

6th French-Chinese Conference on Green Chemistry
第六届中法绿色化学会议
6^{ème} Conférence Franco-Chinoise sur la Chimie Verte



BOOK OF ABSTRACTS

Lyon
26th - 28th October, 2026

CPE Lyon – INSA Lyon – UCBL – ENS de Lyon
LyonTech La Doua Campus
Villeurbanne, France

FC2GChem, Lyon, October 26-28, 2026

Monday Oct 26			Tuesday Oct 27			Wednesday Oct 28		
	7:30 – 8:30	Registration						
	8:30 – 9:15	Opening ceremony						
Session 1	9:15 – 10:00	Opening Lecture Marc FONTECAVE	Session 5	8:30 – 10:00	Florent ALLAIS Shigang SUN Céline CHIZALLET	Session 9	8:30 – 10:00	Haichao LIU Christophe COPERET Peng WU
	10:00 – 10:30	Group picture & coffee break		10:00 – 10:30	coffee break		10:00 – 10:30	coffee break
Session 2	10:30 – 12:00	Can LI Jean-Marie TARASCON Suojiang ZHANG	Session 6	10:30 – 12:30	<i>Early career invited lectures</i> Dawei ZHANG - Noémie PERRET Gaixiu YANG - Grégory CHATEL Longfei LIN - Maïwenn JACOLOT Sébastien LIVI	Session 10	10:30 – 11:00	Aurélien BOULEGUE-MONDIERE
	12:00 – 13h15	Buffet lunch		12:30 – 13:30	Buffet lunch		11:00-12:30	<i>Early career invited lectures</i> Laetitia CHAUSSET-BOISSARIE - Yue LIU Egon HEUSON - Qingqing MEI Marie VUILLEMIN - Bo PENG
Session 3	13:15 – 15:15	Lorie HAMELIN Licheng SUN Hong NIE Sergio MASTROIANNI		12:30 – 14:30	Poster session	Session 11	12:30 – 13h45	Buffet lunch
	15:15 – 15:45	coffee break	Session 7	14:30 – 16:00	Yunhui WANG Carine MICHEL Fengshou XIAO		13:45 – 15:15	<i>Early career invited lectures</i> Wenbin CHEN - Clément CAMP Yang SONG - Léa VILCOCQ Frédéric GUEGAN
Session 4	15:45 – 16:30	FC2GChem - SYENSQO Lecture Ben L FERLINGA		16:00 – 16:30	coffee break		15:15 – 15:45	coffee break
	16:30 – 18:00	Dongyuan ZHAO Alessandra QUADRELLI Buxing HAN	Session 8	16:30 – 18:00	Industrial Roundtable	Session 12	15:45 – 16:15	Baolian SU
	19:00 21:30	Conference dinner Hotel-Dieu Lyon					16:15 – 17:00	Closing Lecture Guy BERTRAND
				19:00 21:00	FC2GChem event Nouvel Institut franco-Chinois		17h00 – 17:15	Closing Ceremony
								End of the meeting
							19:00 21:00	FC2GChem Steering committee dinner



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Welcome / 欢迎词 / Bienvenue

The 6th French-Chinese Conference on Green Chemistry (FC2GChem 2026) takes place in Lyon from October 26th to 28th, 2026 on the LyonTech La Doua Campus in Villeurbanne. The conference is hosted by CPE Lyon and Université Claude Bernard Lyon 1, in collaboration with INSA Lyon and ENS de Lyon, continuing a series of successful the editions held in Shanghai, Wuhan, and Lyon since 2014.

Building on the longstanding friendship between France and China, and partnership between the Region Auvergne Rhône-Alpes and Shanghai, which celebrates its 40th anniversary this year, we are delighted to welcome you once again to Lyon for FC2GChem 2026.

This French-Chinese Conference on Green Chemistry aims to highlight scientific advances and collaborative the efforts towards **“A better Chemistry for a Better Life”**.

We wish you an enjoyable and fruitful conference!

第六届中法绿色化学会议（FC2GChem 2026）将于2026年10月26日至28日在法国维勒班市的里昂科技拉杜阿校区举行。本届会议由里昂高等化学、物理与电子学院（CPE Lyon）和里昂第一大学主办，里昂国立应用科学学院（INSA Lyon）与里昂高等师范学校（ENS de Lyon）协同承办。自2014年以来，该系列会议已先后在上海、武汉和里昂举办多届。

适逢奥弗涅-罗讷-阿尔卑斯大区与上海及其地区缔结友好合作关系四十周年，秉承中法两国源远流长的传统友谊，我们热忱欢迎各位再次莅临里昂，参加第六届中法绿色化学会议。本次会议以“化学使生活更美好”为愿景，旨在集中展示各方为此付出的努力。

祝参会愉快！

La 6^{ème} conférence Franco-Chinoise sur la Chimie Verte, FC2GChem 2026 se tient à Lyon du 26 au 28 octobre, précisément sur le campus LyonTech La Doua à Villeurbanne, accueillie par CPE Lyon et Lyon 1 Université en coordination avec l'INSA Lyon et l'ENS de Lyon, après les éditions organisées à Shanghai, Wuhan et Lyon depuis 2014.

Dans la continuité des relations historiques d'amitié entre la France et la Chine, et de partenariat entre la Région Auvergne-Rhône-Alpes et Shanghai et sa région, dont on célèbre cette année le 40^{ème} anniversaire, nous sommes heureux de vous souhaiter la bienvenue à l'occasion de la conférence FC2GChem 2026, Conférence Franco-Chinoise sur la Chimie Verte, destinée à illustrer les efforts vers « Une Chimie Meilleure pour une Vie Meilleure ».

Bonne conférence !

Prof. Florence POPOWYCZ (INSA Lyon), **Prof. Bruno ANDRIOLETTI** (Univ Lyon 1 & CPE Lyon)
Co-Chairs, Lyon,

Prof. Buxing HAN (ECNU & CAS), **Prof. Peng WU** (ECNU), Co-Chairs, Shanghai

Prof. Yves QUENEAU (CNRS & Univ Lyon), **Prof. Laurent BONNEVIOT** (ENSL),
Prof. Mingyuan HE (ECNU), Honorary Chairs

Preface / (序言) 主旨 / Préface

Sustainable or Green Chemistry, which aims to develop cleaner and safer chemical processes and products with a reduced environmental impact, is a key priority in scientific collaboration between China and France. Organized with the support of the French Chemical Society, the Auvergne Rhône Alpes Region and the Métropole de Lyon, Lyon's academic institutions, and several industrial partners, this conference showcases the joint efforts of both countries to contribute to the transition towards the chemistry of tomorrow.

发展可持续化学或绿色化学，研发环境影响更低、更加清洁安全的化工工艺与产品，始终是中法两国科学合作的优先方向。本届会议得到法国化学会、奥弗涅-罗讷-阿尔卑斯大区、里昂大都会、里昂各高校科研机构以及多家工业合作伙伴的支持，集中展现两国为推动面向未来的化学转型所付出的共同努力。

La Chimie Durable ou Chimie Verte, qui consiste à développer des procédés et produits chimiques plus propres, plus sûrs et de faible impact environnemental, est une des priorités des collaborations scientifiques Franco-Chinoises. Organisée avec l'appui de la Société Chimique de France, de la Région Rhône-Alpes, de la Métropole de Lyon, des établissements académiques de Lyon et plusieurs partenaires industriels, cette conférence est la vitrine des efforts des deux pays pour contribuer à la transition vers la chimie de demain.

The conference brings together more than 120 scientists from academia and industry, covering all areas of sustainable chemistry, including synthesis, catalysis, theoretical chemistry, materials, and chemical engineering. Thanks to the support of numerous institutions and sponsors, the conference will welcome internationally renowned scientists and feature a rich scientific program comprising more than 40 presentations, as well as a dedicated poster session.

