solvents like N,N-dimethylformamide (DMF) or dimethyl sulfoxide (DMSO), which influences the final properties, particularly for biomedical applications. Alternatively, a green synthetic method using mechanochemistry, specifically ball milling with 1,1-carbonyldiimidazole as the crosslinker, has been developed. This method produces a polymer with similar characteristics to those synthesized in solvents. Additionally, a green synthesis of citric acid nanosponges using sodium hypophosphite monohydrate as a catalyst and distilled water as the solvent is achieved under vacuum at specific temperatures and times.

FTIR spectroscopy confirmed the formation and stability of the carbonate bonds in the synthesized nanosponges, with spectra showing a consistent band around 1750 cm⁻¹ for carbonyl groups. Even after hours of treatment in water at 40 °C, the structure remained stable. Thermogravimetric analysis revealed that the degradation patterns of nanosponges synthesized by both methods were similar, with significant mass loss starting above 300 °C and peaking around 345 °C, indicating a similar molecular structure. Initial mass loss was attributed to absorbed environmental water, common in hygroscopic cyclodextrin-based nanoparticles. However, the formation of citrate NSs is confirmed by FTIR measurements, occurrence of a C=O band at 1720 cm⁻¹ in the FTIR spectrum is the characteristic feature of citrate NSs with a β -cyclodextrin.

In conclusion, cyclodextrin nanosponges represent a versatile and biocompatible cross-linked polymer with cost-effective green synthesis methods. Their unique properties, including high encapsulation ability, biocompatibility, and solubilization capacity, make them ideal for various nanomedicine applications.

References

- [1] Rubin Pedrazzo A, Trotta F, Hoti G, Cesano F, Zanetti M. Sustainable mechanochemical synthesis of β -cyclodextrin polymers by twin screw extrusion. *Environ Sci Pollut Res Int.* 2022 Jan;29(1):251-263.
- [2] Rubin Pedrazzo A, Caldera F, Zanetti M, Appleton SL, Dhakar NK, Trotta F. Mechanochemical green synthesis of hyper-crosslinked cyclodextrin polymers. *Beilstein J Org Chem.* 2020 Jun 29;16:1554-1563.

Metal-Organic Frameworks Impregnated with Ionic Liquids as Adsorbent Materials for Phenol and Phenol Derivatives

Marcela IOSIVONI^{1*}, Aurelia VISA¹, Bianca MARANESCU², Lavinia LUPA³

¹ „Coriolan Dragulescu” Institute of Chemistry, 24 Mihai Viteazul Blv., 300223 Timisoara, Romania, *e-mail: miosivoni@gmail.com

² Department of Biology-Chemistry, Faculty of Chemistry, Biology, Geography, West University of Timisoara, 16 Pestalozzi Street, 300115 Timisoara, Romania

³ Faculty of Industrial Chemistry and Environmental Engineering, Politehnica University Timisoara, 6 Vasile Parvan Blv, 300223 Timisoara, Romania

As a result of petrochemical activity, phenol and phenol derivatives can be found in water, which increases toxicity not only to the environment, but also to humans. These pollutants are difficult to remove from water due to their solubility and the costs are extremely high. Therefore, we need materials that can adsorb the phenol and phenol derivatives, that are low cost, reusable and synthesized with minimal to none hazard effects on the environment. This study aimed to synthesize different solid materials, considering the 12 principles of green chemistry, achieving materials with high adsorbent capacities for phenol and phenol derivatives. The phosphonate metal-organic frameworks were obtained from the reaction between etidronic acid (HEDP)- as the organic component, and divalent (Co^{2+} , Ni^{2+} , Cu^{2+}) and trivalent (Ce^{3+}) metal salts- as the inorganic component, in hydrothermal conditions [1] using water as solvent. As a second step in the synthesis, the materials were impregnated with imidazolium based ionic liquids, namely 1-ethyl-3-methylimidazolium chloride and 1-hexyl-3-methylimidazolium chloride to increase their adsorption capacities, named IL@MOFs. The phenol and phenol derivatives adsorption have been tested and the following order illustrates the increased adsorption capacity of the studied materials: $\text{CuHEDP} < \text{NiHEDP} < \text{CoHEDP} < \text{CeHEDP}$. The highest adsorption capacity was obtained by materials impregnated with 1-hexyl-3-methylimidazolium chloride; best result was observed on CeHEDP (23,1 mg/g for 2,6-dimethylphenol). Experimental data showed strong concordance with Langmuir and Redlich-Peterson isotherms, indicating that phenol adsorption involves physical sorption [2].

Keywords

Phosphonate metal-organic frameworks, ionic liquids, physical adsorption, phenol and phenol derivatives

Acknowledgments

This work is partially supported by Program no 2, from the „Coriolan Dragulescu” Institute of Chemistry Timisoara, Romania and by a grant of the Ministry of Research, Innovation and Digitization, CNCS-UEFISCDI, project number PN-III-P4-PCE-2021-0089, within PNCDI III.

References

- [1] Y. Zhao, Z. Wang, Z. Bao, H. Xing, Z. Zhang, B. Su, Q. Yang, Y. Yang, Q. Ren, *Separation and Purification Technology*. **2018**, *195*, 238-243.
- [2] L. Lupa, N. S. Tolea, **M. Iosivoni**, B. Maranescu, N. Plesu, A. Visa, *RSC Advances*. **2024**, *14*, 4759-4777.

A Breakthrough in Wearable Electronics: Flexible Natural Rubber Hydrogel Electrolytes

Fathiah KAMARULAZAM¹, M. PERSHAANAA¹, Zhi Ling GOH¹, G. SURENDER¹, N.K. FARHANA¹, S. RAMESH^{1*}, K. RAMESH¹

¹Centre for Ionics Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur, Malaysia

*Corresponding author: rameshtsubra@gmail.com

The rapid development of supercapacitors towards achieving the world's energy demand are suitable for flexible, wearable, and portable electronic applications. Typically, liquid electrolytes have been crucial due to their high ionic conductivities and good contact with electrodes, but they have brought risks of electrolyte leakage. Solid electrolytes are remarkably safe and might avoid the leakage issue of liquid electrolytes, but they encounter low ionic conductivity. For a new generation of flexible and lightweight energy storage systems, hydrogel electrolytes have emerged as the ideal electrolyte material. Their advantageous properties of stretchability, good ionic conductivities due to water content, and resistance to leakage, are promising candidates for supercapacitor. However, striking a balance between stretchability, remarkable ionic conductivity, and self-healing ability remains challenging. In this research. Thus, a novel approach involving the utilization of epoxidized natural rubber (ENR)/acrylamide (AAm)/acrylic acid (AA) copolymer hydrogel electrolytes formed through a free radical mechanism was performed. To enhance the conductivity, hydrogel electrolytes were immersed in 1 M sodium sulfate (Na_2SO_4) salt solutions for varying periods. By capitalizing on the hydrogen bonding and electrostatic interactions within the hydrogels and the hydrogel-salt interaction, the resulting hydrogel exhibited an impressive ionic conductivity of 19.4×10^{-2} S/cm, a stretchability of 550 % from its initial length and demonstrated self-healing capabilities. By employing symmetrical porous carbon electrodes, the hydrogel-based electric double layer capacitor (EDLC) achieved an outstanding specific capacitance of 55.65 F/g, enduring stable cycling over 3500 cycles without significant discharge.

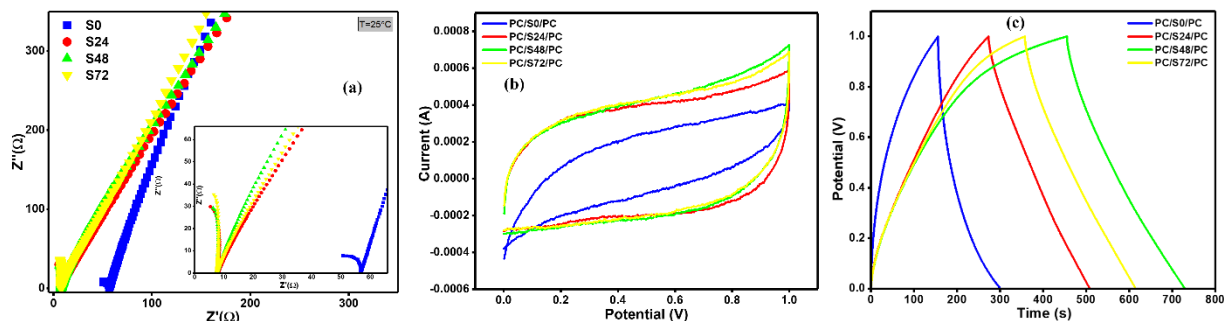


Figure 1. (a) Imaginary versus real impedance (Nyquist Plot) of all samples (b) CV curves of symmetric EDLCs of PC/S0/PC, PC/S24/PC, PC/S48/PC, PC/S72/PC at scan rate 5 mV/s (c) Comparison of GCD curves of PC/S0/PC, PC/S24/PC, PC/S48/PC and PC/S72/PC at 100 mA/g.

Keywords: Hydrogel electrolytes, Natural rubber, Electric double-layer capacitors, Sodium Sulfate

References

- [1] Guo, L.; Ma, W. Bin; Wang, Y.; Song, X. Z.; Ma, J.; Han, X. D.; Tao, X. Y.; Guo, L. T.; Fan, H. L.; Liu, Z. S.; et al. A Chemically Crosslinked Hydrogel Electrolyte Based All-in-One Flexible Supercapacitor with Superior Performance. *Journal of Alloys and Compounds*, **2020**, *843*, 155895.
- [2] Bashir, S.; Omar, F. S.; Hina, M.; Numan, A.; Iqbal, J.; Ramesh, S.; Ramesh, K. Synthesis and Characterization of Hybrid Poly (N, N-Dimethylacrylamide) Composite Hydrogel Electrolytes and Their Performance in Supercapacitor. *Electrochimica Acta*, **2020**, *332*, 135438.

Synthesis of Cyclometalated Platinum(II) Complex in a Green Solvent: Biological Evolutions

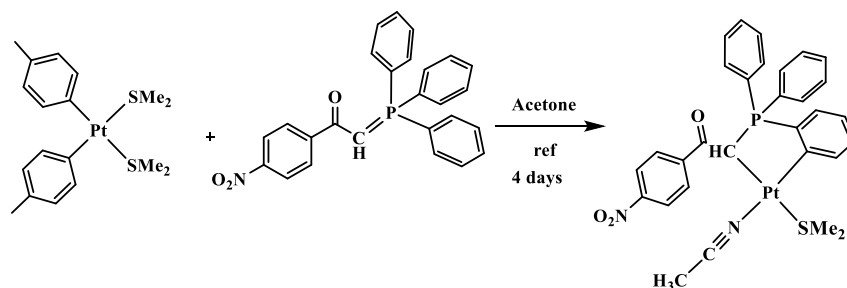
Faeze KAZEMI-ANDALIB, Hamid R. SHAHSAVARI*

Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, 45137-66731, Iran

*Corresponding author: shahsavari@iasbs.ac.ir

Cancer remains a leading cause of mortality worldwide, prompting extensive research efforts into the development of new treatment modalities and anticancer drugs. Among these, platinum-based chemotherapy drugs hold prominence, driving the quest for complexes with reduced side effects and comparable cytotoxicity.¹ This study focuses on the synthesis and characterization of a cyclometalated Pt(II) complex, [Pt(*p*-MeC₆H₄)(YPN)(CH₃CN)], **1**, derived from [Pt(*p*-MeC₆H₄)₂(SMe₂)₂],² and a phosphonium ylide ligand, YPN, Ph₃PC(H)C(O)C₆H₄NO₂.³ Notably, the use of acetone as a green solvent for synthesis highlights eco-friendly synthesis practices.

The cytotoxicity of **1** was evaluated across various human cancer cell lines, including A549 (lung), MCF-7 (breast), and HeLa (cervical), alongside a normal lung fibroblast cell line (MRC-5).⁴ Results indicate promising anticancer activity with a selective effect on cancerous cells, particularly evident in MCF-7 cells. Interestingly, **1** demonstrated greater selectivity towards cancer cells compared to cisplatin while also inducing apoptosis, thereby elucidating its potential as an effective anticancer agent.



Scheme 1. Synthetic routes for the preparation of **1**.

Keywords:

Organometallic, Platinum, Green solvents.

Acknowledgments

This work was supported by the Institute for Advanced Studies in Basic Sciences (IASBS) Research Council and the Iran National Science Foundation (Grant no. 4015454).

References

- [1] S. Alassadi, M. J. Pisani, N. J. Wheate, *Dalton Trans.*, **2022**, 51, 10835-10846.
- [2] M. Rashidi, M. Hashemi, M. Khorasani-Motlagh, R. J. Puddephatt, *Organometallics.*, **2000**, 19, 2751-2755.
- [3] S. J. Sabounchei, F. Kazemi Andalib, M. Hosseinzadeh, A. Sedghi, A. Hashemi, R. Karamian, K. Van Hecke, *Appl. Organomet. Chem.*, **2020**, 34, e5265.
- [4] M. Fereidoonzhad, H. R. Shahsavari, S. Abedanzadeh, A. Nezafati, A. Khazali, P. Mastrorilli, M. Babaghasabha, J. Webb, Z. Faghieh, Z. Faghieh, *New J. Chem.* **2018**, 42, 8681-8692.

Enzymatic Synthesis of Amino Acid-Based Surfactants

Dmitrii KURNOSOV¹, Luca BANFI¹

¹Università di Genova – Dipartimento di Chimica e Chimica Industriale, Via Dodecaneso, 31, 16146 Genova

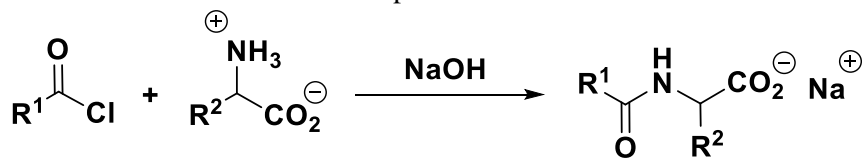
*Corresponding author: kurnosov.dimitri@gmail.com

Surfactants are chemical substances, that reduce surface and interfacial tension due to the hydrophilic and hydrophobic parts of the molecules. They are widely used in various fields of human activity: cosmetic, food, textile industries; cleaning; oil and gas extraction.

Generally, oil is the main source of raw material for their production. However, oil is non-renewable and its extraction is not environmentally friendly. Also, surfactants with petrochemical origin are not biodegradable, and once in ecosystems can damage it. Therefore, recent time growing interest in developing of eco-friendly surfactants with low toxicity, high biodegradability and efficiency.

Over the past twenty years, interest in amino acid-based surfactants has strongly increased due to its excellent properties and possibility of using renewable raw materials – amino acids and plant oils¹.

The most common method for synthesis of N-acyl amino acids is Schotten-Baumann acylation of amino acids (Scheme 2). This reaction can be carried out at low temperature in water.

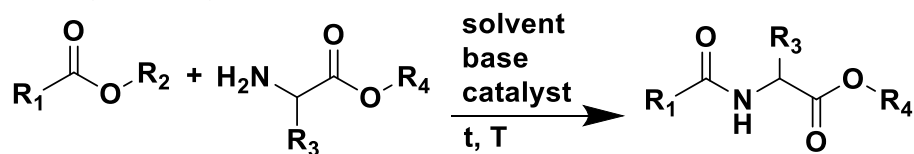


Scheme 1. Schotten-Baumann acylation.

However, the synthesis of acyl chlorides is environmentally unfriendly, toxic reagents are used (SOCl₂, COCl₂, PCl₃, POCl₃, PCl₅) in stoichiometric quantities to form them².

Catalytic routes allow to improve atom economy and reduce the environmental impact. Enzymatic alternatives led to use nontoxic and biodegradable wild-type and engineered enzymes as the catalyst³.

Due to catalytic mechanism acyl chlorides can be replaced with fatty acid esters; as the acyl acceptor can be used esters of amino acids (Scheme 2).



Scheme 2. Enzymatic amide formation.

In this work, it was identified the best solvent, enzyme, base, initial reagents and reaction conditions to obtain the highest yield.

References

- [1]. Danyelle Khadydja F Santos, Raquel D Rufino, Juliana M Luna, Valdemir A Santos, Leonie A Sarubbo, Biosurfactants: Multifunctional Biomolecules of the 21st Century, International Journal of Molecular Sciences, **2016**, 17 (3), 401.
- [2]. Christian A. G. N. Montalbetti, Virginie Falque, Amide bond formation and peptide coupling, Tetrahedron, **2005**, 61, 10827–10852.
- [3]. Roger A. Sheldon, John M. Woodley, Role of Biocatalysis in Sustainable Chemistry, Chemical Reviews, **2018**, 118 (2), 801–838.

The Evolution of MXene Synthesis: Towards Using Green Solvent

Jerome LIEW¹, Prasankumar THIBORCHEWS^{1,2}, Shahid BASHIR³, Ramesh KASI¹, Ramesh SUBRAMANIAM^{1,4*}

¹Centre of Ionics Universiti Malaya, Department of Physics, Faculty of Science, Universiti Malaya, 50603 Kuala Lumpur, Malaysia

²Institute of Power Engineering, College of Engineering, University Tenaga Nasional (UNITEN), 43000 Kajang, Selangor, Malaysia

³Higher 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

⁴Department of Chemistry, Saveetha School of Engineering, Institute of Medical and Technical Science, Saveetha University, Chennai 602105, Tamilnadu, India

*Corresponding author: ramesh@um.edu.my

In the past decade, the research volume of MXenes has been increasing due to its exceptional properties arising from its peculiar nature. MXenes are a group of two-dimensional (2D) transition metal carbides (nitride, or carbonitride); with transition elements as their core and unique morphology and surface termination, MXene possesses outstanding conductivity, mechanical integrity, and aspect ratio. Its inherent properties have caused the research and applications of MXenes to bloom in the fields of energy storage and harvesting systems, and electromagnetic applications. Combined with its benignity towards human biology, MXene has been explored in the applications of biosensors and drug delivery systems. Nonetheless, despite the potential MXene can bring about, its commercialization is not without challenges, one of which is the toxicity involved in the synthesis of MXenes. The use of hydrofluoric acid (HF) as an etchant remains prominent and widespread for its etching prowess. Regardless, the dangers of HF exposure can never be understated. Even though HF-forming mixtures (*in situ* HF) are popular alternatives, their etching efficiency is limited, and therefore the possible MXene configurations can be safely produced. Hence, to progress in the commercialization of MXenes, a safer and more efficient solution must be used. We have optimized safe and efficient MXene synthesis by hydrothermal-assisted etching, whereby high temperatures and pressures are utilized to enhance the etching efficacy of *in situ* HF, and even green solvents. The increased etching prowess has greatly improved the extent of exfoliation of MXene precursors (mostly known as MAX phases), as shown in Figure 1. This enables the widespread use of green solvents as etchants and hydrothermal-assisted etching, and the production of highly exfoliated MXenes without the negatives of using HF. The progress made is a great step forward in the commercialization of MXenes and unleashing their potential.

Evolution of MXene Synthesis – From HF Etching to Green Solvent Etching

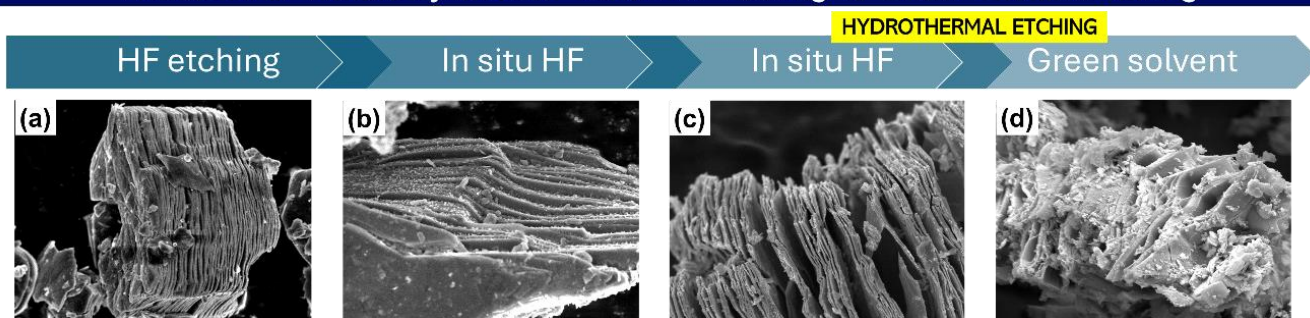


Figure 1. FESEM images of MXene synthesized by different etchants and etching approaches.

Reuse of Textile Effluents Treated by Electrooxidation with Green Hydrogen Cogeneration: A Sustainable Solution for the Textile Industry

Herbet LIMA OLIVEIRA^{1*}, Myllena Kelly PEREIRA FERREIRA², José Heriberto OLIVEIRA DO NASCIMENTO¹, Carlos Alberto MARTÍNEZ-HUITLE¹, Elisama VIEIRA DOS SANTOS¹

¹Federal University of Rio Grande do Norte, Natal/RN, Brazil

*Corresponding author: herbet.lima.097@ufrn.edu.br

The textile industry is one of the industrial sectors that consumes the most water and generate contaminated effluents in the world [1], requiring around 30 to 50 L of water for each kilogram of fiber in the dyeing process [2]. Furthermore, wet processes in the textile industry consume large amounts of energy, especially for dyeing and washing, which use thermal energy [1]. In this context, it is essential to seek new strategies to develop a more sustainable textile production system. The present work aimed to develop a hybrid process for treating textile effluents from dyeing, with the cogeneration of green hydrogen through electrochemical technology. Furthermore, the dyeing process reused the treated effluent. The effluents used were obtained from a dyeing process in a proportion of 200 mL for 5 g of cotton fiber in a Mathis ALT-1-B machine, using a dye bath with BG-4G yellow reactive dyes (0.15 g/L), blue DC-2G (0.15 g/L) and/or red BG-3B (0.20 g/L), in addition to Na₂SO₄ (10.0 g/L), Na₂CO₃ (25.0 g/L) and NaOH (1.5 g/L). Monochromatic and trichromic (mixture of the three dyes) dyeings were carried out. The electrochemical system was composed of a cell divided by an anion exchange membrane. The divided electrochemical reactor is made up of anodic and cathodic compartments, separated by an anion-exchange membrane (AEM) with a DSA electrode (Ti/RuO₂IrO₂TiO₂) electrode as an anode (10 cm²) and a stainless steel (SS, Ni-Fe based) mesh as a cathode. The electrolysis of 1 L of textile effluent in the anodic compartment was carried out via recirculation at a constant flow rate of about 167 mL min⁻¹ using a peristaltic pump. The cathodic compartment was connected to an additional reservoir (5) to collect the green H₂ produced, which was measured at predetermined time intervals, parallel to the analysis of the anode compartment [3]. All energy in the system was supplied by solar energy. To determine the level of oxidation j of 100 mA/cm² was applied and each treatment lasted 10 h. Initially, the removal of organic matter, in terms of COD rates of 97.23%, 99.30%, 99.81% and 98.16% were achieved, and COD rates of 54.92%, 57.92%, 71.31% and 46.53% for yellow, red, blue and trichrome dyes, respectively. Regarding green H₂, there were no significant discrepancies between the different effluents, with an approximate production of 7.35 L of H₂ in 10 h. The reuse of the effluent treated in dyeing was based on trichromic dyeing, carrying out three dyeing cycles: the first with fresh water, the second with treated water from the first dyeing and the third with treated water from the second dyeing. In each cycle, dyes were added, but it was not necessary to add more salts. The dyed fabrics demonstrated uniformity in color between cycles. Color removal in each treatment decreased with increasing cycles, being 98.16%, 97.52% and 95.81% for the first, second and third cycles, respectively. These results demonstrate the feasibility of a highly sustainable and economical approach to the textile dyeing process, allowing to treat the effluent and reuse the treatment water in new dyeing cycles, with just the addition of dyes and without the need to add salts. Furthermore, the green hydrogen produced can be applied in energy processes within the textile industry or as a clean fuel for transport.

References

- [1] K. Farhana, K. Kadirgama, A.S.F. Mahamude, M.T. Mica, *Materials Circular Economy* **2022**,4, 15.
 [2] F. Uddin, *Cellulose* **2021**, 28, 10715-10739.
 [2] H.L. Oliveira, T.M. Barros, J.E.L. Santos, A.D. Gondim, M.A. Quiroz, C.A. Martínez-Huitile, E.V. dos Santos, *Electrochemistry Communications* **2023**, 154, 107553.

Energy-Saving Electrochemical Green Hydrogen Production Coupled With Active Chlorine Species Valorization

Karen G. Duarte MAGALHÃES^{1,*}, Maiara B. FERREIRA¹, Jussara C. CARDOZO¹, José Heriberto O. DO NASCIMENTO¹, Carlos A. MARTINEZ-HULTLE¹ Elisama V. DOS SANTOS¹

¹Federal University of Rio Grande do Norte, Natal/RN, Brazil

*Corresponding author: karen.magalhaes.700@ufrn.edu.br

The goal of diversifying energy has become a global priority, driven not only by the need to mitigate greenhouse gases, but also by the urgent need to combat global warming. In this context, the green hydrogen is increasingly becoming a target for commercial exploitation for application in the industrial, residential, commercial and transportation energy sectors. (Nazir *et al.*, 2020; Karmaker *et al.*, 2022). There is also a growing debate about the adoption of other hydrogen production routes with a focus on carbon neutrality. Brito (2015) analyzed the evolution of active chlorine species in NaCl solutions, to degrade and mineralize total organic load and the percentage of color removal of the textile dye to evaluate the applicability of this electrochemical technology. In this research, both green hydrogen and sodium hypochlorite were produced by electrochemical treatment of synthetic 0.025, 0.043 and 0.06 M NaCl solutions. The electrochemical system was realized using a solar-powered cationic membrane cell with a DSA-type electrode (Ti/RuO₂IrO₂TO₂) as anode and a Ni-Fe-based SS (stainless steel) mesh as cathode, applying a current density of 50 mA/cm². As a result, there was a production of hydrogen that followed the linear compartment (Figure 1a), and the parameters of energy consumption and faradaic efficiency varied in a range from 0.0260 to 0.0406 kWh and 81.43 to 90.79 %, respectively, according to the concentration of NaCl. In the production of chlorinated species, Figure 1b illustrates the production of sodium hypochlorite by time, and it can be seen that from 30 min onwards production stabilizes in all experiments with concentrations of approximately 0.6 mM. Therefore, the electrochemical treatment of saline effluents, as well as producing an energy vector (H₂) and value-added products. To conclude, future experiments are expected to use real effluents from the salt industry.

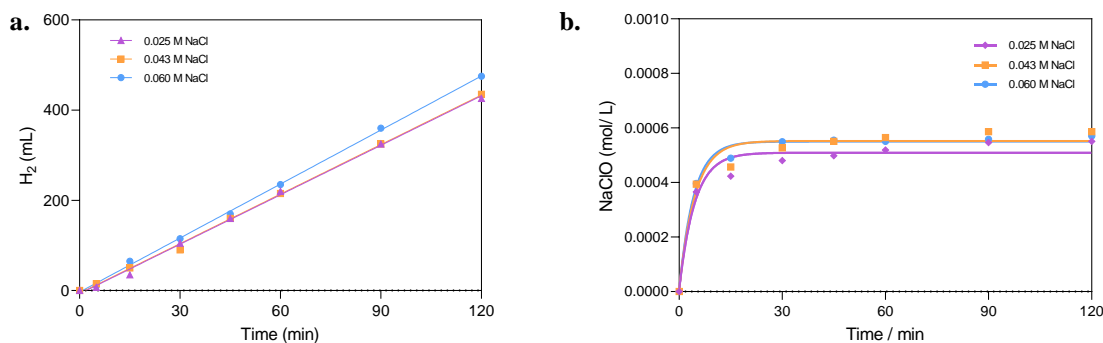


Figure 1a. Volume of dry H₂ produced **b.** Evolution of sodium hypochlorite concentration over time.

References

- [1] C. do Nascimento Brito, D.M. de Araujo, C.A. Martinez-Huitle, M.A. Rodrigo. Understanding active chlorine species production using boron doped diamond films with lower and higher sp³/sp² ratio, *Electrochem. Commun.*, **2015**, 55, 34–38.
- [2] Karmaker *et al.* Renewable energy pathways toward accelerating hydrogen fuel production: evidence from global hydrogen modeling. *Sustainability*, **2022**, v. 15, n. 1.
- [3] Nazir *et al.* Is the H₂ economy realizable in the foreseeable future? Part I: H₂ production methods. *International Journal of Hydrogen Energy*, **2020**, v. 45, n. 27, p. 13777-13788.

Sustainable valorization of cherry (*Prunus avium* L.) pomace waste via the combined use of (NA)DESs and bio-ILs

Angelica MERO¹, Andrea MEZZETTA^{1,2}, Marinella DE LEO^{1,2,3,*}, Alessandra BRACA^{1,2,3}, Lorenzo GUAZZELLI^{1,2,*}

¹Department of Pharmacy, Via Bonanno 33, Pisa, Italy

²Centre for Instrumentation Sharing, University of Pisa (CISUP), Lungarno Pacinotti 43, Pisa, Italy

³Interdepartmental Research Center Nutrafood “Nutraceuticals and Food for Health”, University of Pisa, Via del Borghetto 80, Pisa, Italy

*Corresponding authors: marinella.deleo@unipi.it, lorenzo.guazzelli@unipi.it

Sweet cherry pomace waste (CPW) still contains significant amounts of dietary fiber and added value compounds like polyphenols. Hence, in line with the circular economy concept, CPW can be employed as renewable feedstock to produce novel commodities, bioactive compounds and bio-functional materials. In this study, a sustainable biorefinery approach was developed using natural deep eutectic solvents (NADESs) to recover polyphenolic compounds^[1] and bio-based ionic liquids (bio-ILs) to treat and convert the remaining lignocellulosic residue into an ionogel^[2] (Fig. 1). The efficiency and selectivity of various (NA)DESs were assessed by varying both the hydrogen bond acceptor and donor, HBA and HBD. The extracted phenolic compounds were qualitatively and quantitatively analyzed by UHPLC-HR-ESI-MS, leading to the identification of over 25 compounds, classified into four main subclasses (phenolic acids, flavonoid glycosides, flavonoid aglycones, and anthocyanins). Choline chloride:ethylene glycol (ChCl:EG) 1:2 was identified as the best performing system in terms of total phenolic content and was used as the extraction medium for the optimization of the operative conditions and recycling studies. The solvent was quantitatively recovered for three cycles maintaining extraction efficiency. Finally, cellulose enriched material was obtained using cholinium arginate and was subsequently dissolved at 2 wt% in cholinium levulinate to prepare a weak physical ionogel, a functional biomaterial with potential applications in the medical and pharmaceutical sectors.

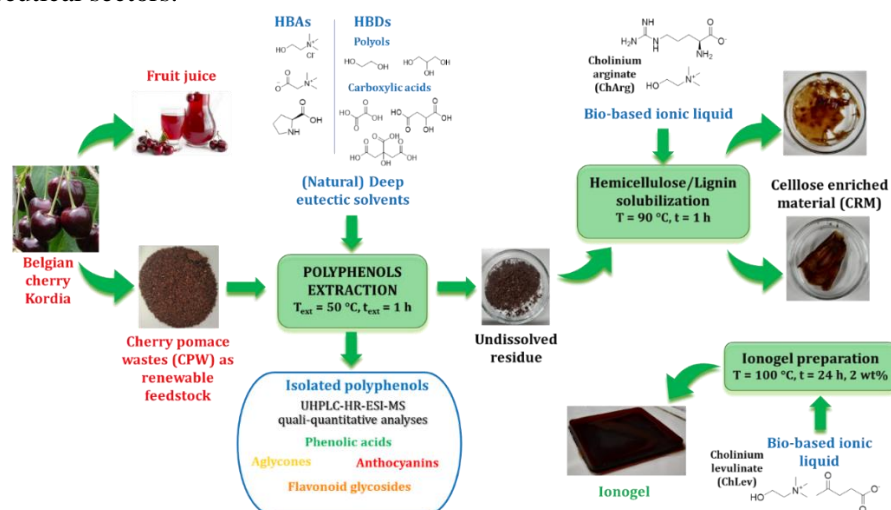


Figure 1. Scheme of the developed biorefinery approach aimed at the complete valorization of CPW.