本次会议云集了120余位来自工业界与学术界的科研专家，涵盖可持续化学的各个领域，包括合成化学、催化、理论化学、材料、工程等。在众多机构与赞助单位的鼎力支持下，众多知名学者将莅临参会，会议议程包含40余场学术报告以及一场海报展示环节。

La conférence rassemble plus de 120 scientifiques issus des milieux académiques et industriels recouvrant toutes les facettes de la chimie durable (synthèse, catalyse, chimie théorique, matériaux, procédés...). Grâce à l'appui de nombreuses institutions et sponsors, la conférence bénéficiera de la présence d'éminents scientifiques dans un programme proposant plus de 40 conférences et 1 session de posters.

We would like to thank all the institutions and companies that have supported the organization of this conference, as well as everyone who has contributed so enthusiastically and efficiently to making this exceptional event possible.

This conference aims to highlight the importance of Green Chemistry and to foster and strengthen interactions between the Chinese and French scientific communities.

在此，我们谨向所有支持本届会议组织的机构、企业，以及为筹办这一盛会高效付出的全体人员致以诚挚谢意。本次会议旨在展示绿色化学领域的重要性，并促进中法科学界之间的互动与交流。

Nous remercions l'ensemble des institutions et entreprises qui ont soutenu financièrement l'organisation du congrès, et les personnes qui se sont investies dans la préparation de cet événement exceptionnel qui a pour but de mettre à jour l'importance du domaine de la Chimie Verte et de catalyser les interactions au sein de la communauté des chercheurs Français et Chinois.

The Chairs of FC2GChem 2026 Lyon

Prof. Florence POPOWYCZ, Prof. Bruno ANDRIOLETTI, Prof. Buxing HAN, Prof. Peng WU, Prof. Yves QUENEAU, Prof. Laurent BONNEVIOT, Prof. Mingyuan HE

Scientific and Organizing Committees / 组委会

Bilateral Scientific Committee

Gilberte CHAMBAUD, Présidente de la Société Chimique de France
Catherine PINEL, CNRS Chimie & IRCELYON
Bruno LINA, Président de Lyon 1 Université
Marie-Christine BAIETTO, Directrice de la Recherche, INSA Lyon
Claude De BELLEFON, CPE Lyon, Directeur Scientifique
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Arnaud BRIOUDE, Vice- président Recherche, Lyon 1 Université
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Estelle METAY, ICBMS et CNRS Chimie Développement Durable
Vivien HENRYON, ACTIVATION
Philippe MARION, SYENSQO
Hélène OLIVIER-BOURBIGOU, Membre de l'Académie des Sciences, IFPEN
Nicolas ROQUES, SYENSQO
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Shi-Gang SUN, Membre de l'Académie des Sciences de Chine, Xiamen University
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Licheng SUN, Membre de l'Académie des Sciences de Chine, Université de Westlake, Hangzhou
Suojing ZHANG, Membre de l'Académie des Sciences de Chine, Université du Henan & IPE, Beijing
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Université de Technologie de Wuhan
Haichao LIU, Université Peking, Beijing
Guoyue SHI, East China Normal University, Shanghai
Yang TIAN, East China Normal University, Shanghai
Yanlong GU, Université Huazhong de Science et Technologie, Wuhan

Local Organizing Committee

Florence POPOWYCZ (INSA Lyon)
Bruno ANDRIOLETTI (UCBL & CPE Lyon)
Claude DE BELLEFON (CNRS & CPE Lyon)
Yves QUENEAU (CNRS)
Laurent BONNEVIOT (ENS de Lyon)
Belen ALBELA (ENS de Lyon)
Pascal FONGARLAND (UCBL)
Angela REA-BOUTROIS (CPE)
Dawei ZHANG (ECNU, Shanghai)

Chinese Organizing Committee

Buxing HAN (Institute of Chemistry, CAS, Beijing)
Peng WU (ECNU, Shanghai)
Dawei ZHANG (ECNU, Shanghai) – conference secretary (Chinese side)

Team of Volunteers

Mathias FONNESU, Tingjun HU, Syhana JOUBERT, Yaping WANG, Yifan ZHANG, Weike ZHU,
Mariam BOU ORM, Peng CHENG, Cyril HACHEMI, Wenjun JIANG, Antoine LE RAY, Chen LI,
Guanghao LI, Anastasiia SUVOROVA, Buqin XU, Anissa YACIN ALI, Zhigang YAN, Wara ECHAZU-
FLORES, Mingjun GU, Karolina KOWALSKA, Lakshmi Prasad SIVADAM, Salah-eddine AKRIAL.

Institutions / Sponsors / 会议赞助

The FC2GChem Organizing Committee is extremely grateful to their partners and sponsors for the financial contribution to the organization of the conference.

Institutional Partners supporting the event:

Région Auvergne Rhône-Alpes
Métropole de Lyon
Société Chimique de France
CPE Lyon
INSA Lyon
Lyon 1 Université
ENS de Lyon
CNRS
East China Normal University
Institute of Chemistry, Chinese academy of Sciences, Beijing

Industrial sponsors:

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Bluestar Silicones
Wanhua Chemicals

Chinese laboratories supporting the event:

State Key Laboratory of Petroleum Molecular & Process Engineering
Shanghai Key Laboratory of Green Chemistry and Chemical Processes
School of Chemistry and Molecular Engineering, East China Normal University

French laboratories supporting the event:

Institut de Chimie de Lyon
Institut de Chimie et Biochimie Moléculaires et Supramoléculaires (ICBMS), UCBL, CNRS, INSA Lyon, CPE Lyon
Laboratoire de Chimie (LCENS), ENS de Lyon, CNRS, UCBL
Institut de Recherche sur la Catalyse et l'environnement (IRCELYON), CNRS, UCBL
Laboratoire Catalyse, Procédés, Polymérisation et Matériaux (CP2M), CPE, CNRS, UCBL
Institut de Chimie des Milieux et Matériaux de Poitiers (IC2MP), CNRS, Université de Poitiers
Institut CARMEN, Université de Rouen Normandie, CNRS, INSA de Rouen, ENSICAen, UniCaen
Laboratoire Environnements, Dynamiques et Territoires de Montagne (EDYTEM Chambéry), Université Savoie-Mont-Blanc, CNRS
Unité de Catalyse et Chimie du Solide (UCCS), CNRS, Université de Lille, Université d'Artois, Centrale Lille
Institut de Chimie, Collège de France, Paris

Social Program / 会议外的其它社会活动

Lunches & Coffee Breaks Monday October 26th, Tuesday October 27th, Wednesday October 28th

Amphitheater I. Joliot-Curie Building, Level -1, in front of Amphitheater entrance.
Accessible to all registered attendees

Conference dinner Monday October 26th, 19h00, on invitation only

Grand Réfectoire de l'Hôtel-Dieu, 3 Cour Saint Henri Grand Hôtel-Dieu, 69002 Lyon.

Transportation for the Chinese delegation and plenary speakers will be organised. Departure from the Campus after the afternoon scientific sessions.
Other invited guests are kindly asked to go by themselves.

Nouvel Institut Franco-Chinois (NIFC) Event: Tuesday October 27th 19h00, on invitation only

Celebrating the 10th anniversary of NIFC and the 40th anniversary of the AURA- Shanghai Régions partnership.

Nouvel Institut Franco-Chinois, 2 Rue Sœur Bouvier, 69005 Lyon

Transportation for the Chinese delegation and plenary speakers will be organised. Departure from the Campus after the afternoon scientific sessions.
Other invited guests are kindly asked to go by themselves.

Chinese delegation & Steering committee dinner Wednesday October 28th, 19h00

on invitation only, Brasserie Bocuse l'EST, 14 place Jules Ferry (Brotteaux), 69006 Lyon

Transportation for the Chinese delegation will be organised. Departure from the Campus after the afternoon scientific sessions.

Gala dinner and NIFC event dinner attendance is on invitation only for members of the Chinese delegation, plenary speakers, and committee members and guests having been invited by the organization team. Transportation will be organized for the Chinese delegation and plenary speakers. Other attendees are kindly required to arrange their own transportation. Please ask for assistance to the Volunteers if necessary.

Scientific Program

All sessions will take place in the **Irène Joliot-Curie Building**. The amphitheater is located on level -1.