References

- [1] R. F. Gonzalez-Laredo, V. I. Sayago-Monreal, M. R. Moreno-Jimenez, N. E. Rocha-Guzman, J. A. Gallegos-Infante, L. F. Landeros-Macías, M. Rosales-Castro, *International Journal of Food Science and Technology* **2023**, 58, 6660-6673.
- [2] E. S. Morais, A. M. da Costa Lopes, M.G. Freire, C. S. R. Freire, J. A. P. Coutinho, *Molecules* **2020**, 25, 365.

Green synthesis of nano hybrids as an alternative against cancer

**Ingrid MEZA¹, Daniela CHÁVEZ², Daniel SÁNCHEZ¹, Demetrio MENDOZA³, Beatriz MORALES⁴,
Elías PÉREZ¹, Daniela SALADO^{1,5*}**

¹*Institute of Physics, Autonomous University of San Luis Potosí, 78210 San Luis Potosí, SLP., México*

²*Faculty of Chemical Sciences, Autonomous University of San Luis Potosí, 78210 San Luis Potosí, SLP, México.*

³*ININ, National Institute of Nuclear Research, 52750 La Marquesa, México.*

⁴*School of Engineering, Autonomous University of San Luis Potosí, 78210 San Luis Potosí, México.*

⁵*Researchers for Mexico, CONAHCyT, Av. Insurgentes Sur 1582, Col. Crédito Constructor, C.P. 03940, México City, México.*

*Corresponding author: daniela.salado@conacyt.mx

Curcumin (CUR), extracted from *Curcuma longa*, is recognized for its antitumoral properties [1]. However, its hydrophobicity limits its clinical efficacy. This work aims to improve the physicochemical properties of CUR through green nano hybrid synthesis using curcumin, iron and trimesic acid as coordinating agents. We implemented two green synthesis routes: a wet-soft technique (SH) and mechanochemistry (SM). Three batches of each type of synthesis were produced to verify their reproducibility, forming polyhedral and spherical structures with average sizes of 87 and 30 nm, respectively. Using EDS, we confirmed the chemical composition of the nano hybrids, which includes carbon, oxygen and iron. X-ray diffraction (XRD) and Raman spectroscopy validated the structure of the materials, highlighting that iron is present in the hematite phase (α -Fe₂O₃). Infrared (IR) spectroscopy detected the characteristic bands corresponding to the complex, retaining the same spectrum as the original materials. Hydrodynamic size analyses (DLS) showed average sizes of 1047.86 ± 186.3 nm for SH and 1265.36 ± 157.27 nm for SM, with polydispersity indices of 0.26 ± 0.03 and 0.45 ± 0.05 , respectively. Zeta potential measurements across a pH range of 3 to 11 revealed that the materials maintain a negative surface charge between -31.68 to -2.5 mV. Turbidity tests indicated higher stability in sulfate buffer supplemented with 4% fetal bovine serum. Additionally, cytotoxic evaluation was performed on normal cell lines (HaCaT and HPrEC), and cancer cell lines (HeLa and PC-3). The results showed that the cytotoxic response of the materials is cell type selective under the evaluated conditions.

The results demonstrate the potential of green, eco-friendly, one-step synthesis methods to improve the properties of curcumin. Promoting a future alternative to conventional cancer treatments. This addresses a significant concern due to the incidence and prevalence of cancer in Mexico.

Acknowledgements: MEZA thanks CONAHCyT for the support provided through the postdoctoral fellowship. The authors also thank CONAHCyT for the funding provided by the Proyectos Ciencia de Frontera CF-2023-I-1196 and 102986. Additionally, they express their gratitude to Bernardo Yáñez Soto of the Laboratorio Nacional de Ingeniería de la Materia Fuera de Equilibrio (LANIMFE) and Luz E. Alcántara Quintana of the Coordinación para la Innovación y Aplicación de la Ciencia y Tecnología (CIACyT) for their facilities.

References

- [1] Y. S. Fu, T. H. Chen, L. Weng, L. Huang, D. Lai, and C. F. Weng, "Pharmacological properties and underlying mechanisms of curcumin and prospects in medicinal potential," *Biomedicine and Pharmacotherapy*, vol. 141. Elsevier Masson s.r.l., Sep. 01, 2021. doi: 10.1016/j.biopha.2021.111888.

Construction of Ru(II) Complexes Bearing Diphosphinoferrocene Ligands: Electrochemical and Biological Investigations

Shadi MOHAMMADIAN, Sayed HABIB KAZEMI,* Hamid R. SHAHSAVARI*

Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, 45137-66731, Iran.

*Corresponding authors: habibkazemi@iasbs.ac.ir; shahsavari@iasbs.ac.ir

Since the antitumor activity of cisplatin was discovered in 1969, inorganic chemists have been motivated to extend their studies in medical science. Despite its high supply and demand as the first clinical anticancer drug, cisplatin has an undeniable side. Therefore, designing an anti-cancer drug with the fewest side effects is a great challenge.¹ For these reasons, the use of platinum-based anti-cancer drugs has decreased, and the efforts to design, prepare, and develop new metallodrugs based on other metals for chemotherapy have increased. Ruthenium-based compounds can be mentioned as one of the best candidates for chemotherapy and clinical development.² The redox-active binuclear ruthenium(II) complexes with the general formula $[(p\text{-cymene})_2\text{Ru}_2\text{Cl}_4(\mu\text{-P}^{\wedge}\text{P})]$, $\text{P}^{\wedge}\text{P} = 1,1'$ -bis(diphenylphosphino)ferrocene (dppf), $1,1'$ -bis(diisopropylphosphino)ferrocene (dippf), and $1,1'$ -bis(dicyclohexylphosphino)ferrocene (dcpf), have been synthesized, Figure 1, and characterized. To evaluate the potential of these complexes as anticancer agents, biological activities including cytotoxic activity, DNA interaction, and molecular docking were accomplished. Based on NMR data, these complexes had good stability in water as a green solvent for biological studies. Furthermore, the redox nature of these complexes was assessed by the cyclic voltammetry (CV) technique.

Keywords:

Ruthenium complexes, Anti-cancer drugs, Electrochemistry, Water

Acknowledgments

This work was supported by the Institute for Advanced Studies in Basic Sciences (IASBS) Research Council and the Iran National Science Foundation (Grant no. 99023593).

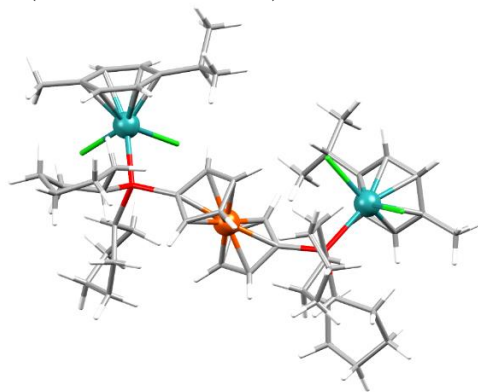


Figure 1. Optimized structure of a ruthenium(II) complex containing dcpf ligand.

[1] H. R. Shahsavari, J. Hu, S. Chamyani, Y. Sakamaki, R. Babadi Aghakhanpour, C. Salmon, M. Fereidoon nezhad, A. Mojaddami, P. Peyvasteh, H. Beyzavi, *Organometallics*, 2021, **40**, 72-82.

[2] S. Yarahmadi, E. Jekar, Z. Shamsi, D. Nahieh, M. Moosavi, M. Fereidoon nezhad, H. R. Shahsavari, *New J. Chem.*, 2023, **47**, 6266-6274.

Computational and Experimental Evaluation of Triazolium and Imidazolium-Based Ionic Liquids as Electrolyte for CO₂ Electrochemical Reduction

Sulafa Abdalmageed Saadaldeen MOHAMMED^{1,2,*}, Wan Zaireen Nisa YAHYA^{2,3*}, Rabea JAFFARI⁴, Manzoor Ahmed HASHMANI⁵, Fasee ULLAH⁵, Mohamad azmi BUSTAM^{2,3}, and Md Golam KIBRIA⁶

¹ Department of Energy, Aalborg University, 9220 Aalborg, Denmark

² Chemical Engineering Department, Universiti Teknologi PETRONAS, Seri Iskandar 32610, Perak, Malaysia

³ Centre for Research in Ionic Liquid, Universiti Teknologi PETRONAS, Seri Iskandar 32610, Perak, Malaysia

⁴ Software Engineering Department Mehran University of Engineering and Technology Jamshoro, 76260, Sindh, Pakistan

⁵ Computer and Information Sciences Department Universiti Teknologi Petronas Seri Iskander, 32610, Perak, Malaysia

⁶ Chemical and Petroleum Engineering, University of Calgary, 2500 University Drive NW, Calgary, AB T2N 1N4, Canada

*Corresponding author: sasm@energy.aau.dk

*Corresponding author: zaireen.yahya@utp.edu.my

Carbon dioxide (CO₂) electrochemical reduction (CO₂ER) shows great promise for mitigating CO₂ emissions and integrating with renewable energy sources. However, it faces technical challenges such as low electrochemical stability, high overpotential, low current density, and low faradaic efficiency, hindering industrial application. Ionic liquids (ILs) have gained attention for CO₂ER due to their high CO₂ solubility, electrochemical stability, reduced overpotential, and increased current density. This study evaluated novel triazolium-based and imidazolium-based ILs for CO₂ absorption and CO₂ER performance. The correlation between the molecular structures and orbitals of cations and anions on CO₂ solubility and CO₂ER performance was analyzed. CO₂ absorption capacity was determined using an isochoric saturation method and compared with predicted solubility using the Conductor-like Screening Model for Realistic Solvents (COSMO-RS). Electrochemical stability and CO₂ER performance were evaluated using cyclic voltammetry and chronoamperometry. Triazolium-based ILs generally showed higher CO₂ solubility compared to imidazolium-based ILs, with the highest capacity of 0.252 mol CO₂/mol IL exhibited by 1,4-dibutyl-1,2,4-triazolium bis(trifluoromethylsulfonyl)imide. The best CO₂ER performance was achieved with 1-ethyl-3-methylimidazolium tetrafluoroborate, reducing the applied potential by 320 mV compared to the reference electrolyte without IL. The computational modeling study reveals that ILs' molecular orbital energy levels significantly influence CO₂ capacity, with the anion's highest occupied molecular orbital (HOMO) having a greater impact on solubility than the cation's (LUMO). The results show that the reduction stability of the ionic liquid is not relying solely on the individual LUMO/HOMO values of cations or anions, but also the molecular interactions such as hydrogen bonds, electrostatic interactions, and van der Waals forces significantly influences the stability. Additionally, machine learning was used to investigate factors affecting CO₂ER performance, utilizing a novel dataset of electronic and geometric properties of 90 ILs formulated using COSMO-RS and TURBOMOLE. Our findings underscore the crucial role of anions with sulfur, fluorine, and oxygen in influencing both CO₂ solubility and catalytic processes, offering an explanation for discrepancies between solubility trends and catalytic activity, emphasizing interaction types.

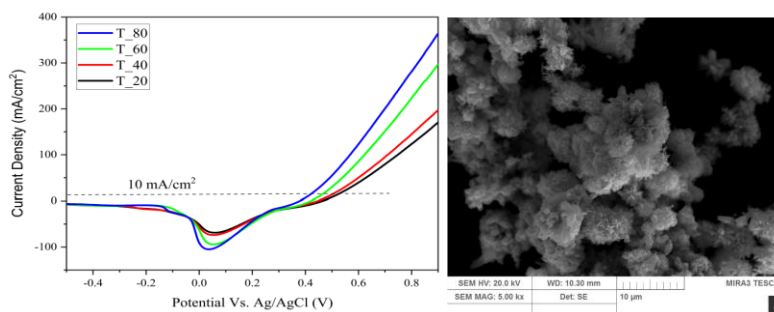
Investigating the Impact of Electrolyte Temperature on the Oxygen Evolution Reaction Efficiency of Ni-Co/NiFelt Nano Composite Electrode

Ataollah NIYATI*, Arianna MORANDA, Ombretta PALADINO**

Department of Civil, Chemical, and Environmental Engineering - Università Di Genova, Via Opera Pia 15, I-16145, Genoa, Italy

Email: ataollah.niyati@edu.unige.it, ombretta.paladino@unige.it

Anion exchange membrane water electrolysis (AEMWE) emerged as a viable alternative for producing eco-friendly-green hydrogen and has been a cornerstone in industrial hydrogen generation particularly through non-noble electrocatalysts [1]. Before testing the fabricated electrode inside the AEMWE, it is of paramount importance to test it inside a three-electrode setup. Many studies focused on a three-electrode setup for studying the electrochemical behavior of electrocatalysts at room temperature (25°C) while some considered the electrolyte temperature at 60-80 °C in the AEMWE cell related to industrial applications [2]. The electrolyte's temperature substantially impacts several aspects of the electrochemical reaction such as double-layer charging, electron charge transfer, diffusion in terms of mass transfer, and overall electrochemical processes at the electrodes. As a result, temperature changes affect the adsorption and dissociation of H₂O or OH⁻ species on electrocatalysts, as well as the production and desorption of H₂ and O₂ molecules from the surface of electrocatalysts [3]. To this end, a nanocomposite of Ni-Co is synthesized with the hydrothermal method followed by calcination and used as a binder-free method to coat this electrocatalyst onto the NiFelt as gas diffusion layer (GDL) [4]. The investigation used a standard threeelectrode setup, employing Pt wire as the counter electrode, Ag/AgCl as the reference electrode, and a selfmade Ni-Co/NiFelt nanocomposite electrode as the working electrode. Temperatures ranging from 20 to 80°C were tested to identify the optimal current density considering the stability. Various tests, including linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), chronopotentiometry, and chronoamperometry, were conducted to assess electrode activity. As expected, an increase in the KOH electrolyte temperature has shown an improvement in Oxygen Evolution Reaction (OER) kinetics. However, this rise in temperature compromised reaction stability due to increased conductivity, heightened hydrophilicity, more active sites, and reduced electrolysis resistance.



Keywords: Green Hydrogen, Non-noble Electrocatalysts, Ni-Co nanocomposite, Oxygen evolution reaction.

References:

- [1] K. Chand, O. Paladino, *Arabian Journal of Chemistry* 16 (2023) 104451.
- [2] M. Nishimoto, Z. Xiong, S. Kitano, Y. Aoki, H. Habazaki, *Electrochim Acta* 427 (2022) 140875.
- [3] A.Niyati, A. Moranda, J.F.Basbus, O. Paladino, "Unlocking the Potential of NiCo₂O₄ Nanocomposite: Morphology Modification via Urea Quantity, Hydrothermal and Calcination Temperature." *New Journal of Chemistry* (2024).
- [4] A. Niyati, A. Moranda, F. Navarra, A. Riva, M. Campione, G. Schiappelli, O. Paladino, *E3S Web of Conferences* 414 (2023) 01002.

Optimization of Phosphate and Nitrate Ions Adsorption Using LDH-Alginate Composite Beads: A Response Surface Methodology Approach

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

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

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

*Corresponding author: nouaasafa.pro@gmail.com

Phosphate and nitrate are essential micronutrients that play a critical role in biomass growth, energy storage, and agricultural activities. However, their elevated concentrations pose significant health risks to humans and other living organisms. Layered double hydroxides (LDHs) are known for their high selectivity and efficiency in removing phosphate and nitrate ions from water. Nonetheless, their tendency to agglomerate due to high surface properties makes recovery from aqueous solutions challenging. Functionalizing LDHs with biopolymeric materials, such as alginate, offers a promising solution to these issues.

In this study, we investigated the adsorptive removal of phosphate and nitrate ions from water using MgFe-LDHs assembled in alginate beads. We evaluated the removal efficiency and percentage, considering various influencing factors including sorbent dosage, solution pH, contact time, and the presence of co-ions. Additionally, we employed Response Surface Methodology (RSM) to optimize the adsorption conditions and maximize the adsorption capacity of the beads. Our results demonstrated that MgFe/Alginate beads exhibited exceptionally high removal efficiencies for both phosphate and nitrate ions under optimized conditions.