Monday October 26th

8:30 Opening Ceremony

Host: Prof. Bruno ANDRIOLETTI, Lyon 1 Université, Conference co-Chair

- **Welcome address by Prof. Florence POPOWYCZ**, INSA Lyon, Conference co-Chair,
- **M. Alexandre MOULIN**, Director of CPE Lyon
- **Prof. Raphaël TERREUX**, Vice-President of Lyon 1 Université, International Relationships, representing **Prof. Bruno LINA**, President of Lyon 1 Université
- **Mme Sophie BLACHERE**, Conseillère déléguée au campus région du numérique, representing **M. Fabrice PANNEKOUCKE**, Président de la Région Auvergne-Rhône-Alpes
- **M. Jiang YU**, General Consul of China to Lyon
- **Prof. Guoyue SHI**, Vice-President of East China Normal University, Shanghai
- **Prof. Peng WU**, East China Normal University, Shanghai, Conference Co-chair
- **Prof. Emmanuel TRIZAC**, President of Ecole Normale Supérieure de Lyon
- **Prof. Catherine PINEL**, Deputy-Director of CNRS Chimie
- **Prof. Yves QUENEAU, CNRS**, representing **Prof. Gilberte CHAMBAUD**, President of the Société Chimique de France

Group photo of all attendees in the Amphitheater

Session 1 Chair: Alessandra QUADRELLI

15:45 PL8 **Marc FONTECAVE**

Laboratoire de Chimie des Processus Biologiques, Collège de France, CNRS, Sorbonne Université, Paris, France

From Nature to Chemistry : Artificial Enzymes for CO₂ Valorization

10:00 Coffee break

Session 2 Chairs: Shi-Gang SUN & Alessandra QUADRELLI

10:30 PL1 **Can LI**

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China

Green Hydrogen and Liquid Sunshine

11:00 PL2 **Jean-Marie TARASCON**

Collège de France, Paris, France

Better Li(Na)-ion Batteries through Chemistry

11:30 PL3 **Suojiang ZHANG**, Yawei LIU and Yao LI

Institute of Process Engineering, Chinese Academy of Sciences, Beijing, and Henan University, Zhengzhou, China

Ionic Liquids: Functional Design and Process Innovation

12:00 Lunch

Session 3 Chairs: Hong NIE & Claude DE BELLEFON

13:15 **PL4** **Lorie HAMELIN**

TBI, Université de Toulouse, CNRS, INRAE, INSA, Toulouse, France

Beyond Individual Technologies: Designing Coherent and Sustainable Strategies for GHG Neutrality at the National Scale

13:45 **PL5** **Licheng SUN**

Center of Artificial Photosynthesis for Solar Fuels and Department of Chemistry, School of Science, Westlake University, Hangzhou, China

Water Splitting Catalysis—From Natural to Artificial Photosynthesis

14:15 **PL6** **Hong NIE and Wenbin CHEN**

SINOPEC Research Institute of Petroleum Processing CO., LTD, Beijing, China

Catalytic Hydrotreating Technology Innovation towards Green and Low-Carbon Development of Oil Refining

14:45 **PL7** **Sergio MASTROIANNI**, Philippe MARION and Nicolas ROQUES

Syensqo Research and Innovation Center of Lyon, Saint-Fons, France

From Renewable Carbon to Circular Materials: Industrial Pathways for Sustainable Chemistry

15:15 Coffee break

Session 4a Chair: Philippe MARION

15:45 **FC2GChem SYENSQO Lecture**

Ben L. FERINGA, 2016 Nobel Prize winner in Chemistry

Stratingh Institute for Chemistry, University of Groningen, Groningen, The Netherlands

Exploring Sustainable Catalytic Space

Session 4b Chairs: Can LI & Karine DE OLIVEIRA VIGIER

16:30 **PL9** **Dongyuan ZHAO**

Laboratory of Advanced Materials, Fudan University, Shanghai, and College of Energy Materials and Chemistry, Inner Mongolia University, Hohhot, China

Controllable Synthesis and Application of Mesoporous Crystalline Frameworks

17:00 **PL10** **Alessandra QUADRELLI**

IRCELYON, CNRS Université Claude Bernard Lyon 1, Villeurbanne, France

Situated Green Chemistries, Sustainability, and Ending the Myth of Neutral Research in Green Chemistry

17:30 **PL11** **Buxing HAN**

Institute of Chemistry, Chinese Academy of Sciences, Beijing, China

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

19:00 Conference dinner (on invitation only)

Tuesday October 27th

Session 5 Chairs: Florence POPOWYCZ & Vivien HENRYON

8:30 **PL12 Florent ALLAIS**

Université Paris-Saclay, AgroParisTech, URD Agro-Biotechnologies Industrielles, CEBB, Pomacle, France

Integrating Green Chemistry, Biotechnology and Downstream Processing for Biomass Valorization

9:00 **PL13 Shigang SUN**

State Key Laboratory of Physical Chemistry of Solid Surfaces, College of Chemistry and Chemical Engineering and College of Energy, Xiamen University, Xiamen, China

Electrochemical Energy Processes investigated by In-situ/Operando Spectroscopy

9:30 **PL14 Céline CHIZALLET**

IFP Energies nouvelles, Rond-point de l'échangeur de Solaize, Solaize, France

Alcohol Dehydration Mechanisms by Brønsted acidic Zeolites unraveled by Atomic-Scale Calculations

10:00 Coffee break

Session 6 *Early Career Invited Lectures*

Chairs: Dongyuan ZHAO & Nicolas ROQUES

10:30 **IL1 Dawei ZHANG**

State Key Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Harnessing Supramolecular Confinement: Functionalities from Macrocycles to Cages

10:45 **IL2 Noémie PERRET, Alberto J. REYNOSO, Kamila KAŻMIERCZAK, Carine MICHEL, Laurent DJAKOVITCH**

Université Lyon 1, CNRS, IRCELYON, UMR 5256, Villeurbanne, and CNRS, ENS de Lyon, LCH, UMR 5182, Lyon, France

Dehydrogenation of Alcohols and Polyols in Liquid Phase with Metal Catalysts

11:00 **IL3 Gaixiu YANG**

School of Ecology and Environment, Xizang University, Lhasa, and Guangdong Provincial Key Laboratory of High-Quality Recycling of End-of-Life New Energy Devices, Guangzhou Institute of Energy Conversion, Chinese Academy of Sciences, Guangzhou, China

The Green Synthesis of Biomass based Carbon Materials via Biomolecular Tailoring and its Application in Energy Storage

11:15 IL4 **Grégory CHATEL**

Laboratoire EDYTEM, Université Savoie Mont Blanc, Chambéry, France

From Residual Biomass to Value-added Products: a Systemic Green Chemistry Approach

11:30 IL5 **Longfei LIN**, Ziyu CEN, Tianrui BI, Wanying HAN and Buxing HAN

Institute of Chemistry, Chinese Academy of Sciences, Beijing, and School of Chemical Sciences, University of Chinese Academy of Sciences, Beijing, China

Conversion of Polyolefins to Fuels and Chemicals

11:45 IL6 **Maïwenn JACOLOT**

Institut de Chimie et Biochimie Moléculaire et Supramoléculaire (ICBMS), INSA Lyon, CNRS, Université Lyon 1, CPE Lyon, Villeurbanne, France

Borrowing Hydrogen Catalysis for the Sustainable Synthesis of High-Value Molecules from Alcohols and Polyols

12:00 IL7 **CANCELED Chengcheng LI** and Jingwen CHU

State Key Laboratory of Chemical Resource Engineering, Beijing Advanced Innovation Center for Soft Matter Science and Engineering, Beijing University of Chemical Technology, Beijing, and Quzhou Institute for Innovation in Resource Chemical Engineering, Quzhou, China

Electrothermal Methane Dry Reforming, beyond Rapid Heat Delivery

12:15 IL8 **Sébastien LIVI**, Jean-François GERARD and Jannick DUCHET-RUMEAU

Université Claude Bernard Lyon 1, INSA Lyon, Université Jean Monnet, CNRS UMR 5223, Ingénierie des Matériaux Polymères, Villeurbanne, France

A new generation of multifunctional and recyclable epoxy networks

12:30 Lunch

12:30 **Poster session**

Location: Level -1, by the entrance of the Amphiteater

Session 7 *Chairs: Haichao LIU & Micheline DRAYE*

14:30 PL15 **Yunhui WANG**, Nicolas LESUEUR and Nicolas LEROY

R&D of Functionalization of Starch, Sugar and Polyol, and Paper and Board Development Center, Roquette, Lestrem, France

Application of Starch and its Derivatives in Paper&Board for Sustainable Packaging Materials

15:00 **PL16** **Carine MICHEL**

CNRS, ENS de Lyon, Laboratoire de Chimie, Lyon, France

Upgrading HMF using Thermal Heterogeneous Catalysis and Electrocatalysis combining Modeling and Experiments

15:30 **PL17** **Feng-Shou XIAO**

College of Chemical and Biological Engineering, Zhejiang University, Hangzhou, China

Design of Efficient Zeolite-Based Catalysts from Surface Sorption Equilibrium

16:00 Coffee break

16:30 *Session 8* *Industrial Roundtable*

"How green chemistry principles can be integrated in the industrial and R&I strategies".

Sergio MASTROIANNI SYENSQO, Vivien HENRYON (ACTIVATION), Yunhui WANG (ROQUETTE), Yang SONG (SINOPEC), Pierre BECCAT (BLUESTAR SILICONES), Tao YU (PDC-WANHUA CHEMICALS)

19:00 Nouvel Institut Franco-Chinois (NIFC) reception & cocktail (on invitation only)

Wednesday October 28th

Session 9 *Chairs: Bao-Lian SU & Estelle METAY*

8:30 **PL18** **Haichao LIU**

Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing, China

Catalytic Conversion of Cellulosic Biomass to Chemicals

9:00 **PL19** **Christophe COPERET**

Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland

Understanding Catalysis, One Atom at a Time

9:30 **PL20** **Peng WU and Hao XU**

State Key Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Design Synthesis of Novel Metallosilicates for Selective Oxidation

10:00 Coffee break

Session 10 Chairs: Peng WU & Belen ALBELA

10:30 **PL21** Aurélie BOULEGUE-MONDIERE

R&D, Bluestar Silicones, 9 rue Spécia, 69190 Saint -Fons, France

Chemical Recycling of Silicones: Back to Circularity

Early Career Invited Lectures

11:00 **IL9** Laetitia CHAUSSEY-BOISSARIE

Institut CARMen UMR CNRS 6064, Rouen, France

Electrocatalytic Generation of Alkyl Radicals from Organoboron Compounds for C–C Bond Formation

11:15 **IL10** Yue LIU

State Key Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Influence of Water on the Acidity of Zeolite

11:30 **IL11** Egon HEUSON, Lucas BISEL, Aurélie FOSSEY-JOUEENNE, Richard MARTIN, Jonathan BASSUT, Antoine LANCIEN, Louis MOUTERDE, Vivien HERRSCHER, Carine VERGNE-VAXELAIRE, Renato FROIDEVAUX, Manuel ANTUCH and Anne ZAPARUCHA

Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181-UCCS-Unité de Catalyse et Chimie du Solide, Lille; Génomique Métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry; UMR Transfrontalière BioEcoAgro N° 1158, Univ. Lille, INRAE, Univ. Liège, UPJV, JUNIA, Univ. Artois, Univ. Littoral Côte d'Opale, Institut Charles Viollette, Villeneuve d'Ascq ; URD Agro-Biotechnologies Industrielles (ABI), CEBB, AgroParisTech Innovation, Pomacle, France

Unlocking new Biobased Chemicals and co-Substrate in situ Production through Chemo- and Biocatalysts Combination

11:45 **IL12** Qingqing MEI, Siyu ZHANG and Minghao ZHANG

College of Environmental and Resource Sciences, Zhejiang University, Hangzhou, Zhejiang, China

Challenges and Strategies for the Chemical Recycling of Polyester-Based Waste Plastics

12:00 **IL13** Marie E. VUILLEMIN

Université Lyon 1, CNRS, ICBMS, UMR 5246, Villeurbanne, France

One Solvent, Many Opportunities: 2-Methyltetrahydrofuran-3-one as a Multifunctional Solvent for Biomass Valorization

12:15 **IL14** Bo PENG

State Key Laboratory of Petroleum Molecular & Process Engineering, SINOPEC Research Institute of Petroleum Processing Co., Ltd., Beijing, China

Changes on Reaction Pathways during C-C Bond Cleavage via Metal Addition to Zeolites

12:30 Lunch

Session 11 *Early Career Invited Lectures*

Chairs: Licheng SUN & Pascal FONGARLAND

13:45 **IL15** **CANCELED Wenbin CHEN**, Xueyan JU, Hong NIE, Rui ZHANG, Qinghe LIU, Feng LIU, Yuanbing XI, Mingfeng LI

SINOPEC Research Institute of Petroleum Processing CO., LTD, Beijing, China

Catalyst Design for Diesel Hydrotreating towards Low Carbon Production

14:00 **IL16** **Clément CAMP**

Laboratory of Catalysis, Polymerization, Processes and Materials (CP2M UMR 5128), CNRS, Université Lyon 1, CPE-Lyon, Villeurbanne, France

Engineering Heterobimetallic Catalysts for C-H Activation: from H/D Exchange to Methane Valorization

14:15 **IL17** **Yang SONG** and Wei LIN

SINOPEC Research Institute of Petroleum Processing CO., LTD., Beijing

Development and Application of PEM Water Electrolysis for Hydrogen Production

14:30 **IL18** **Léa VILCOCQ**

IRCELYON, CNRS-Université Claude Bernard Lyon 1, Villeurbanne, France

Innovative Catalytic Processes for Black Liquor Valorisation

14:45 **IL19** **CANCELED Wei ZHANG**

State Key Laboratory of Petroleum Molecular & Process Engineering, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai 200062, China

Low-temperature Catalytic Upcycling of Mixed Polyolefins via Tandem Catalysis

15:00 **IL20** **Frédéric GUEGAN**, Richail Dubien MOULANDOU KOUMBA, Adrien RATIER, Karine DE OLIVEIRA VIGIER and François JEROME

IC2MP, UMR CNRS 7285 Université de Poitiers, Poitiers, France

From Rationalization to Prediction of Reactivity and Selectivity through DFT Simulations : The Case of Diels-Alder Reactions of Biobased Furanic Derivatives

15:15 Coffee break

Session 12 Chairs: Buxing HAN & H       OLIVIER-BOURBIGOU

15:45 **PL22 Bao-Lian SU**

Laboratory of Inorganic Materials Chemistry (CMI), University of Namur, Namur, Belgium, and State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan, China

Photothermal Catalytic Reduction of CO₂

16:15 **Closing lecture**

Guy BERTRAND

UCSD-CNRS Joint Research Laboratory, Department of Chemistry and Biochemistry, University of California San Diego, La Jolla, USA

Could Carbenes and related Low-valent Carbon Species Replace Transition Metals

17:00 **Closing Ceremony**

Conference summary and perspectives by Conference Chairs

Hosts: Prof Laurent BONNEVIOT, ENS de Lyon and **Prof. Yves QUENEAU**, CNRS

**Adresses by Prof. Florence POPOWYCZ, Prof. Bruno ANDRIOLETTI,
Prof. Buxing HAN, Prof. Peng WU**

19h00 Steering Committee and Delegation Dinner (on invitation)