These findings suggest that MgFe/Alginate beads can serve as an effective and selective sorbent for the remediation of toxic ions from water and wastewater. The use of RSM for optimization not only enhanced the adsorption performance but also aligns with the principles of green chemistry by utilizing sustainable and environmentally friendly materials.

Sustainable Production of Activated Carbon From Waste Coconut Shells and Its Application in Wastewater Treatment

OGUNLETI DANIEL¹, k.O BADMUS BADMUS²

Department of Industrial Chemistry, First Technical University, Nigeria

INTRODUCTION Water pollution due to industrialization and improper waste disposal introduces toxic metals like lead, cadmium, and mercury into natural water sources, posing serious environmental and health risks. Conventional removal methods, such as precipitation and ion exchange, have drawbacks like secondary pollution and high costs. Activated carbon (AC) emerges as a superior alternative due to its sustainable production from coconut shells, offering high adsorption capacity and recyclability without generating additional pollutants. This approach supports environmental sustainability by repurposing waste materials and reducing energy consumption in water treatment processes.

ABSTRACT

The carbonized shells was chemically characterized during activation and the subsequent products was analyzed with FTIR by our team at First Technical University, Nigeria. The treatment processes was carried out with the best product and utilized under various conditions including varied pH, contact time and amount of product used with the corresponding results analyzed with UV spectrophotometer to emphasize optimal conditions.

MATERIALS & METHODS

The study utilized coconut shells as a carbon precursor and calcium chloride (CaCl₂) as an activating agent to produce activated carbon. Coconut shells were cleaned, dried, and thermally treated at 250°C to remove moisture and volatile components. After blending and sieving, carbonization was conducted at 650°C in an oxygen-limited environment. Chemical activation involved mixing CaCl₂ with carbonized biochar, followed by sonication and washing. FTIR analysis characterized functional groups, crucial for adsorption properties. UV-spectrophotometry calibrated with copper sulfate solutions measured adsorption efficiency under varied conditions: activated carbon quantity, pH, metal concentration, and contact time. These methods aimed to optimize activated carbon performance in removing toxic metals from wastewater.

RESULTS & DISCUSSION

The activated carbon exhibited low ash content (0.76%) and high carbon content (72.4%), indicating suitability for effective adsorption without interference from minerals. FTIR analysis identified functional groups like hydroxyl (-OH) and carbonyl (C=O), crucial for adsorption capacity. UV spectroscopy calibration showed a strong linear relationship ($R^2 = 0.9985$) between absorbance and CuSO₄ concentration, validating its use in quantifying metal ions in treated wastewater. Optimal conditions for CuSO₄ removal included acidic pH (pH 3) and higher amounts of activated carbon (3 grams), with extended contact time (30 minutes) enhancing efficiency. The study recommends utilizing waste coconut shells for sustainable activated carbon production and underscores the material's versatility in treating wastewater with varying heavy metal concentrations.

Optimization of MOF-199-Based Solid-Phase Microextraction Coatings Synthesis for an Efficient Quantification of Volatile Organic Compounds in Air

Anara OMAROVA¹, **Nassiba BAIMATOVA**^{1*}, **Hossein KAZEMIAN**^{2,3*}

¹ Center of Physical Chemical Methods of Research and Analysis, Faculty of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty, Kazakhstan

² Northern Analytical Lab Services (Northern BC's Environmental Solutions Innovation Hub), University of Northern British Columbia, Prince George, BC, Canada

³ Chemistry Department, Faculty of Science and Engineering, University of Northern British Columbia, Canada

*Corresponding authors: baimatova@cfhma.kz,
hossein.kazemian@unbc.ca

Solid-phase microextraction (SPME) is an eco-friendly sample preparation technique used in combination with various methods including gas chromatography (GC). Unlike conventional methods that involve time-consuming extraction, concentration, and filtration processes, and require large sample volumes and toxic solvents, SPME combines these steps into a single stage. This is achieved using SPME fibers, with thicknesses ranging from 7 to 100 μm , which are inserted into the sample or the headspace above the sample in a hermetically sealed vial during extraction. Extraction is performed under pre-optimized conditions, including time and temperature, until equilibrium between analyte concentrations in the sample and in the SPME coating is reached. Afterward, the fiber is transferred to the GC inlet to desorb the analytes at high temperatures for further analysis and quantification of their levels [1].

Commercially available SPME coatings have several drawbacks, including low surface area and selectivity. These limitations have increased interest in developing coatings based on various materials such as metal-organic frameworks, ionic liquids, layered double hydroxides, molecularly imprinted polymers and conductive polymers [2].

In this study, the synthesis of SPME coatings based on the metal-organic framework MOF-199 was optimized to develop alternatives to commercially available fibers, featuring advanced properties such as higher surface area and porosity. Several parameters, including solvent, copper salt, and the addition of a modulator, were optimized. The developed MOF-199-based SPME coatings, with thicknesses varying from 6 to 62 μm , were applied for the quantification of volatile organic compounds (VOCs) in air [3]. The application of the obtained MOF-199 coatings enabled the development of an analytical method using gas chromatography with mass spectrometry detection for the quantification of benzene, toluene, ethylbenzene, and xylenes in air. This method achieved low detection limits (0.03–0.09 $\mu\text{g}/\text{m}^3$), high reproducibility (4.5–8.0%) and repeatability (1.0–6.4%) [3].

References

- [1] J. Pawliszyn, Handbook of solid-phase microextraction, Elsevier 2012.
- [2] A. Omarova, N. Bakaikina, A. Muratuly, H. Kazemian, N. Baimatova, Microchemical Journal 2022, 175, 107147.
- [3] A. Omarova, N. Baimatova, H. Kazemian, Microchemical Journal 2023, 185, 108263.

5,5'-[oxybis(methylene)]bis-2-Furfural (OBMF) One-Pot Green Synthesis from D-Fructose

Greta PALOMBELLA^a, Giacomo TRAPASSO^a, Fabio ARICÒ^{a,*}

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

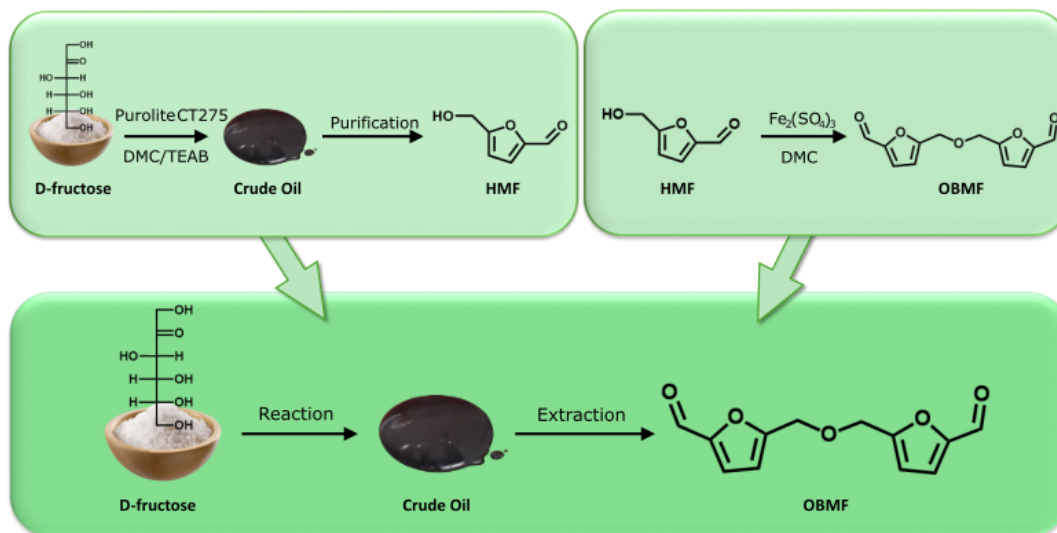
*Corresponding author: fabio.arico@unive.it

Bio-based platform chemicals are compounds obtainable from biomass that can be employed as starting materials for the production of chemical intermediates, building blocks and polymers. Among them, 5,5'-[oxybis(methylene)]bis-2-furfural (OBMF) is a bio-based platform chemical obtainable either via the self-etherification of 5-hydroxymethyl furfural (HMF) or as a side product from HMF synthesis. OBMF finds various applications mainly in the synthesis of macrocycles and as a precursor of polyurethanes, polyamides and polyamines.¹

Previous works have shown that it is possible to obtain OBMF from HMF with high yields applying a green synthetic approach.² However, this approach relies on high-purity HMF isolated via cold precipitation in the form of yellow crystals. In fact, reactions performed with raw HMF in the form of a brown oil did not yield comparable results.^{1,2}

From these premises, the present work aims to the one-pot green synthesis of OBMF from D-fructose with the in-situ formation of HMF. This approach will therefore avoid the isolation of HMF with consequent savings in term of solvents and work-up materials.

According to the best-found reaction conditions, OBMF could be detected by dissolving D-fructose in a mixture of dimethyl carbonate (DMC) and tetraethylammonium bromide (TEAB) in the presence of an acid heterogeneous sulfonic resin. A Dean-Stark apparatus seems to be necessary to remove water molecules forming both from the triple dehydration of D-fructose and after the self-etherification of HMF, thus promoting the thermodynamics of the process. These reaction conditions allowed the isolation of OBMF for the first time directly from D-fructose in *ca* 35 % yield.



References

- [1] M. Annatelli, G. Trapasso, D. D. Torre, L. Pietrobon, D. Redolfi-Bristol, F. Aricò, *Adv. Sustainable Syst.* 2022, 6, 2200297. <https://doi.org/10.1002/adsu.202200297>.
- [2] G. Trapasso, G. Mazzi, B. Chícharo, M. Annatelli, D. Dalla Torre, F. Aricò, *Org. Process Res. Dev.* 2022, 26, 10, 2830–2838. <https://doi.org/10.1021/acs.oprd.2c00196>.

Green Hydrogen production exploiting Capnophilic Lactic Fermentation pathway in the anaerobic hyperthermophilic bacterium *Thermotoga neapolitana*

Irene PASERO¹, Leonardo SETTI²

¹*Alma Mater Studiorum, University of Bologna*

²*Alma Mater Studiorum, University of Bologna*

*Corresponding author: irenepasero237@gmail.com

In today society, the necessity to fulfill the energetic demand worldwide has highlighted the need for new, renewable and sustainable sources of energy; among the possibilities, hydrogen drawn increasing attention as the only fuel not containing carbon, especially taking into consideration the possibility to produce it via fermentative pathways.

This research, entirely carried out in the laboratories of the Institute of Biomolecular Chemistry (CNR) in Pozzuoli, investigated the potential of the bacterium *Thermotoga neapolitana* to produce hydrogen, alongside acetic acid and lactic acid, by consuming glucose through two different metabolic pathways: Dark Fermentation and Capnophilic Lactic Fermentation (CLF).

The differentiation between the two pathways arises right after the step involving the glycolysis via EMP: in a Dark Fermentation, the produced pyruvate is further oxidized to acetate and the reducing equivalents (NADH) are consumed to produce hydrogen, while the lactate is only formed from the pyruvate in a side reaction after inhibition of the main one, when H₂ saturates the atmosphere (closed system), in order to keep consuming the NADH (in this fermentation H₂ and lactic acid compete for reducing equivalents).

In a CLF (requiring CO₂), instead, the formation of a bond between CO₂ and AcetylCoA allows to increase the production of lactic acid while maintaining unaltered the yield of hydrogen (particularly interesting because lactate is commercially more valuable than acetate).

The anaerobic systems for the analyses, were prepared by inoculating the bacterium in 120 mL sealed serum bottles filled with a liquid standard medium called TN and, then, the atmosphere was saturated by bubbling either N₂ or CO₂ in order to differentiate the performed pathway, Dark Fermentation and Capnophilic Lactic Fermentation respectively.

The production capacities of the systems were then further assessed over a range of different temperatures, more specifically at 65, 70, 80 and 85°C, taking into consideration the production of hydrogen, of main interest, alongside other important parameters, using the following procedures:

- pH, using a pHmeter, which shows an inhibiting property toward the biosynthesis if too acidic with respect to the optimal value of 7.5-8
- cellular growth. Measuring the change in optical density with an UV-Vis spectrophotometer
- glucose consumption, using an UV-Vis spectrophotometer, via DNS assay (colorimetric technique)
- hydrogen concentration in the headspace of the serum bottles, using a gas chromatograph
- organic acids concentration, with Nuclear Magnetic Resonance (¹H-NMR)

References

Pasero, & Setti, L. (2024). Green Hydrogen exploiting Capnophilic lactic Fermentation pathway in the anaerobic hyperthermophilic bacterium *Thermotoga neapolitana*. Alma Mater Studiorum - Università di Bologna.

Dipasquale, Laura, Giuliana D'Ippolito, and Angelo Fontana. 2014. "Capnophilic Lactic Fermentation and Hydrogen Synthesis by *Thermotoga Neapolitana*: An Unexpected Deviation from the Dark Fermentation Model." In International Journal of Hydrogen Energy

Design of Novel Heterogeneous Biocatalysts for the Enantioselective Synthesis of β -Hydroxy Acids

Giulio POTA^{1*}, Daniel ANDRÉS-SANZ², Marta GALLEGO², Giuseppe VITIELLO^{1,3}, Fernando LÓPEZ-GALLEGO^{2,4}, Aniello COSTANTINI¹, Valeria CALIFANO⁵

¹ Department of Chemical, Materials and Production Engineering, University of Naples Federico II, Piazzale Tecchio 80, 80125 Fuorigrotta, Naples, Italy.

² Center for Cooperative Research in Biomaterials (CIC biomaGUNE), Basque Research and Technology Alliance (BRTA), 20014 Donostia-San Sebastián, Spain

³ CSGI, Center for Colloid and Surface Science, Sesto Fiorentino (FI), Italy.

⁴ IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

⁵ Institute of Science and Technology for Sustainable Energy and Mobility (STEMS), National Research Council of Italy (CNR), Viale Marconi 4, 80125 Naples, Italy.

*Corresponding author: giulio.pota@unina.it

Lipases are industrially attractive biocatalysts for green organic chemistry, being involved in the synthesis of enantiopure precursors of drugs, cosmetics and polymers like β -hydroxy acids. However, substrate accessibility is regulated by the lid, a polypeptide chain which opens and frees the active site as the enzyme is adsorbed onto a hydrophobic surface (interfacial activation).¹ This study examines the adsorption of lipases from *Candida antarctica B* (CALB) and *Rhizomucor miehei* (RML) onto hydrophobic wrinkled silica nanoparticles (WSNs), which have been hydrophobized using chemical vapor deposition. Both lipases are evenly distributed within the nanoparticle pores, as confirmed by Transmission Electron Microscopy and Energy Dispersive X-ray measurements. The maximum enzyme load of CALB is twice that of RML. Fourier Transform Infrared Spectroscopy confirms that the secondary structure of both enzymes remains intact after immobilization. Adsorption isotherms follow a Langmuir model, with RML exhibiting a binding constant (K_L) 4.5 times higher than CALB, indicating stronger binding. Kinetic analysis shows a positive correlation between RML activity and enzyme load, while CALB activity decreases with increasing enzyme load. Moreover, the analysis of catalytic efficiency k_{cat}/K_m reveals stronger hyperactivation and higher sensitivity to interfacial activation on the superhydrophobic surface of WSNs for RML, due to the bigger lid size this protein exhibits with respect to CALB's. CALB demonstrates superior performance in the hydrolysis of ethyl-3-hydroxybutyrate (E3HB), yet immobilized CALB produces 20% less 3-HBA than its free form, whereas immobilized RML yields three times more 3-hydroxybutyric acid (3-HBA) compared to the free enzyme. Furthermore, soluble enzymes are both enantioselective towards the hydrolysis of (R)-E3HB, whereas adsorption leads RML to become (S)-selective. Finally, immobilization enhances both thermal, pH and operational stability of both lipases, being fully reusable in 10 consecutive reaction cycles.²

In the end, chemical vapor deposition proved to be a successful strategy to hydrophobize the surface of mesoporous silica nanoparticles, paving the way for the design of effective heterogeneous lipase-based biocatalysts to be used in the synthesis of enantiopure fine chemicals.

References

[1] P. Adlercreutz, *Chem. Soc. Rev* **2013**, 42, 6406-6436.

[2] G. Pota et al. *International Journal of Biological Macromolecules* **2024**, 131022.

Exploring the potential of Levoglucosenone: from cellulose biomass to the synthesis of aminosugar derivatives

Debora PRATESI¹, **Francesca CLEMENTE¹**, **Massimiliano MARVASI²**, **Andrea GOTI¹**, **Francesca CARDONA¹**, **Camilla MATASSINI^{1,*}**

¹ Dipartimento di Chimica ‘Ugo Schiff’ (DICUS), Università degli Studi di Firenze, via della Lastruccia n. 3-13, Sesto Fiorentino (FI) 50019, Italy.

² Dipartimento di Biologia (BIO), Università degli Studi di Firenze, via Madonna del Piano n. 6, Sesto Fiorentino (FI) 50019, Italy.

*Corresponding author: camilla.matassini@unifi.it

Pyrolysis is one of the more promising technologies for using biomass in the production of high added value synthetic intermediates. In particular, levoglucosenone (**1**),¹ a small molecule with a highly functionalized structure, is obtained from the pyrolysis of cellulose, as well as of urban and industrial residual materials containing cellulose, such as wastepaper. Levoglucosenone (**1**) is a valuable intermediate to produce high added value biologically active synthetic compounds, such as aminosugars, nitrogenated glycomimetics known as antibacterial agents.² In this context, we were able to obtain a series of aminosugar derivatives **4** through the sigmatropic cyanate to isocyanate rearrangement reaction starting from levoglucosenone-derived carbamate **2** (Figure 1). The process involves three steps, which are usually performed in one-pot: initial dehydration of the carbamate to the corresponding elusive cyanate, followed by spontaneous [3,3]-sigmatropic rearrangement to the isocyanate, which is conveniently trapped with a nucleophile (*O*-, *N*- or *S*-nucleophiles) to afford nitrogen-containing products **3**. This methodology follows the Green Chemistry principles, allowing the metal-free insertion of the nitrogen atom under mild conditions, and with complete control of the stereoselectivity.³ After dihydroxylation of the double bond and opening of the 1,6-bridge, new precursors of 4-aminosugars were obtained in a stereocontrolled way. Furthermore, *N*-alkyl aminosugars were obtained from mesylated levoglucosenone derivative **5** through: i) introduction of the nitrogen atom by nucleophilic substitution; ii) dihydroxylation of the double bond; iii) *N*-alkylation with long alkyl chain. The 4-aminosugar derivatives and the *N*-alkyl aminosugar derivatives have been tested on different bacterial strains including *Escherichia Coli* and *Bacillus Subtilis*. The presence of a lipophilic chain is essential for antibacterial activity. Preliminary data suggest the potential use of *N*-alkyl aminosugar derivatives as levoglucosenone-derived antibacterial agents.

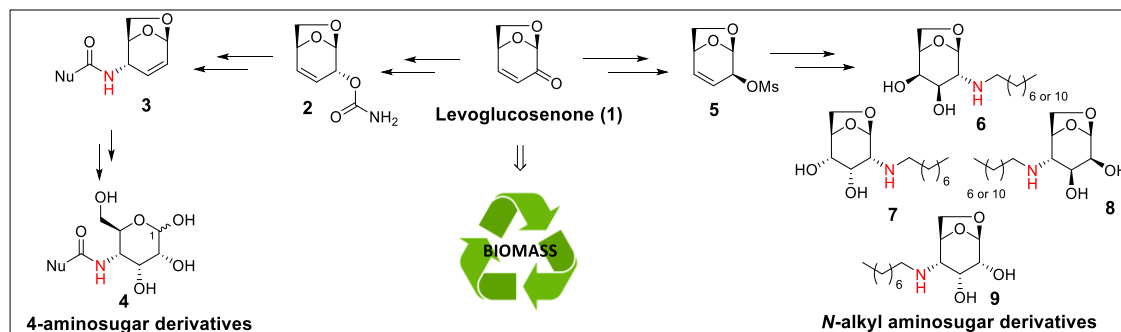


Figure 1. Use of levoglucosenone (**1**) to obtain biologically relevant compounds.

References

- [1] A. M. Sarotti, R. A. Spanevello, A. G. Suárez, *Green Chem.* **2007**, *9*, 1137–1140.
- [2] C. Nicolas, O. R. Martin, *Molecules* **2018**, *23*, 1612–1641.
- [3] Y. Ichikawa, *Synlett* **1991**, *4*, 238-240.

Straightforward Methods to Design Advanced Materials Using Melamine Foams

Ana-Isabel QUILEZ-MOLINA^{1,2,*}, Suset BARROSO-SOLARES^{1,2}, Sergio ACOSTA³, Antonio VICO-PADILLA³, Miguel-Ángel RODRÍGUEZ-PÉREZ^{2,4}, Javier PINTO^{1,2,*}

¹*Study, Preservation, and Recovery of the Archaeological, Historical, and Environmental Heritage (AHMAT) Research Group, Condensed Matter Physics, Crystallography and Mineralogy Department, Faculty of Science, University of Valladolid (Spain)*

²*BioEcoUVa Research Institute of Bioeconomy, University of Valladolid (Spain)*

³*BIOFORGE Lab, Bioengineering, Biomaterials and Nanomedicine Networking Biomedical Research Center (CIBER-BNN), University of Valladolid (Spain)*

⁴*Cellular Materials Laboratory (CellMat), Condensed Matter Physics, Crystallography, and Mineralogy Department, Faculty of Science, University of Valladolid (Spain)*

*Corresponding author: anaisabel.quilez@uva.es; anaquilezm@gmail.com

Melamine foams (Me) can be considered one of the most important chemical raw materials to date due to the great benefits it has brought in construction, aeronautics, cleaning and transportation, etc... Their unique morphological and chemical characteristics have prompted their use as building blocks for developing new materials with advanced properties. Me presents a tridimensional porous structure with high porosity (up to > 0.99) that fosters the material's functionalization and provides a large active surface for attaining high performance in environmental remediation approaches. On the other side, its chemistry involves functional groups rich in nitrogen with distinguished anchoring properties that facilitate the activation of the foam surface. **Figure 1** displays two outstanding methods to endow Me with highly beneficial properties for water purification.

Figure 1(A) displays a unique in situ method to functionalize Me with metallic silver nanoparticles¹. In our previous work², the synthesis pathway and the influence of the processing parameters were optimized to phase out 100% of polluting solvents, obtaining active melamine foams with bactericide properties processed with water as the only solvent.

Figure 1(B) highlights the benefits obtained from activating the Me via pyrolysis. The thermal degradation reactions triggered the formation of active N-doped carbonaceous molecules with outstanding catalytic properties to remove polluting dyes in water. As a result, calcined foams were shown to be up to six times more effective in removing the pollutant dye methylene blue (MB) in 24 hours independently of the environmental conditions of light than the pristine Me.

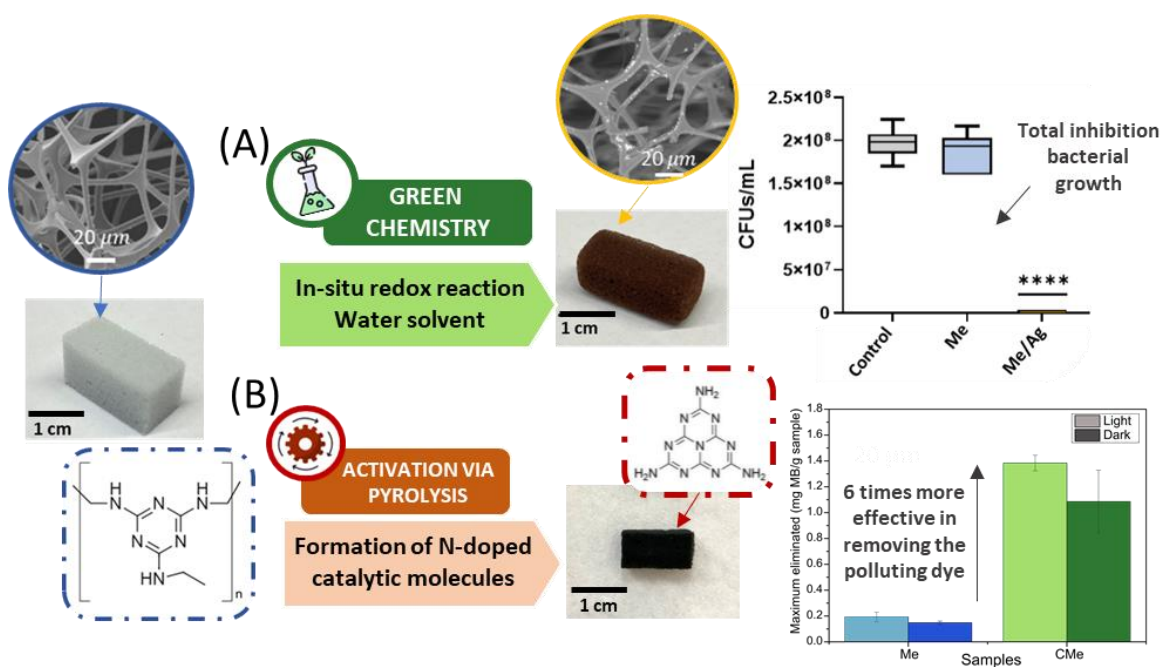


Figure 1. Scheme of the two pathways for activating Me: (A) in situ functionalization of Me with metallic silver nanoparticles to obtain Me with antibacterial properties through a green approach. (B) pyrolysis to trigger the formation of active N-doped molecules that improve the capability to remove polluting dyes in water.

References

- [1] P. Javier, M. Davide, V. Paola, P. Francisco, H.G. José Antonio, L. Simone, B.S. Suset, C. Luca, P. Pier Paolo, A. Athanassia, F. Despina, *ACS Applied Materials and Interfaces* **2018**, 10, 16095-16104
- [2] Q.M. Ana Isabel, B.S. Suset, R.P. Miguel Ángel, P. Javier, *Macromolecular Materials and Engineering* **2023**, 308, 2300178.

Sustainable Synthesis of Functionalized Glycerol Oligoesters

Francesco RABONI¹, Andrea GALATINI¹, Luca BANFI¹, Renata RIVA¹, Alessandro PELLIS^{1*}

Università degli Studi di Genova, Dipartimento di Chimica e Chimica Industriale, via Dodecaneso 31, 16146, Genova, Italy

**Corresponding author: alessandro.pellis@unige.it*

Glycerol based oligoesters are a class of useful molecules of potential application in different areas, such as the cosmetic and pharmaceutical industries. Their main advantage lies in the properties imparted by glycerol itself that, being a triol, can not only render the molecule more hydrophilic but also be used to further functionalize and fine tune the polymer's properties, by attaching pendant groups to the residual free hydroxyl moiety. To do so we tried to apply as much as possible the 12 principles of Green Chemistry, starting by biobased molecules, glycerol and various aliphatic diesters, we developed a synthetic protocol devoid of harmful chemicals, dedicating great effort to replace and circumvent reaction pathways using toxic substances while also employing quick yet effective purification methods to avoid column chromatography.

Furthermore, we made extensive use of biocatalysis both to synthesize and functionalize the polymers, obtaining molecules that not only are biodegradable but also compatible and well tolerated by the human body¹.

The synthesized molecules, shown in Figure 1, were thoroughly analyzed by means of both organic and polymer chemistry to better understand their properties and potential applications, mainly as emulsifiers and peptide delivery system².

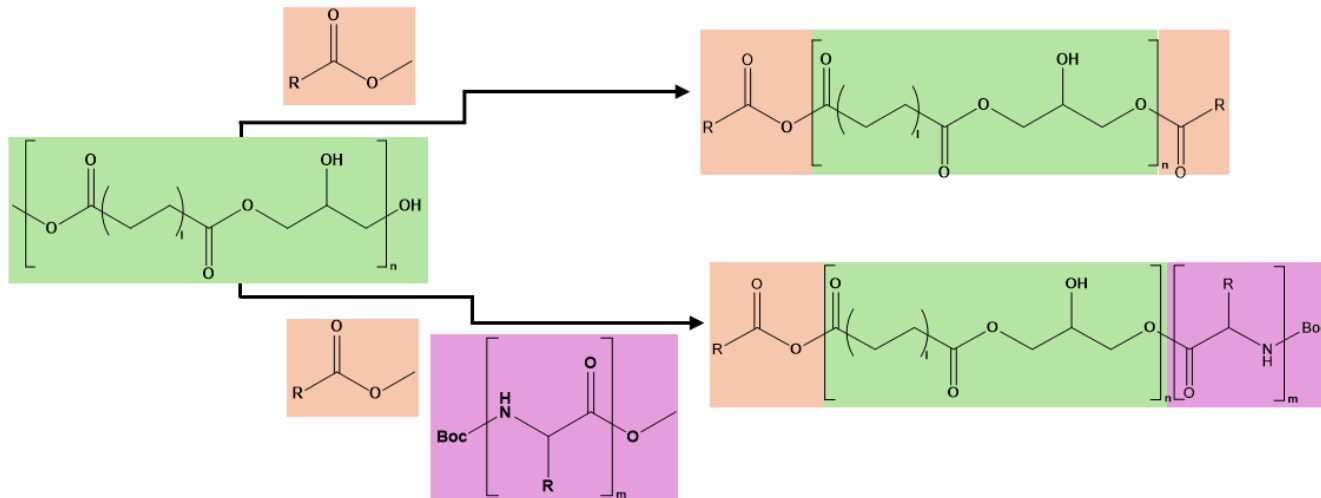


Figure 1. Glycerol oligoesters and their functionalized products.

References

- [1] Weiss VM, Lucas H, Mueller T, Chytil P, Etrych T, Naolou T, Kressler J, Mäder K. *Macromolecular Bioscience*. **2018**.
- [2] Raboni, F., Galatini, A., Banfi, L., Riva, R., Pellis, A. *ChemBioChem* **2024**, vol 25, issue 6, e202300839.

Aminolysis of Polycarbonate under UV Irradiation to Obtain Ionic Liquids

Giovanna Raia¹, Fleana SABATINO¹, Salvatore MARULLO¹, Francesca D'Anna^{1*}

¹ *Università degli Studi di Palermo, Dipartimento STEBICEF, Sezione di Chimica. Viale delle Scienze, Ed. 17
90128 Palermo (Italy)*

**Corresponding author: francesca.danna@unipa.it*

Nowadays, the majority of daily objects are made up by plastic, it is ubiquitous in different fields such as construction, electronics and packaging. Plastic has some advantages such as versatility and low cost; on another hand, poor management of plastic waste poses the issue of accumulation of plastic debris in environment.^[1] Chemical recycling to monomers is a viable strategy to tackle this problem.^[2] In this regard, we investigated the depolymerization of polycarbonate into bisphenol A. In the framework of our interest in plastic chemical recycling, we used ultrasound to promote the aminolysis of polycarbonate (PC). We used *N,N*-dimethylethylenediamine, *N,N*-dimethylpropylenediamine and 3-aminopropylimidazole as nucleophiles. The use of ultrasound allowed to carry out the reaction at low temperature, according to the holistic approach.^[3] In addition, in order to obtain value products we alkylated the obtained amides with different alkyl iodide to obtain Ionic Liquids.