POSTER SESSION

- P1 *How do Alkali Cations Affect Alkaline HER Activity of Nickel and Platinum?*
Sumit BAWARI, Nicolas A. ISHIKI, Mingjun GU, Gaëlle KHALIL, Marion GIRAUD, Jennifer PERON, Stephan N. STEINMANN
- P2 *Design and Development of a Tandem Photoelectrochemical Device for the Solar Valorization of Biomass-Derived Furanic Compounds*
Mariam BOU ORM, Mathieu PREVOT, Philippe VERNOUX
- P3 *Thermodynamic modeling of CO₂ absorption with aqueous potassium lysinate and organocatalyzed mineralization*
Axel CHANCRE, Deborah ROMITO, Julien LECLAIRE
- P4 *Total Synthesis of Miyabeacin B. Is Ansarane a potential 3D Bioisostere of Naphthyl group?*
Lisenn DORE, Fabienne FACHE, Olivier PIVA
- P5 *Molecular and Macromolecular Heterocyclic Compounds formed during the Transformation of Sugars into Caramel*
Mathias FONNESU, Florence POPOWYCZ, Bruno ANDRIOLETTI, Yves QUENEAU, Cédric MORETTON, Henri NIGAY
- P6 *Boranil-based Molecular Emitters for the Development of Responsive Supramolecular Materials with Enhanced Chiroptical Properties*
Romain DUWAT, Samuel DECORPS, Rayan HACHEM, Juichi BAINVEL-SATO, Laure GUY, Christophe BUCHER, Denis FRATH
- P7 *Electrochemically-Driven Auto-Tandem Nickel Catalysis for the Production of Butafulvenes*
Tingjun HU, Camille BELUZE, Coralie DUCHEMIN, Didier BOUYSSI, Julien C. VANTOUROUT, Nuno MONTEIRO, Abderrhamane AMGOUNE
- P8 *Valorization of 5-HMF for the Synthesis of Novel Spirocycles using aza-Piancatelli Reaction*
Syhana JOUBERT, Malvina LARDUINAT, Adrien DELOCHE, Eman DOKMAK, Lucie GRAND, Charlie VERRIER, Sylvie MOEBS-SANCHEZ, Florence POPOWYCZ
- P9 *Efficient and Sustained Electrocatalytic Methanol Production from CO₂ on Heterogenized Butoxy-substituted Cobalt Phthalocyanines*
Chen LI, Camile TABARIÈS, Gloria ZANOTTI, Laurent PICCOLO, Mathieu S. PREVOT
- P10 **CANCELED** *Stable Electrothermal Methane Dry Reforming Using Structured Ni/CHA Zeolite*
Jingwen CHU, Chengeng LI
- P11 *Screening of Catalysts for the Heterogeneous Fenton Process for Plastics Degradation*
Guanghao LI, Peng CHENG, Jing SUN, Frederic DAPPOZZE, Jesús GONZÁLEZ-COBOS, Sonia GIL
- P12 *Conversion of Polyesters and CO₂ to Monomers and Carbonates*
Cong LUO, Ziyu CEN, Longfei LIN, Buxing HAN

- P13 *Chemical Recycling of Polyolefin Plastics under Mild Conditions via GaCl₃-based Molten Catalysts*
Yue LIU
- P14 *Selective and Synergistic Upcycling of Mixed Plastic Waste*
Qingqing MEI, Yunkai YU, Shaoyu ZHANG, Yue Zhu
- P15 *Efforts for paradigm shift of basic research with industrial orientation - examples at Basic Research Department @ RIPP*
Bo PENG, Qi OU
- P16 *Engineering Catalytic Sites and Reaction Pathways for CO₂ Electroreduction to Value-Added Chemicals*
Yang SONG, Xue YANG, Wei LIN
- P17 *Computational Investigation of the Glucose-Fructose Isomerization Catalyzed by a Base*
Charlyne VOGEL, S.N. STEINMANN, Carine MICHEL
- P18 *Photoredox-Catalyzed Synthesis of Aromatic Difluoroacyl Spirocycles*
Yaping WANG, Chérif ADOUAMA, Noémie MURARD, David GUEYRARD, Guillaume PILET, Marcelo PUIATTI, José BORIONI, Anis TLILI, Jérémy MERAD, Maurice MÉDEBIELLE
- P19 *The Green Synthesis of Biomass based Carbon Materials via Biomolecular Tailoring and its Application in Energy Storage*
Gaixiu YANG
- P20 *Cyclic BODIPY Arrays: A Class of Macrocyclic-Based Molecular Solids for Hydrogen Isotope Separation and Iodine Capture*
Dawei ZHANG
- P21 *Enzymatic Depolymerization of Lignin as Nanoparticles*
Yifan ZHANG, Marjorie OCHS, Bastien DOUMECHE, Marie E. VUILLEMIN
- P22 *Iron-Promoted Sulfided NiW Catalysts with Synergistic Ni-Fe-W Interaction for Boosting Hydrodeoxygenation of Lipids*
Weitao ZHAO, Xiao ZHANG, Xiaoyi SANG, Dadong Li, Hong NIE
- P23 *Photocatalytic β -C-H Functionalization of Alcohol Derivatives via 1,5-HAT*
Wei-ke ZHU, Abderrahmane AMGOUNE, Jérémy MERAD
- P24 *AI-Driven Design of SrTiO₃:Al Photocatalysts for Overall Water Splitting*
Hong WANG, Abdoulatif CISSE, Mengjia ZHU, Rob CLOWES, Xenophon EVANGELOPOULOS, Charlotte E. BOOTT, Can LI, Andrew I. COOPER
- P25 *Characterization of an Antiviral Malagasy Plant Extract for Viral Infection Control*
Rojo Koloina RAZAFINDRALAMBO, Marjolaine REY, Gilles COMPTES, Chaker EL KALAMOUNI, Voahangy RAMANANDRAIBE, Marc LEMAIRE, Estelle METAY

Plenary Lectures

Exploring Sustainable Catalytic Space

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Facing the future of chemistry, being the creating science par excellence, chemical synthesis is confronted with major challenges regarding catalysis, precision chemical transformations and adopting the principles of green chemistry. In this lecture we will explore chemical activation discussing recent advances in our program on asymmetric catalysis and adaptive catalysts using metal- based catalytic approaches. Catalytic enantioselective synthesis with organolithium reagents are presented as well as ultrafast Pd-catalyzed cross coupling methodology, illustrating fast, high precision and stereoselective C-C bond formation. Towards sustainable chemical transformations the waste-free synthesis of alkylamines, using hydrogen borrowing catalysis and ultrafast photoclick reactions are described. Finally, a bio-based route to polymers and coatings using photocatalytic oxidation as a key transformation and multitasking chiral catalyst based on light-powered rotary motors are discussed.



Fig. 1: Phosphoramidite ligands for sustainable catalysis

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Green Hydrogen and Liquid Sunshine

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The overuse of fossil energy has led to serious problems which threaten the sustainable development of the mankind and the environmental and ecological civilization. Among the feasible routes to overcome difficulties in the sustainable development, solar fuel utilization has been considered as an ideal solution to replace the fossil energy with renewable energy.

This lecture presents the progress made in solar fuel production via artificial photosynthesis, including a two-step process: the CO₂ reduction with green hydrogen which is produced from water splitting by electrolysis with renewable energy. As a example, the lecture will introduce a Liquid Sunshine project which is based on photovoltaic-electrolysis hydrogen production and CO₂ hydrogenation to methanol. It has been demonstrated that green hydrogen and liquid sunshine methanol would be a promising strategic path to achieve net-zero emission, i.e., carbon neutrality.

Liquid sunshine refer to solar fuel synthesis from CO₂ and H₂O with renewable energy. Practically, this process can be divided into two steps: water splitting to generate green hydrogen as the first step, and then CO₂ is hydrogenated to solar fuel, like methanol, with the green hydrogen. To meet the demand for inducing large scale alkali water electrolysis (>1000 Nm³/h) technology was developed based on advanced cathode and anode electrocatalysts; Meanwhile, a bimetal oxide solid solution catalyst, ZnZrO₂ was discovered to be highly active and selective for CO₂ hydrogenation ever under industrial conditions. Liquid sunshine strategy has been extended to the DMF synthesis on a ZnTiO₂ solid solution catalysts. Liquid sunshine methanol (or solar methanol) as the solar energy carrier has been utilized in bio-manufactures, such as starch synthesis, and L-lactic acid (L-LA) synthesis. This is becoming a promising route to synthesis the biomolecules efficiently utilizing CO₂ and renewable energy.

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Better Li(Na)-ion Batteries through Chemistry

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Due to their high energy density, rechargeable lithium-ion batteries have become the standard for most portable electronics today and are the optimal choice for electric vehicles. However, greater autonomy and faster charging times are still needed. There is great hope for the development of solid-state batteries, provided positive electrode materials with higher energy density and solid-state electrolytes with higher ionic conductivity can be identified. This is what this lecture will aim to address by focussing on new halides and oxyhalides compounds.

Firstly we will report on the synthesis of crystalline LiMCl_6 and derivatives together with their reactivity against Li in both solid state and liquid cells prior to demonstrate a universal self-assembly reaction between halide solid electrolytes and glyme-based solvents that produces a new universal class of cubic crystalline alkali organic-inorganic halide-glymes of formula $\text{AMX}_6.m\text{Gn}$ ($A = \text{Li, Na, K}$; $M = \text{Ta, Nb}$; $X = \text{Cl, Br}$; $\text{Gn} = \text{mono- to tetraglyme}$; $m = \text{number of Gn}$). We will comment on their assembly mechanism and their chemical-physical properties.

Turning to oxyhalides, we will report on a new crystalline phase of $\text{Li}_2\text{TaOCl}_{10}$, synthesized via a simple, low-temperature process, that is composed of isolated $[\text{Ta}_2\text{OCl}_{10}]^{2-}$ dimers. We demonstrate that this new phase exhibits a room-temperature ionic conductivity of up to 11 mS cm^{-1} via partial ball milling, and can be used to assemble solid-state batteries that retain 80% of their initial capacity through 800 cycles. Lastly, we will discuss how structures built from dimer units provide a rich chemical design space for the next generation of high-ionic-conductivity solid-state electrolytes.

Ionic Liquids: Functional Design and Process Innovation

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As an emerging class of green media with unique structures and tunable properties, ionic liquids (ILs), offer new avenues for functional material design and process innovation^{1,2}. This report presents a systematic review of IL development from fundamental breakthroughs to industrial applications. It clarifies key scientific concepts including Z-bonds, quasi-liquids, ionic clusters, and ionic microenvironment, that form the basis for rational molecular design and precise process regulation of ILs. Using industrial cases, the report surveys IL-driven transformative technologies and industrializations in areas such as CCUS, photoelectric conversion, energy storage, and biomedicine^{2,3}. Looking forward, an AI-driven cross-scale research paradigm should be established to enable precision fabrication of functional ILs and to innovate reaction-separation processes, thereby accelerating the transformation and upgrading of the chemical engineering industry.

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Beyond Individual Technologies: Designing Coherent and Sustainable Strategies for GHG Neutrality at the National Scale

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Sustainably achieving greenhouse gas (GHG) neutrality is not simply a matter of identifying the best-performing technologies in isolation. At the national scale, transition choices are interconnected through limited supplies of biomass, renewable electricity, land, nutrients, infrastructure and carbon-storage capacity. A technology that appears environmentally attractive on its own may perform differently once its deployment scale, resource requirements and interactions with other sectors are considered.

This lecture will examine how environmental assessment can contribute to the transition from evaluating individual technologies to designing more coherent and sustainable strategies for GHG neutrality. It will address three complementary pillars: reducing GHG emissions from existing systems; replacing fossil carbon in applications where carbon remains functionally necessary; and generating additional removals of carbon dioxide from the atmosphere, combined with sufficiently durable storage. It will also consider the accounting methodologies needed to represent emissions, substitution effects and carbon removals consistently, and the challenge of reconciling practical applicability with scientific robustness.

Particular attention will be given to a research programme developed for France under the presidential Make Our Planet Great Again initiative. The programme investigates how France's limited residual biomass resources could be prioritised among competing uses, including food and feed[1–3], bio-based materials and chemicals[4,5], aviation and maritime fuels[6–7], and domestic and industrial energy production[9–10], as part of a broader effort (e.g. [11]) to ground national transition strategies in robust scientific evidence (e.g. [12]).

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Water Splitting Catalysis—From Natural to Artificial Photosynthesis

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One important challenge in converting sustainable energy, such as solar and wind power, into fuels is directly coupling a PV and a wind turbine to a water electrolyser for green hydrogen production. In this process, the design and synthesis of catalysts to promote water oxidation and proton reduction are important. This talk will present research progress on developing anion exchange membranes (AEMs), bioinspired water-oxidation catalysts, hydrogen-generation catalysts, and their membrane electrode assemblies. Inspired by watermelon skins, several synthetic polymers have been designed and prepared as AEMs. Together with NiFe-based water oxidation catalysts and NiMo-based hydrogen generation catalysts, these AEMs are used in functional devices and demonstrate excellent performance for sustainable, energy-driven green hydrogen production at low cost. The mechanisms of O-O bond formation in pure Ni-based and NiFe-based water oxidation catalysts, revealing the important role of Fe, will be presented. In addition to AEM-WE, the use of water as a green solvent and oxygen source for electrochemical HMF oxidation to FDCA will also be demonstrated.

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Catalytic Hydrotreating Technology Innovation towards Green and Low-Carbon Development of Oil Refining

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The oil refining industry plays a pivotal role in the global energy and chemical supply system. Driven by the initiative of green development and "carbon neutrality" goals, the transformation and upgrading of the oil refining industry is accelerating at an unprecedented pace. Catalytic hydrogenation technology stands as a critical enabler for the green and low-carbon development of the oil refining industry. Focusing on the key challenges involved in the carbon reduction targets covering raw materials, processes and products, a series of new catalysts and advanced processes have been developed and commercialized. Extensive researches have been carried out in the key directions including the production of sustainable biofuels, energy conservation in the production processes, the improvement of yield of high value chemical products and jet fuel, which promotes the efficient and low-carbon development of refining and chemical technologies.

Regarding the sustainable biofuel production technology, this study introduced a "two-stage three-zone" reaction system for molecular directional reconstruction. High-stable hydrodeoxygenation and high-selective isomerization catalysts were developed to address the challenges as the proneness of conventional catalysts to deactivation, severe exothermic effects during reaction, and excessive cracking that affects jet fuel yield. Based on these technical breakthroughs, a bio-jet fuel production technology with independent intellectual property rights was developed and commercially applied for the first time in China.

To achieve energy conservation and emission reduction in diesel production, the stable hydrogenation catalysts and low-energy consumption hydrogenation processes were developed by focusing on defining the high efficient active phase structure and optimizing the reaction environment. This enabled forming key technologies for efficient and low-carbon production of clean diesel, which can extend the operation cycle of diesel hydrogenation units and deliver remarkable energy conservation as well as emission reduction benefits.

For the production of various chemicals and yield enhancement of jet fuel, this research clarified the conversion rules of S and N impurities, as well as aromatics, cycloalkanes, and chain alkanes during the hydrocracking process, and revealed the mechanism of zone-specific conversion of hydrocarbons. By constructing different reaction zones and designing suitable catalysts, a series of hydrocracking technologies were developed for the production of high-value clean jet fuel and the maximized output of high-value chemical raw materials, forming the core technology of a chemical-type refinery.

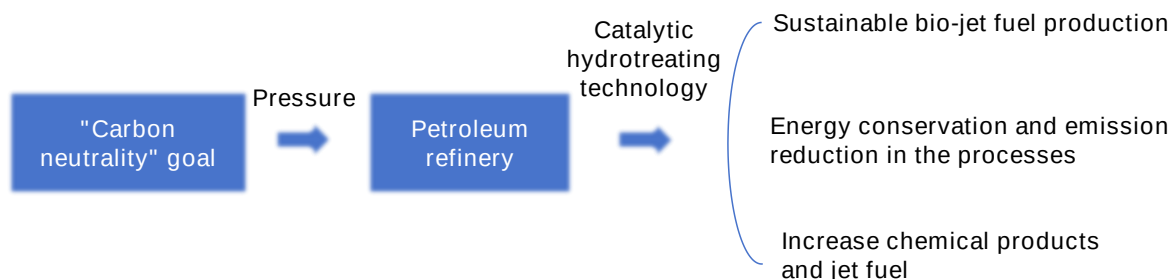


Fig. 1: Solutions for green development of petroleum refinery

From Renewable Carbon to Circular Materials: Industrial Pathways for Sustainable Chemistry

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The transition toward a low-carbon and circular economy is reshaping the chemical industry and accelerating the development of renewable, biodegradable, and circular solutions. As a leading specialty chemical company, Syensqo is leveraging the combined power of chemistry, biotechnology, and sustainability-by-design approaches to accelerate this transition and deliver high-performance solutions with reduced environmental footprints.