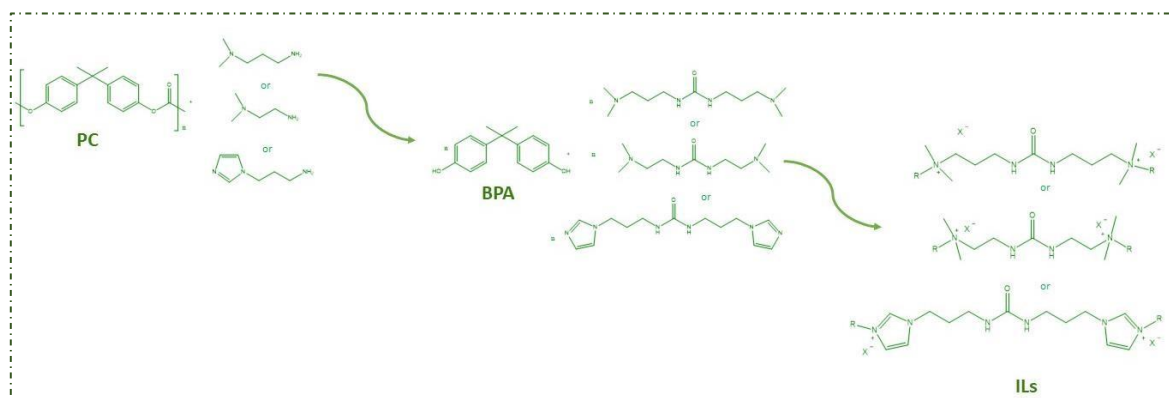


Figure 1. General process

References

- [1] Barnes, D. K. A.; Galgani, F.; Thompson, R. C.; Barlaz, M. *Philos. Trans. R. Soc. Lond., B, Biol. Sci.* **2009**, *364*, 1985–1998.
- [2] Coates, Geoffrey W; Getzler, Yutan D. Y. L. *Nature Reviews Materials*, **2020**, *5*, 501-516. [3] C. Robert McElroy, Andri Constantinou, Leonie C. Jones, Louise Summerton, James H. Clark, *Green Chem.*, **2015**, *17*, 3111–3121.

Search for Photoactivated Antimicrobial Compounds from South American Plant Species

Eugenia RODRIGUEZ RISTAU*, Viviana NICOTRA, Carina CASERO

Multidisciplinary Institute of Plant Biology (IMBIV – CONICET), Department of Organic Chemistry, Faculty of Chemical Sciences, UNC, Ciudad Universitaria, Córdoba, X5000HUA, Argentina.
eugenia.ristau@mi.unc.edu.ar*

The extensive use of antimicrobials has led to the emergence of resistance genes in pathogenic microorganisms, surpassing the rate of development of new treatments and threatening global public health, especially against nosocomial pathogens of the "ESKAPE" group [1]. Antimicrobial Photodynamic Therapy (aPDT) emerges as a promising strategy, using photosensitizer compounds that could generate reactive oxygen species (ROS) under light irradiation, inducing cell death [2]. Recent research suggests that natural-origin compounds with light-activated antimicrobial properties may offer innovative solutions [3].

This work began with a screening of 25 plant species from South America, based on photoinduced antibacterial activity against ATCC strains of *S. aureus* and *E. coli*. This assay was performed using the disk diffusion method. The results obtained led to the selection of species with promising bioactivity to perform a bioguided phytochemical study aimed at the isolation of photosensitizing metabolites. Subsequently, the most active isolated compounds were characterized by NMR to identify their molecular structure.

The hexane fraction obtained from *Erythrina crista-galli* flowers showed high inhibitory activity against the evaluated gram-positive strain, *S. aureus*. From this fraction, a bioactive (21.5 mm) mixture of free fatty acids was isolated and characterized by ¹H-NMR. The ethyl acetate extract of *Berberis johnstonii* also showed good bioactivity values against the same bacterial strain (11 mm).

The *Berberis* genus is characterized by its content of berberine, a metabolite with reported antimicrobial activity [4]. Spectroscopic characterization, determination of singlet molecular oxygen (¹O₂) production, and cell viability studies under irradiation and dark conditions were performed on this metabolite.

White light irradiation (λ_{\max} 446 and 542 nm) allowed us to determine a half-life of berberine of 49 min. in Mueller-Hinton Broth (MHB) and photostability in dimethylformamide (DMF). The kinetics of dimethylantracene (DMA) oxidation in front of berberine showed the generation of ¹O₂ triggered by photoactivation of the metabolite under study. In addition, our results showed a reduction of 4 log CFU/mL of *S. aureus*, under irradiation conditions.

References:

- [1]. X. Zhen, C.S. Lundborg, X. Sun, X. Hu, H. Dong. *Antimicrob. Resist. Infect. Control*, **2019**, 8, 137.
- [2]. Q. Jia, Q. Song, P. Li, W. Huang. *Adv. Healthc. Mater.* **2019**, 1900608.
- [3]. D.J. Newman, G. M. Cragg. *J. Nat. Prod.* **2020**, 83, 770-803.
- [4]. M.A. Mujtaba, M.H. Akhter, Alam MS, Ali MD, Hussain A. *Curr Pharm Biotechnol.* **2022**, 23, 60-71.

Heterogeneous Palladium-Catalysed C(sp³)-H α -Arylation for the Green Synthesis of Fused N-Heterocycles

Tian SANG¹, Tommaso SCARABOTTINI¹, Francesco MINIO¹, Luigi VACCARO^{1,*}

¹ Laboratory of Green SOC, Dipartimento di Chimica, Biologia e Biotecnologie Università degli Studi di Perugia Via Elce di Sotto, 8, 06124 Perugia (Italy)

*Corresponding author: Luigi Vaccaro@unipg.it

One of the most effective strategies for reducing environmental pollution associated with chemical production is the use of efficient catalytic reactions. Transition-metal-catalyzed C-H functionalization technologies have emerged as a valid alternative to traditional cross-coupling reactions for the effective formation of carbon-carbon and carbon-heteroatom bonds. In particular, heterogeneous palladium catalysts have received widespread attention because they can be easily separated from the reaction mixture and reused.

N-containing heterocyclic compounds, such as oxindoles and pyrrole derivatives, are important structural motifs in many molecules of biological and pharmaceutical interest. In previous work, we present the development of a waste-minimized protocol for the synthesis of oxindoles using cyclopentyl methyl ether (CPME) as a safe and green reaction medium and palladium on carbon (Pd/C) as a reusable catalyst.¹ Then this work, we developed an effective waste-minimized approach for the intramolecular Pd-catalyzed C(sp³)-H activation of methyl pyrrole derivatives by using a heterogeneous recyclable palladium(II)-bis(N-heterocyclic carbene) catalyst and CPME, the heterogeneous catalytic system could be recovered and reused up to representative five runs without any loss in efficiency. The target products have been obtained selectively and with excellent isolated yields. Other green metrics have been calculated and the data collected demonstrate that our newly developed protocol is very promising in terms of its environmental impact profile.²

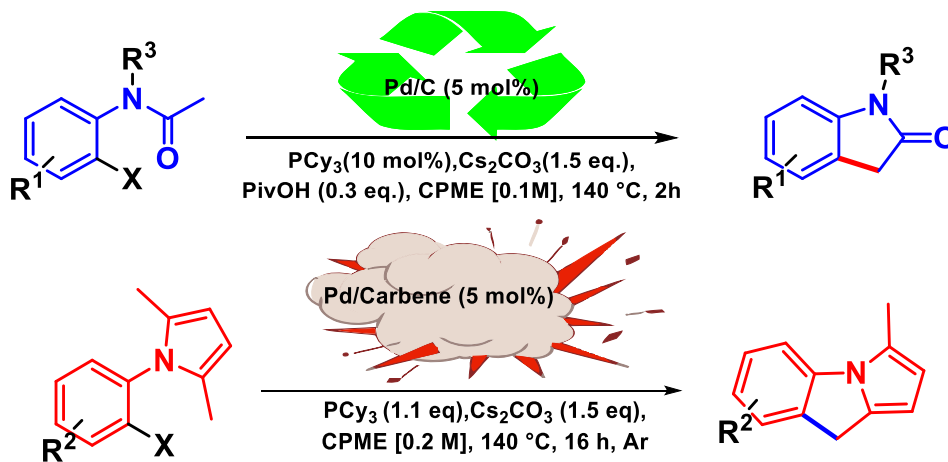


Figure 1. Heterogeneous palladium-catalysed C(sp³)-H α -arylation for the green synthesis of fused N-heterocycles.

References

- [1] N. Salameh, I. Anastasiou, F. Ferlin, F. Minio, S M. Chen, S. Santoro, P. Liu, Y L. Gu, L. Vaccaro, *Mol. Catal.* **2022**, 522, 112211.
 [2] N. Salameh, F. Minio, G. Rossini, A. Marrocchi, L. Vaccaro, *Green Synth. Catal.* **2023**, 4, 240-245.

Chemical Recycling of Polylactide Promoted by Zinc-Complexes

Federica SANTULLI,* Marina LAMBERTI, Mina MAZZEO

University of Salerno, Department of Chemistry and Biology "A. Zambelli", Fisciano, Salerno, Italy

*fsantulli@unisa.it

Biodegradable plastics synthesized from renewable resources offer an appealing alternative to traditional petroleum-based plastics. Among these green polymers, polylactide (PLA) stands out as the most successful example. Thanks to its good mechanical properties, PLA is already widely used in various sectors, including agriculture, textiles, and packaging.

However, despite its green credentials, PLA still contributes to the plastic waste crisis because its waste management strategy is currently aligned with a linear economic model. Developing efficient chemical recycling strategies towards the production of monomers and/or value-added materials is the way for creating a circular economic model of PLA that supports the growing use of this plastic. [1]

Currently, hydrolysis and alcoholysis reactions represent the two most successful techniques for treating PLA waste. Hydrolysis produces lactic acid, thus closing the life cycle of PLA (*route a*). Alcoholysis is an effective upcycling strategy for PLA waste, which through methanol or ethanol, transforms it into alkyl lactate, widely used as green solvents (*route b*). Additionally, the use of diols such as ethylene glycol and 1,4-butanediol enables the production of polyols (*route c*), which are valuable in the preparation of polyurethanes. [2]

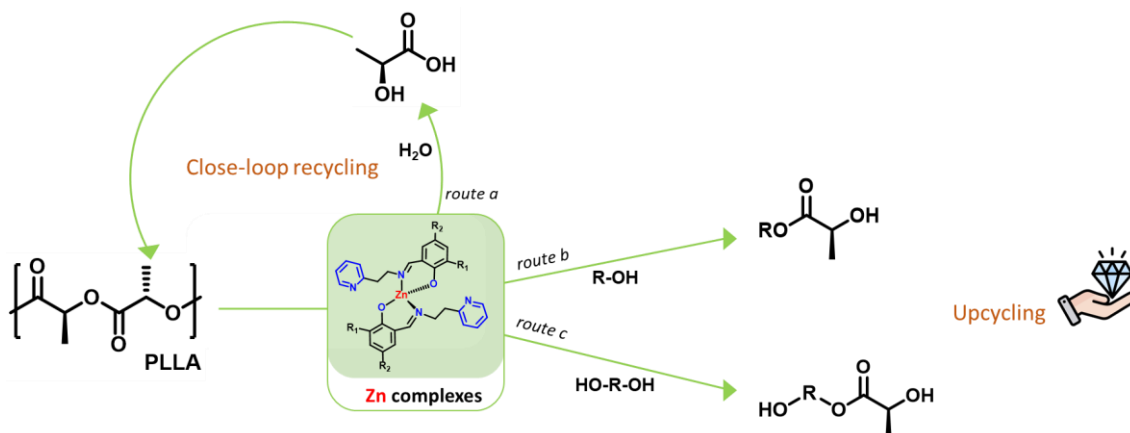


Figure 1. Chemical recycling reactions of polylactide waste.

Here, new homoleptic zinc complexes based on phenoxy-imine pyridine ligands have been synthesized and used in chemical recycling reactions of polylactide. [3] The microwave-assisted catalyst exhibited outstanding activity and selectivity toward the targeted products. Furthermore, recyclability tests of the catalyst supported its potential for continuous use in these processes. [4]

References

- [1] Y. Li, S. Wang, S. Qian, Z. Liu, Y. Weng, Y. Zhang, *ACS Omega* **2024**, 9, 13509.
- [2] B. Nim, M. Opaprakasit, A. Petchsuk, P. Opaprakasit, *Polym. Degrad. Stab.* **2020**, 181, 109363.
- [3] F. Santulli, G. Gravina, M. Lamberti, C. Tedesco, M. Mazzeo, *Mol. Catal.* **2022**, 528, 112480.
- [4] S. D'Aniello, S. Laviéville, F. Santulli, M. Simon, M. Sellitto, C. Tedesco, C. M. Thomas, M. Mazzeo, *Catal. Sci. Technol.*, **2022**, 12, 6142.

Valorisation of Coffee Silverskin Through Extractions and Pyrolytic Processes

Anna SCETTRI^{1,2*}, Elisabetta SCHIEVANO³, Roberto VOLPE², Paolo SGARBOSSA¹, Roberta BERTANI^{1*}

¹Department of Industrial Engineering, University of Padova, Padova, Italy

²Queen Mary University of London, London, UK

³Department of Chemical Sciences, University of Padova, Padova, Italy

*Corresponding author: anna.scettri@phd.unipd.it; roberta.bertani@unipd.it

Coffee silverskin (SK) is the coffee integument and is collected as coffee by-product from roasting process. At present, SK is used as a direct fuel and for composting and soil enrichment.¹ However, due to its rich organic content, SK is also potentially suitable for the extraction of organic compounds² for industrial purposes, such as caffeine and phenolic compounds, the creation of porous biochar^{1,3}, which can be applied in several environmental application such as water and soil remediation, and the extraction of cellulose for food packaging or paper production⁴.

We explored the extraction processes of SK carried out at room temperature (RT) as well as through microwave-assisted extraction (MAE) and ultrasound-assisted extraction (UAE) using water, ethanol, chloroform, and the mixture acetone:hexane (1:1). Several compounds were recovered, including caffeine, chlorogenic acids, trigonelline, glucose, and sucrose, particularly with water, and identified using ¹H-NMR, as illustrated in Figure 1. Among the methods employed, RT yielded the highest amounts of extracted compounds; however, MAE and UAE offer the advantage of significantly reduced reaction times, taking 30 and 15 minutes, respectively. Moreover, in a circular economy purpose, we investigated the extraction of cellulose from the residue and pyrolytic processes to achieve activated carbons and biochars.

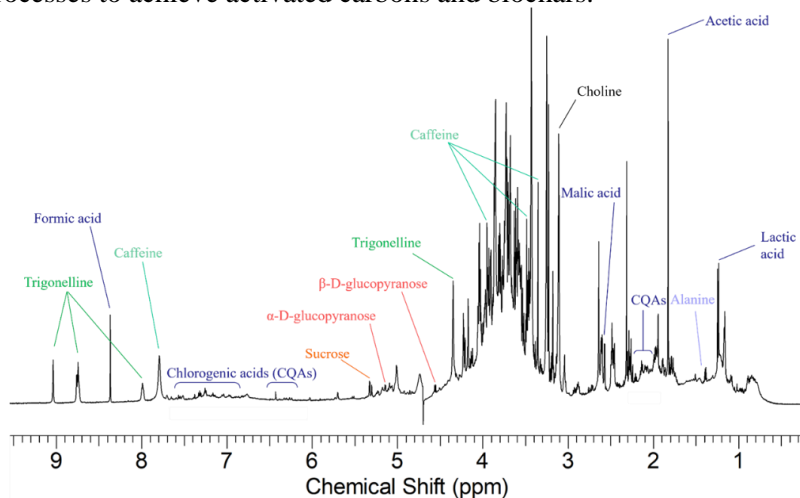


Figure 1. ¹H-NMR spectrum of SK water extract.

References

- [1] J. Fernández-Ferreras, T. Llano, M.K. Kochaniec, A. Coz, *Energies* 2023, 16, 2300.
- [2] X. Wang, D.-F. Hong, G.-L. Hu, Z.-R. Li, X.-R. Peng, Q.-Q. Shi, M.-H. Qiu, *Molecules* 2021, 26, 4914.
- [3] C. Del Pozo, F. Rego, Y. Yang, N. Puy, J. Bartrolí, E. Fàbregas, A.V. Bridgwater, *Fuel Process. Technol* 2021, 214, 106708.
- [4] Overturf, E. Pezzutto, S. Boschiero, M. Ravasio, N. Monegato, A. *Sustainability* 2021, 13, 9069.