This presentation will provide an industrial perspective on how renewable carbon sources, biotechnology, and circularity principles can be leveraged to develop high-performance materials and specialty ingredients with reduced environmental impact. Syensqo's strategy combines the use of renewable feedstocks, biodegradable-by-design technologies, and circular material approaches to support the transition away from fossil-based resources while maintaining product performance and competitiveness.

Several industrial case studies will be presented, including natural aromatic ingredients, biodegradable functional polymers, bio-based formulation ingredients, and circular material solutions. These examples illustrate how sustainability considerations are integrated from early research through industrial deployment using science-based assessment methodologies and life-cycle thinking.

The presentation will conclude with perspectives on the key scientific and industrial challenges associated with scaling sustainable chemistries and on the role of industry-academia collaborations in advancing the bioeconomy and circular economy.

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From Nature to Chemistry : Artificial Enzymes for CO₂ Valorization

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While developed in a number of directions, bioinspired molecular catalysis has been explored only very recently for CO₂ reduction, a challenging reaction, of prime importance in the context of the energetic transition to be built up. This approach is particularly relevant as Nature teaches us that CO₂ reduction is possible, at low overpotentials, high rates and large selectivity, and gives us unique clues to design and discover new interesting molecular catalysts. Indeed, based on our relatively advanced understanding of the structures and mechanisms of the active sites of fascinating metalloenzymes such as formate dehydrogenases and CO dehydrogenases, it is possible to design original bioinspired molecular catalysts for CO₂ electro- and photo-reduction.

Here we specifically discuss our recent efforts, failures and successes, in developing artificial metalloenzymes for CO₂ reduction, so-called Artificial CO₂ reductases, combining an appropriate host protein and synthetic organometallic complexes [1,2]. Recently, we succeeded in creating such an artificial enzyme using a metallic cofactor mimicking the heterodinuclear sites found in natural “CO₂ reductases” (unpublished).

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Controllable Synthesis and Application of Mesoporous Crystalline Frameworks

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Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) have emerged as classical crystalline porous materials assembled by microscopic building block, showing a great promise in various areas such as catalysis, gas storage and separation, and energy storage. Owing to the inherent microporosity of such frameworks, the applications that involve large molecules are greatly hindered. The introduction of mesopores (size of 2 ~ 50 nm) into MOFs/COFs can effectively mitigate transport limitations, enhancing accessibility and utilization of deeply embedded active sites. Nonetheless, realizing mesoporous MOFs/COFs is hampered by imbalance in structural tension at the micro-scale of the crystalline MOF framework and the meso-scales of surfactant-composite self-assembly. The mismatch between the MOF/COF framework crystallization and co-assembly of micelles with the building blocks, normally could lead to decreased crystallinity, disordered pore structures, and even post-synthesis collapse. Recently, we have demonstrated a novel cooperative assembly strategy by precisely regulating crystallization kinetics and template interactions, enabling the formation of highly crystalline mesoporous MOFs/COFs with tunable, ordered mesopore architectures. This new methodology has been extended to more complex hierarchical porous networks. Based on this, we have constructed a library of meso-MOFs that covers a wide range of morphologies (such as cubes and 2D nanosheets), compositions and architectures (including hollow and core-shell structures), expanding the diversity of mesoporous materials. By integrating mesoscale channel networks while preserving long-range order and site-definability at the micro-scale, we have successfully reduced diffusion resistance and enhanced interfacial exchange, thereby promoting efficient combination of reaction kinetics and ion transport with internal active centers. In summary, highly ordered mesoporous MOFs/COFs offer unique advantages in cross-scale mass transport and improved site availability, providing structurally robust, high-flux platforms for membrane-based separations, selective transport, photo-electrocatalysis, and energy storage devices. Such advances further drive the integration of crystalline framework materials in the form of thin films, electrodes, and reactor components.

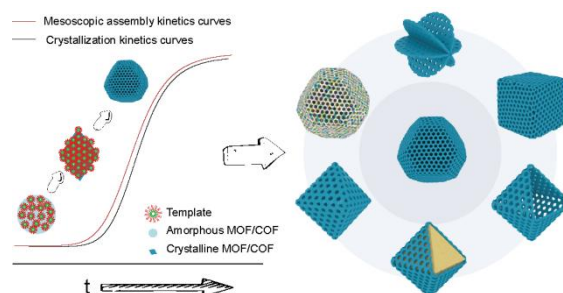


Fig. 1: Scheme illustration of the formation of the mesoporous MOFs/COFs.

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Situated Green Chemistries, Sustainability, and Ending the Myth of Neutral Research in Green Chemistry

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The research in chemistry we perform is not neutral regarding its topics, its contributions or its practices.[1] This lack of neutrality is not a surmountable hindrance, a bias, but a defining feature of science that, if embraced—keeping in mind the values of transparency, rigor, reliability and quest for objectivity— could allow the improvement of our scientific endeavors toward a level less inadequate with respect to our current poly-crises predicament.

In this lecture I will defend the necessity for scientists, including chemists, to pay attention to the conditions, assumptions, and perspectives that shape research. Learning how to acknowledge the context in which and the context *for* which the research is performed -and checking that the knowledges developed are pertinent for the situation addressed - strengthens rather than weakens scientific practice. In this context, the connected proposal developed for green chemistry, the "situated green chemistries" framework, will be shared. [2].

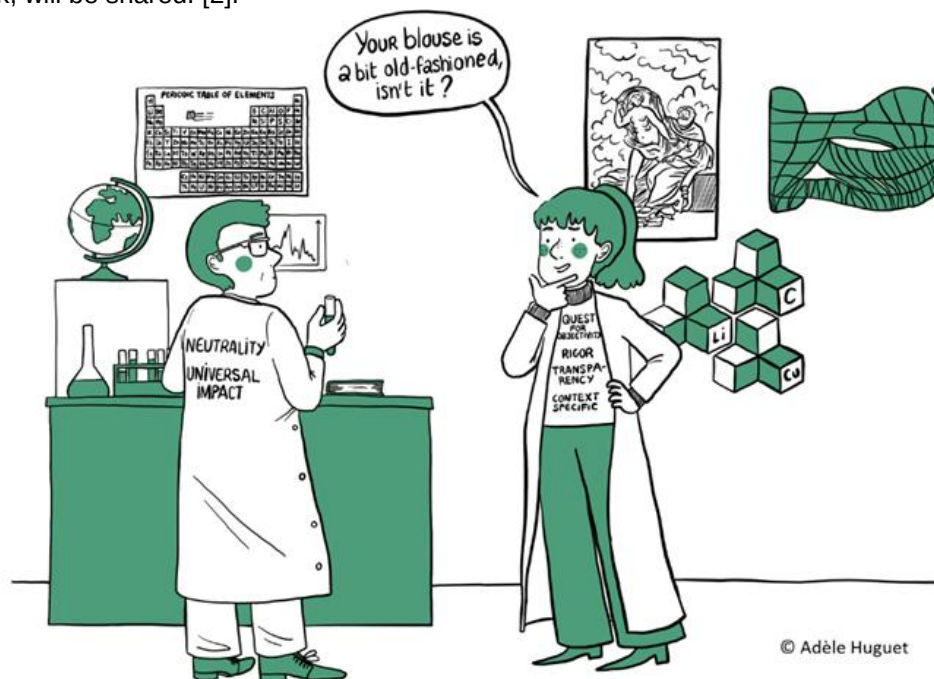


Fig. 1: Illustration about invitation to shift from claims of neutrality and universal impact in research to other scientific epistemologies -situated, context-specific, transparent and rigorous- in a laboratory-based science such as chemistry. CC BY NC SA and inspired from ref 2.