Efficient Conversion of L-Rhamnose into 5-Methylfurfural Combining Performance of Ionic Liquids and Zeolites

Martina SILACO, Salvatore MARULLO, Francesca D'ANNA^{1,*}

¹Università degli Studi di Palermo, Dipartimento STEBICEF, Palermo, Italy

*Corresponding author: francesca.danna@unipa.it

Most carbon-based products that our society uses daily, derive from petroleum, and therefore require the exploitation of fossil fuels; this leads to a consequent increase in carbon dioxide emissions and global warming.¹ For this reason, interest in alternative and renewable energy sources has grown in recent years. Biomass resources including carbohydrates are an ideal petroleum alternative to produce fuels, chemicals, and materials. 5-Methylfurfural (5-MF) is an important intermediate widely used in pharmaceuticals, cosmetics, pesticides, and other applications. Thanks to the presence of several functional groups, 5-MF can be used to produce value-added product, such as 2,5-Dimethylfuran and 2,5-Furandicarboxylic acid. On the other hand, the industrial production of 5-MF involves 2-Methylfuran, phosgene and *N,N*-dimethylformamide, resulting in high production cost. However, 5MF can be obtained from biomass-derived carbohydrates.² L-Rhamnose is a deoxyhexose carbohydrate, and it is the cheapest deoxy sugar. The conversion to 5-MF involves two steps, in particular the isomerization gives L-rhamnulose and the following dehydration form 5-MF.³ In this study, we worked on the direct conversion of L-Rhamnose to 5-MF using Ionic Liquids (ILs) as solvents (Figure 1) and zeolite as catalyst.

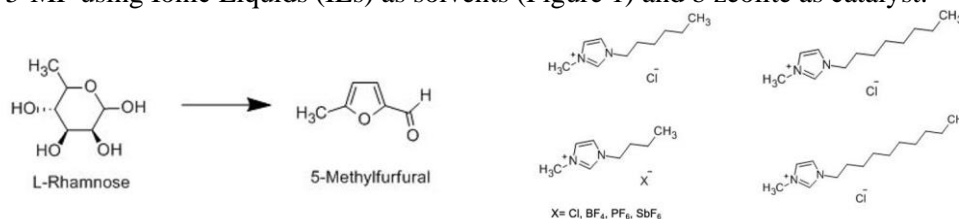


Figure 1. Synthesis of 5-MF from L-Rhamnose and structures of ILs tested.

Reaction conditions such as temperature, the amount of L-Rhamnose and catalyst loading were optimized. To illustrate the effect of solvent, ILs different for both anion and cation were tested, along with mixtures of ILs. Finally, using the best operating conditions, thanks to a biphasic system, we evaluated the possibility of extracting 5-MF and reusing the solvent-catalyst system.

References

- (1) Raud, M.; Kikas, T.; Sippula, O.; Shurpali, N. J. Potentials and Challenges in Lignocellulosic Biofuel Production Technology. *Renewable Sustainable Energy Rev.* **2019**, *111*, 44–56.
- (2) Peng, Y.; Li, X.; Gao, T.; Li, T.; Yang, W. Preparation of 5-Methylfurfural from Starch in One Step by Iodide Mediated Metal-Free Hydrogenolysis. *Green Chem.* **2019**, *21* (15), 4169–4177.
- (3) Tuteja, J.; Nishimura, S.; Ebitani, K. One-Pot Synthesis of Furans from Various Saccharides Using a Combination of Solid Acid and Base Catalysts. *Bull. Chem. Soc. Jpn.* **2012**, *85* (3), 275–281.

ACKNOWLEDGEMENTS

This study was carried out within the MICS (Made in Italy – Circular and Sustainable) Extended Partnership and received funding from the European Union Next-GenerationEU (PIANO NAZIONALE DI RIPRESA E RESILIENZA (PNRR) – MISSIONE 4 COMPONENTE 2, INVESTIMENTO 1.3 – D.D. 1551.11-10-2022, PE00000004). This manuscript reflects only the authors' views and opinions, neither the European Union nor the European Commission can be considered responsible for them.

Sustainable Development of Nano-Adjuvants for Radiotherapy in Mexico

Fernanda Abigail SILVA MELGAREJO¹, Nuria ZÁRATE VILET¹, Lluvia Itzel LÓPEZ LÓPEZ², Ingrid Guadalupe MEZA PARDO³, Daniela Edith SALADO LEZA^{3,4*}

¹Faculty of Chemistry, Autonomous University of San Luis Potosi. 78210, SLP, Mexico

²Research Institute of Desert Areas. Autonomous University of San Luis Potosi. 78377, SLP, Mexico.

³Institute of Physics, Autonomous University of San Luis Potosi. 78295, SLP, Mexico.

⁴Researchers for Mexico, CONAHCyT, 03940, CDMX, Mexico.

*Corresponding author: daniela.salado@conahcyt.mx

Half of all diagnosed cancer patients receive radiotherapy during their treatment. However, this non-invasive therapeutic modality is still limited by radiation damage induced to nearby tissues; thus, nanomedicine is sustainably developing functional materials capable of enhancing the local delivered dose of radiotherapy and minimizing the damage of surrounding normal cells. The main objective of this work is to develop a bismuth-based nano-hybrid containing natural extract, this last obtained from the revalorization of Mexican citrus industry waste, which we named BiNar. The extraction of crude and purified natural compounds is obtained from US-assisted ethanolic extraction of simulated grapefruit waste and characterized to have a comprehensive knowledge about the antioxidant activity and total polyphenols and flavonoids content. The nano-hybrid is synthesized by using a simple one-step green route assisted with solar light, and characterized by complementary physicochemical (DLS, Z-potential), spectroscopic (IR, UV-Vis) and microscopic (light and fluorescence) techniques. The results show that the purified extract (PE) has a highest amount of polyphenols, flavonoids and highest antioxidant activity than the crude extract (CE). On the other hand, using commercial naringin for infrared spectroscopy, it is observed that PE has a best fit than CE, furthermore, comparing the chemical composition by HPLC, the results indicate that the purification was successfully achieved. BiNar obtained by green synthesis using sunlight as the energy source, is composed from micro-aggregates of spherical metallic nanoparticles surrounded by needle-like nanonaringin, which possesses fluorescent properties. In conclusion, based on these findings, PE has the best qualities to be used in the sustainable synthesis of BiNar, whose synthesis methodology is being optimized to subsequently, evaluate in normal and cancerous prostate cell lines; the internalization, localization, and toxicity of the nano-adjuvant before and after being irradiated.

Keywords: functionalized nanoparticle; radiotherapy; sustainability.

References

- [1] J. E. Wong-Paz, J. Contreras-Esquivel, R. Rodríguez-Herrera, M. L. Carrillo-Inungaray, L. I. LópezLópez, G. V. Nevárez-Moorillón, & C. N. Aguilar. Total phenolic content, in vitro antioxidant activity and chemical composition of plant extracts from semiarid Mexican region. *Asian Pacific Journal of Tropical Medicine*. **2015**, 8(2), 104–111.
- [2] N. Jara, N. S. Milán, A. Rahman, L. Mouheb., D. C. Boffito, C., Jeffryes & S.A. Dahoumane. Photochemical Synthesis of Gold and Silver Nanoparticles—A Review. *Molecules*. **2021**, 26(15), 4585.

Aknoledgments

To CONAHCyT for funding the Frontier Science Project CF-2023-I-1196 and for the scholarship (CVU 1319724) that facilitates my master's studies in chemical sciences. To my colleagues at the Bionanotechnology Laboratory (BiNaT) of the Institute of Physics for their contribution and to PhD. Gabriela Navarro and PhD. Luz Alcántara for their guidance and support in different parts of the project.

Multilayer Packaging Delamination Process Using CO₂-Switchable Surfactants

Vanessa SPADAVECCHIA*, Vincenzo ARPAIA¹, Roberta MASTRODDI¹, Martina VAGNONI¹,
Chiara SAMORI¹, Emilio TAGLIAVINI¹, Paola GALLETTI¹

¹ Dipartimento di chimica "Giacomo Ciamician", Università di Bologna, Via Pietro Gobetti 85, 40129 Bologna

*Corresponding author: vanessa.spadavecchi2@unibo.it

Around 25.8 Mt of plastic waste is produced in Europe each year, 59% of which is plastic packaging. At present, multilayer flexible packaging waste represents the largest portion of non-recyclable packaging, accounting for around 20% of all flexible packaging [1].

The MERLIN European project focuses on multilayer rigid, non-metalized flexible, and metalized flexible packaging, developing processes for sorting and recycling each material.

In this framework, this study aimed to find out the most effective process to delaminate a conventional coffee packaging composed of PE, PET and Al (a typical metalized flexible packaging) by using nontoxic, recyclable solvents while preserving high-quality of the recovered material.

After an initial screening of aqueous solutions of various SAS (switchable anionic surfactants), triethanolammonium laurate aqueous solution was selected as the solvent system of choice. The water solubility of this surfactant can be tuned by adding and removing CO₂, reversibly switching from an insoluble form (when pH is decreased by the addition of CO₂) to a soluble one (when pH is increased by CO₂ removal), thus allowing its recovery and recycling at the end of the process.

The delamination was performed at 100°C for 30 min, by using a waste amount of 1 wt% in a SAS concentration of 0.5 wt%. A complete mass balance of the recovered materials (LDPE and aluminium/PET) was obtained. The recovered LDPE did not differ in terms of thermal and mechanical properties from the LDPE initially present in the multilayer waste before the delamination, as demonstrated by the comparable values of elongation at break, tensile strength at break, degradation temperature, melting temperature and crystallinity degree. Finally, by adding CO₂ at ambient pressure, it was possible to recycle more than 90% of the surfactant used for the delamination [2].

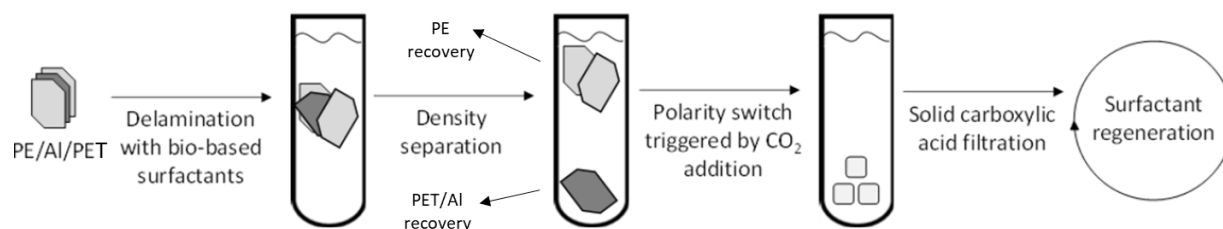


Figure 1. Scheme of the process.

References

- [1] Kaiser, K.M., 2020. Recycling of multilayer packaging using a reversible cross-linking adhesive. <https://mediatum.ub.tum.de/doc/1547705/document.pdf> J. Appl. Polym. Sci. 137 (40)
- [2] Vagnoni M., et al., 2023. Recycling of multilayer packaging waste with switchable anionic surfactant. <https://doi.org/10.1016/j.resconrec.2023.107141>

Colloid-Chemical Features of an Aqueous-Phase Catalytic System for the Direct Hydroxylation of Phenol to Dihydroxybenzenes with Hydrogen Peroxide by Nano/Micro-Sized Iron Containing Silica-Gel

Samira SULEYMANOVA¹, Etibar ISMAILOV¹

¹*Institute of Catalysis and Inorganic Chemistry, Baku, Azerbaijan*

Email: suleymanova.samira1990@gmail.com

One of the main directions of modern catalysis is the development of environmentally friendly catalytic processes. Research conducted over the past 10 years shows that iron-containing catalysts exhibit high activity and selectivity in the reaction of liquid-phase hydroxylation of phenol to dihydroxybenzenes with hydrogen peroxide. It should also be noted that the catalytic oxidative destruction of phenol, phenols - organic impurities in aqueous media using hydrogen peroxide (Fenton-type process) is a promising method of wastewater treatment, which is currently being actively developed in many laboratories around the world. In most cases, these systems are ultradisperse and the study of their colloidal chemical features is of great importance, first of all, for elucidating the mechanism of their functioning and developing methods for preparing effective catalytic systems for this reaction [1,2]. This report presents the results of studies of the colloidal chemical characteristics of liquid-phase iron-containing catalytic systems for the hydroxylation of phenol into dihydroxybenzenes depending on the reaction conditions (temperatures in the range of 278-343 K, reaction duration up to 6 hours) using a combination of dynamic light scattering (DLS) methods, Fourier transform infrared spectroscopy (FTIR) and electron magnetic resonance (EMR). Iron-containing nano- and micro-sized catalysts based on tetraethylorthosilicate (C₂H₅O)₄Si and sodium silicate Na₂SiO₃ were prepared by the autoclave method via hydrothermal synthesis. Cationic gemini surfactants N,N'-bis(alkyl)-N were used as a complexing agent N'-bis(2-hydroxypropyl)ethylenediammonium dibromide, [C_nH_{2n+1}(CH₃CH(OH)CH₂)-NH(CH₂)₂NH(CH₂CH(OH)CH₃) C_nH_{2n+1}]Br₂, where n is the tail part of the chain length, n = 9, 12 and 14, denoted as C_nC₂C_n[iso-Pr(OH)] and iron(III) chloride as an iron precursor. Next, the resulting samples were calcined in air at 400 °C and reduced in a stream of hydrogen at the same temperature and dispersed using a PM200 planetary mill, Retsch, Germany. A Hielscher UP 200S ultrasonic device with a frequency of 26 kHz and a power of 200 W (USA) was used as an ultrasound source (USA). It has been shown that the effect of ultrasonication on the activity of the catalytic system during the liquid-phase hydroxylation of phenol to dihydroxybenzenes with hydrogen peroxide is to reduce the average particle size, the range of their distribution and maintain the highly dispersed state of the catalyst particles and cleanse its surface from reaction products. Catalytically active in this reaction are nano-sized Fe₃O₄ particles formed during the reduction of Fe₂O₃ particles in oxidized samples in a stream of hydrogen, which initially react with hydrogen peroxide, forming the •OH radical. It has been shown that exposure to ultrasound makes it possible to restore almost the original activity of the catalyst after its operation for 4 hours and maintain the ultradispersed state of the catalyst.

References

- [1] Alma D. Salazar-Aguilar, Gonzalo Vega, Jose A. Casas, Sofía Magdalena Vega-Díaz, Ferdinando Tristan, David Meneses-Rodríguez, Manuel Belmonte and Asunción Quintanilla. Direct Hydroxylation of Phenol to Dihydroxybenzenes by H₂O₂ and Fe-based Metal-Organic Framework Catalyst at Room Temperature. *Catalysts* **2020**, 10, 172
- [2] Choi J.S., Yoon S.S., Jang S.H., Ahn W.S. Phenol hydroxylation using Fe-MCM-41 catalysts. *Catal. Today* **2006**, 111, 280–287

Copper-Catalyzed Transfer Hydrogenation in Flow Reactors: Advancing Green Aniline Production

Mikhail TRUKHAN*, Katia MARTINA, Giancarlo CRAVOTTO

University of Turin — Department of Science and Pharmaceutical Technology,
via Pietro Giuria 9, 10125 Turin (Italy)

* e-mail: mikhail.trukhan@unito.it

In the present investigation, a novel synthetic approach for the production of anilines, which are among the most prevalent compounds utilized across various industrial sectors, is introduced. This pathway involves the transfer hydrogenation of nitro compounds executed within a continuous-flow reactor employing a heterogeneous copper-based catalyst. A pivotal innovation of this methodology is the substitution of traditional gaseous hydrogen to bio-solvents—specifically ethylene glycol and glycerol—which function concurrently as hydrogen donors and solvents with high-boiling point [1,2]. This is facilitated by a copper-based catalyst system, which represents a cost-effective alternative to traditional noble metal catalysts, thereby enhancing the reaction's stability and safety while maintaining high operational efficiency [3]. The application of flow chemistry technology in this context enhances the reaction kinetics by augmenting mass transfer rates and enhance the stoichiometric ratio of the catalyst to the reactant at any given instance.

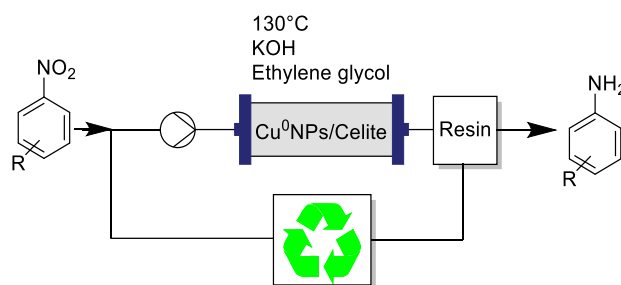


Figure 1. Cu(0)NPs/Celite-catalyzed transfer hydrogenation of nitrobenzene.

The methodology employs copper nanoparticles anchored on a celite surface, with the dual-role playing ethylene glycol or glycerol ensuring high reactivity. The process achieves complete conversion within 7-minute residence time in the reactor, maintaining an efficiency of at least 90% over five days of operation (employing 500 mg of catalyst with a 5% copper by mass, equating to approximately 0.4 mol%). Efficient separation of the reaction products is achieved via ion-exchange resin, significantly reducing the isolation costs associated with the end products. This innovative approach not only markedly reduces the environmental footprint but also diminishes the E-factor of the process to as low as 8.3. The process has demonstrated linear scalability from producing 100 mg to 3 grams per hour under laboratory conditions [4].

References

- [1] T. Zhang, C. Liu, Y. Gu. *Green Chemistry* **2021**, 23(20), 7865-7889.
- [2] MJ Moran, K Martina, G. Cravotto et al., *Front Chem.* **2020**, 8: 34
- [3] MJ. Moran, K. Martina, G. Cravotto et al., *Advanced Synthesis & Catalysis* **2020**, 362, 2689
- [4] K. Martina, MJ. Moran, MV.Trukhan et al., *Org. Process Res. Dev.* **2024**, 28, 5, 1515–1528

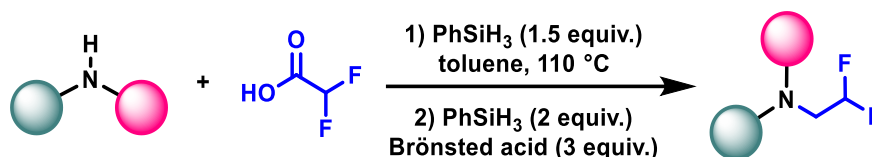
Practical, Metal-Free Synthesis of Difluoroethylamines using Difluoroacetic Acid

Alexander UNER, Oska PUGH and Ross DENTON

School of Chemistry, University of Nottingham, UK

pcyaul@nottingham.ac.uk

www.dentonchemistry.com



Metal-free ✓ Benign, readily available fluorine source ✓ No column chromatography ✓

Difluoroethylamines are an emerging functionality in the pharmaceutical and agrochemical sectors,^{1,2} employed for their ability to fine-tune the basicity, lipophilicity and conformational restraint of a molecule.^{3,4} Despite their increasing use, methods for the synthesis of difluoroethylamines are limited to the use of expensive, inconvenient, and oftentimes toxic reagents and solvents.^{5,6}

We have developed a one-pot synthesis of difluoroethylamines *via* reductive amination of difluoroacetic acid, which is a readily available, shelf stable and low-hazard fluorine source. The reaction proceeds through silane-mediated amidation followed by amide reduction enabled by a Brønsted acid-activated silane species formed *in situ*. The reaction can be performed in conventional laboratory glassware without inert atmospheres or dried solvents and demonstrates tolerance of a variety of functional groups, with both simple and drug-like tertiary amine examples synthesised. Products of the reaction usually do not require chromatographic purification and low-boiling products can be isolated directly from the reaction mixture as Brønsted acid salts.

- (1) R. Nauen, P. Jeschke, R. Velten, M. E. Beck, U. Ebbinghaus, Kintscher, W. Thielert, K. Wölfel, M. Haas, K. Kunz and G. Raupach, *Pest Manag. Sci.*, 2015, **71**, 850–862
- (2) Cephalon Inc., Pharmacopeia Drug Discovery, W.O. Pat., 051 547 A1, 2008
- (3) E. Isabel, C. Mellon, M. J. Boyd, N. Chauret, D. Deschênes, S. Desmarais, J.-P. Falgueyret, J. Y. Gauthier, K. Khougaz, C. K. Lau, S. Léger, D. A. Levorse, C. S. Li, F. Massé, M. David Percival, B. Roy, J. Scheigetz, M. Thérien, V. L. Truong, G. Wesolowski, R. N. Young, R. Zamboni and W. Cameron Black, *Bioorg. Med. Chem. Lett.*, 2011, **21**, 920–923.
- (4) S. Swallow, in *Progress in Medicinal Chemistry*, eds. G. Lawton and D. R. Witty, Elsevier, 2015, vol. 54, pp. 65–133.
- (5) A. T. Brusoe and J. F. Hartwig, *J. Am. Chem. Soc.*, 2015, **137**, 8460–8468
- (6) M. Epifanov, P. J. Foth, F. Gu, C. Barrillon, S. S. Kanani, C. S. Higman, J. E. Hein and G. M. Sammis, *J. Am. Chem. Soc.*, 2018, **140**, 16464–16468.

Physicochemical Characterization of the Water in Pagbanganan River, Baybay City, Leyte, Philippines

Jerald VILLARMINO¹, Elizabeth QUEVEDO²

¹Department of Arts and Sciences, Visayas State University Tolosa

²Department of Pure and Applied Chemistry, Visayas State University Baybay

*Corresponding author: jerald.villarmino@vsu.edu.ph

Pagbanganan River is the major river that traverses Baybay City, Leyte and plays a significant role in catering the necessities for all types of organism's dependent on it. This study was conducted in order to establish baseline data and characterize the water index of Pagbanganan River through its pH, water temperature, dissolved oxygen (DO), biochemical oxygen demand (BOD), total suspended solids (TSS), total hardness (as CaCO₃), total alkalinity, total dissolved solids (TDS), water conductivity, chlorides, phosphates (as reactive phosphorous) and sulfates level among sampling sites and compare it with the standard limits set by Department of Environment and Natural Resources (DENR) [1] and United States Environmental Protection Agency (USEPA) [2]. Sampling was done in a one-month interval from August 2016 to December 2016 following standard method. Results revealed that the water in Pagbanganan River system had an average pH of 7.4±0.3, water temperature of 27.8±0.3°C, DO of 5.6±0.4ppm, BOD of 2.6±1.6 ppm, TSS of 67.7±45.8mg/L, total hardness (as CaCO₃) of 128.6±5.9ppm, total alkalinity of 151.1±6.7ppm, TDS of 25.6±15.2ppm, water conductivity of 195±2.2µS, chlorides of 10.4±1.1mg/L, phosphate (as reactive phosphorous) of 0.04±0.01ppm, and sulfates of 14.7±5.8ppm. This further implies that the water quality of Pagbanganan river is concordant with DENR's Class C Surface water.

Table 1. Physicochemical parameters of the river water between sampling sites compared with the standard limits of DENR and USEPA.

| Sampling Site | pH | Water Temp. (°C) | DO (ppm) | BOD (ppm) | TSS (mg/L) | TH (ppm) | TA (ppm) | TDS (ppm) | Cond (µS) | Cl ⁻ (mg/L) | PO ₄ ³⁻ (ppm) | SO ₄ ²⁻ (ppm) |
|---------------|------------------|------------------|-------------------|------------------|--------------------|---------------------|----------|--------------------|--------------------|------------------------|-------------------------------------|-------------------------------------|
| Ciabu | 7.7 ^a | 28.0 | 6.0 ^a | 1.1 ^c | 20.5 ^c | 121.8 ^b | 157.8 | 108.1 ^b | 169.2 ^b | 8.9 ^c | 0.04 ^a | 9.92 ^c |
| Bubon | 7.3 ^b | 27.9 | 5.5 ^{ab} | 4.3 ^a | 70.5 ^b | 131.6 ^{ab} | 144.5 | 135.0 ^a | 209.2 ^a | 10.2 ^b | 0.03 ^b | 12.98 ^b |
| Canipa | 7.2 ^b | 27.4 | 5.2 ^b | 2.5 ^b | 112.0 ^a | 132.4 ^a | 151.1 | 133.7 ^a | 206.5 ^a | 12.2 ^a | 0.04 ^a | 21.23 ^a |
| DENR (2016) | 6.5 – 9.0 | 25 – 31 | 5 | 7 | 80 | no data | no data | no data | no data | 350 | no data | 250 |
| USEPA (2005) | 6.5 – 9.0 | 32 | 5 | 7 | 30% increase* | 500 | 20 -200 | 500 | no data | 250 | no data | 250 |

¹Averages followed with the same letter are not significantly different from each other based on the 5% level of Tukey's HSD test

*Thirty percent (30%) increase of TSS values compared with the previous data obtained

References

- [1] Department of Environment and Natural Resources. 2016. Revised water quality guidelines. Administrative Order No. 2016. pp. 5-9.
- [2] U.S. Environmental Protection Agency. 2005. Quality Criteria for Water (Gold Book). Office of Water Regulations and Standards.

Synthesis and Characterization of a Robust Ga-MOF Catalyst for the Epoxidation of *cis*-Cyclooctene Using H₂O₂ as a Green Oxidant

Gabriela Tuono Martins XAVIER^{1*}, Gustavo Felix BITENCOURT¹, Wagner Alves CARVALHO¹, Dalmo MANDELLI¹

¹Centro de Ciências Naturais e Humanas, Universidade Federal do ABC - UFABC, Av. dos Estados, 5001, Santo André – SP, 09210-580, Brazil *Corresponding author: gabriela.xavier@ufabc.edu.br

The catalytic oxidation of olefins is a significant pathway for producing epoxides, essential building blocks used to fabricate pharmaceuticals, epoxy resins, paints, fragrances, and other industrial products. Achieving high selectivity, efficiency, and catalyst stability remains challenging in developing more efficient and sustainable chemical processes for these reactions ¹. Metal-organic frameworks (MOFs) appear as potential heterogeneous catalysts due to their singular properties and the simplicity in synthesis, modification, and tailoring, which allows the use of different metals and organic ligands ². In this study, gallium and terephthalic acid were used to synthesize a Ga-MIL-53 type MOF through the solvothermal method, using milder conditions compared to the current procedure ³. The material was characterized using various techniques, including X-ray diffraction, scanning electron microscopy, infrared spectroscopy, surface area analysis, and elemental analysis. The Ga-MIL-53 type MOF was evaluated as a catalyst for the epoxidation of *cis*-cyclooctene with aqueous H₂O₂ 60%, using a metal-ligand cooperative approach in the presence of 1-methylimidazole ⁴. The heterogeneity of the catalyst was confirmed through a hot filtration test ⁵, and its selectivity and productivity were assessed over two consecutive cycles. Reaction kinetics showed that Ga-MIL-53 produced 2.4 mmol of the corresponding epoxide, with a conversion rate of 93%, and epoxide selectivity of 71%.

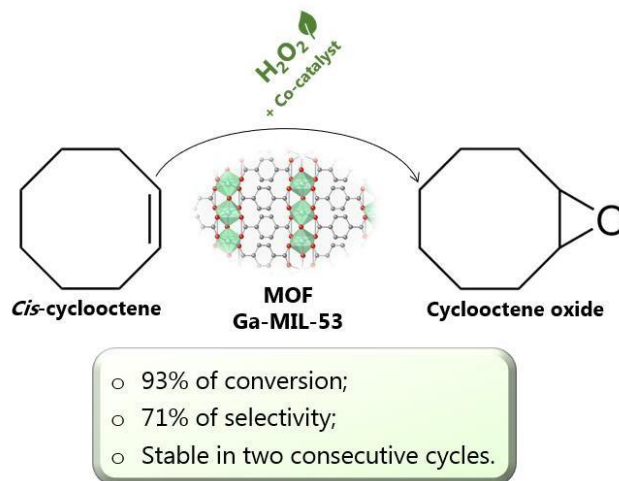


Figure 1. Epoxidation of *cis*-cyclooctene using Ga-MIL-53 as catalyst, and H₂O₂ as oxidant.

References

1. Tombesi, A.; Pettinari, C.; *Inorganics* **2021**, *9*.
2. Aguirre-Díaz, L. M.; Reinales-Fisac, D.; Iglesias, M.; Gutiérrez-Puebla, E.; Gándara, F.; Snejko, N.; Monge, M. Á.; *Coord. Chem. Rev.* **2017**, *335*, 1.
3. Liu, J.; Ran, Z.; Cao, Q.; Ji, S.; *Chinese J. Catal.* **2021**, *42*, 2254.
4. Correia, G. A.; de Araújo, M. L.; Carvalho, W. A.; Sairre, M.; Cerchiaro, G.; Shul'pina, L. S.; Kozlov, Y. N.; Shul'pin, G. B.; Kirillov, A. M.; Mandelli, D.; *Mol. Catal.* **2022**, *528*, 112457.
5. Lempers, H. E. B.; Sheldon, R. A.; *J. Catal.* **1998**, *175*, 62.

POSTER WINNERS AWARDS

43 Posters were received from in-person participants, and the students had the opportunity to expose their research work at two poster sessions. The poster sessions can be considered a highlight of the Summer School, for the originality and the diverse scientific value of the contributions, of the significant number of young people who shared their research with the other participants and teachers. In the Closing Ceremony, three in-person poster award winners and two online poster award winners were announced. The poster award winners presented their research work in the form of 5-minute oral presentation to the lecturers and students during the Closing Ceremony on the last day of the Summer School 2024.

Three in-person poster award winners of the Green Sciences for Sustainable Development Foundation Awards were:

(1) **Valentina BENAZZI** – *Dipartimento di Chimica Organica, Università degli Studi di Pavia, Via Torquato Taramelli 12, 27100 Pavia, Italy.*

POSTER TITLE: “Carbon Dots as Visible Light Bio-based Photocatalysts in Organic Synthesis”

(2) **Sulafa Abdalmageed Saadaldeen MOHAMMED** – *Department of Energy, Aalborg University, 9220 Aalborg, Denmark.*

POSTER TITLE: “Computational and Experimental Evaluation of Triazolium and Imidazolium-Based Ionic Liquids as Electrolyte for CO₂ Electrochemical Reduction”

(3) **Vanessa SPADAVECCHIA** – *Dipartimento di chimica “Giacomo Ciamician”, Università di Bologna, Via Pietro Gobetti 85, 40129 Bologna, Italy.*

POSTER TITLE: “Multilayer Packaging Delamination Process Using CO₂-Switchable Surfactants”

Two online poster award winners of the Green Sciences for Sustainable Development Foundation Awards were:

(1) **Fernanda Abigail SILVA MELGAREJO** – *Faculty of Chemistry, Autonomous University of San Luis Potosi. 78210, SLP, Mexico.*

POSTER TITLE: “Sustainable Development of Nano-Adjuvants for Radiotherapy in Mexico”

(2) **Faeze KAZEMI-ANDALIB** – *Department of Chemistry, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, 45137-66731, Iran.*

POSTER TITLE: “Synthesis of Cyclometalated Platinum(II) Complex in a Green Solvent: Biological Evolutions”

The in-person poster award carries a cash of 500 USD. The online poster award consists of an original print of Venice, which will be sent to the online poster award winners by a postal service. The prints were purchased from a Bookstore in Venice, which is specialized in antiquities: <https://www.libreriaemiliana.com>



PHOTOS



Prof. Francesco Trotta, Chair of Summer School



The Organizing Committee



In-person poster award winners



Teachers and Students of the Summer School



Teachers of the Summer School in Venice



Teachers of the Summer School 2024, who were students in previous editions of the Summer School (right to left: Fabio Arico, Italy; Aurelia Visa, Romania; Peter Licence, UK; Luigi Vaccaro, Italy; Chiara Samorì, Italy)

Ideated and managed by



In collaboration with



Ca' Foscari
University
of Venice

Department of Environmental
Sciences, Informatics and Statistics



UNIVERSITÀ
DI TORINO

Endorsed by



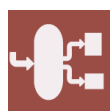
Platinum Sponsors



Sponsors



OPCW



processes

an Open Access Journal by MDPI