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PL11

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

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Carbon dioxide (CO₂) is a major greenhouse gas and also an abundant and low-cost C1 feedstock. Biomass is an abundant renewable carbon resource, and synthetic plastics are indispensable materials in modern life. However, huge amounts of waste plastics are generated every year. Utilizing CO₂, biomass, waste plastics, and kitchen waste as carbon sources to produce value-added fuels, chemicals, and materials is of great importance for achieving green and sustainable development of our society. In recent years, our group has been actively engaged in green chemistry, especially the catalytic conversion of CO₂, biomass, and waste plastics. In this presentation, I will discuss some recent results from our group on the design of green solvent–catalyst systems and their application to the conversion of CO₂, biomass, waste plastics, and kitchen waste into valuable chemicals and fuels.

Keywords: Catalytic transformation, Carbon dioxide, Biomass, Waste plastics, Kitchen waste, Chemicals, Fuels

Integrating Green Chemistry, Biotechnology and Downstream Processing for Biomass Valorization

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The transition toward a sustainable bio-based economy requires the development of innovative processes capable of efficiently converting renewable resources into high-value chemicals and materials. In this talk, a selection of past and ongoing research projects dedicated to the valorisation of biomass and agro-industrial byproducts through integrated and sustainable processing strategies will be presented.

The work discussed focuses on the design of green chemistry and biotechnology-driven approaches, combining biocatalysis, chemo-enzymatic transformations and advanced downstream processing to access functional molecules from lignocellulosic biomass and other renewable feedstocks. Emphasis will be placed on the development of environmentally benign processes that maximize atom economy, reduce waste generation and operate under mild conditions, while remaining compatible with industrial constraints.

Through representative case studies, this talk will highlight how the coupling of green chemistry and biotechnological tools with smart separation and purification strategies enables the efficient transformation of complex bio-resources into valuable platform chemicals, bio-based building blocks and functional ingredients. Perspectives on process integration, scalability and future research directions toward sustainable chemical manufacturing will also be discussed.

Electrochemical Energy Processes investigated by In-situ/Operando Spectroscopy

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Electrochemical energy devices (fuels cells, batteries and supercapacitors) are widely used in today's society with their features of high efficiency, cleanliness, convenience and flexibility. Electrochemical energy plays a vital role in carbon neutralization. The actual rapid development of electric vehicles and large-scale energy storage have put forward increasing demands on high energy density, high power density, high safety, long life, low cost and extreme environmental adaptability on electrochemical energy devices. To meet with these demands, investigation of the electrochemical energy processes and reaction mechanisms is crucial in order to enhance the performance of electrochemical energy devices by controlling the reaction and to regulate the property of electrodes (catalysts, energy storage materials).

In our study, electrochemical energy processes including reaction mechanism and electrode structure evolution were studied by developing a series of in-situ/operando techniques including infrared spectroscopy (In-Situ FTIRS), X-ray diffraction (In-Situ XRD), online electrochemical mass spectrometry (OEMS), magnetic resonance imaging (EC-MRI), and transmission electron microscopic dynamic imaging (EC-TEM) and other techniques. The progress achieved has advanced fundamental understanding at molecular and microstructural level, as well as promoted the development of high-performance electrochemical energy devices.

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Alcohol Dehydration Mechanisms by Brønsted acidic Zeolites unraveled by Atomic-Scale Calculations

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The mechanisms underlying the dehydration of bio-sourced isobutanol into isobutene versus linear butenes remain a subject of considerable debate, primarily because such processes are expected to involve butene isomerization steps that are notoriously slow under typical dehydration operating conditions. Both isobutene and linear alkenes represent high-value-added compounds in the domains of chemistry, polymer production, and fuel synthesis, making precise control of selectivity critical. Proton-exchanged zeolites emerge as highly promising catalysts in these processes, with their selectivity being strongly influenced by their structural topology. While large-pore zeolites predominantly yield isobutene, ferrierite exhibits remarkable selectivity toward linear butenes. Since isobutanol is unable to penetrate the zeolite pores, it is hypothesized that the active sites are located on the external surfaces of the crystallites. To uncover the nature of these active sites across a variety of zeolites, we conducted a density functional theory (DFT) investigation addressing two key challenges: (i) the intricate mechanisms occurring at bridging Si-(OH)-Al groups, and (ii) the complexity of external surfaces, which may host not only bridging OH groups but also other types of active sites.

Our initial static DFT study on bridging OH groups in bulk chabazite revealed novel transformation pathways.[1] Isobutanol isomerization into butan-2-ol emerged as plausible, with linear butenes being subsequently generated from the dehydration of butan-2-ol. Additionally, a previously unreported elementary step was identified, involving synchronous isomerization and dehydration to directly produce linear butenes. Employing the energy span model, we concluded that the dominant reaction pathway under experimentally relevant conditions (500 K) proceeds via butan-2-ol as an intermediate. Similar mechanistic insights were unveiled for the formation of isobutene, with tert-butanol identified as a potential intermediate. While experiments confirmed the presence of butan-2-ol as an intermediate, tert-butanol was not detected, likely due to its rapid dehydration under the reaction conditions.[2]

Further insights were gained through ab initio molecular dynamics (AIMD) simulations, which revealed that competing reaction pathways—(i) isobutanol isomerization into butan-2-ol versus synchronous isomerization-dehydration into linear butenes, and (ii) isobutanol isomerization into tert-butanol versus direct dehydration into isobutene—share dynamic transition states influenced by stochastic atomic fluctuations.[3] These post-transition state bifurcations render traditional static approaches and conventional transition state theory inadequate for accurately describing the reaction dynamics. By combining AIMD with Bennett-Chandler approaches, we quantified rate constants, confirming that large-pore zeolites exhibit high selectivity for isobutene.

However, focusing exclusively on reactive sites within the zeolite bulk may not fully represent the behavior of the real catalyst. Modeling external surfaces is essential. DFT calculations demonstrated that external surfaces of zeolites can host Al-(H₂O) Brønsted acid sites with moderate acidity and strong Lewis acid sites, the nature of which depends on local topology.[4,5] Our ongoing efforts aim to quantify the reactivity of ferrierite's external surfaces for isobutanol dehydration through the application of machine-learning interatomic potentials (MLIPs). This approach reduces computational costs, enabling simulations of thicker slabs. Initial studies focused on bridging OH groups located on the (100) surface orientation of ferrierite.[6] Despite the increased diversity of reaction mechanisms at external surfaces due to the involvement of silanol groups, these sites were still found to preferentially promote isobutene formation. Current investigations are expanding to include alternative active sites and additional crystallographic facets[7] to elucidate the origins of ferrierite's unique selectivity.

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Application of Starch and its Derivatives in Paper&Board for Sustainable Packaging Materials

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As an important raw material from nature, starch and its derivatives have various applications, not only in food and nutrition, but also in many other industrial applications such as pharmaceutical excipients, paper and board, cosmetics, etc. Starch, especially cationic starch, plays an important role in paper and board products, which are widely used in our daily life like printing paper, toilet paper, and packaging materials for transportation as well as for food.



Fig. Main application for paper and board products

During the past decades, Roquette has invested continuous efforts to meet the fast-growing demand on the market for greener, more sustainable starch derivatives which could be applied in paper and board production, not only for new generation food packaging material, but also for customized modified starch for innovative paper recycling process.

The presentation is to introduce the industrial production process of paper and board and how modified starch, especially cationic starch plays an indispensable role in it. In addition, Roquette's recent progress in green chemistry and sustainability would be also presented by a good example, STABILYS® BA 25. This promising product could replace PFAS coating materials for food packaging with comparable barrier properties, which offers an interesting alternative solution for plastic coating materials responsible for microplastic pollution.

Upgrading HMF using Thermal Heterogeneous Catalysis and Electrocatalysis combining Modeling and Experiments

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Hydroxymethyl furfural (HMF) is identified as a key platform molecule in biorefineries. In this communication we will focus on its upgrade through reduction into 2,5-bis(hydroxymethyl)furan (BHMF) using either thermal catalysis or electrocatalysis, combining experimental and modeling approaches.

In collaboration with A. Ruppert, we explored how a change in solvent (dioxane vs. water) can tune the selectivity of the hydrogenolysis of HMF using Ru/TiO₂ catalysts. In dioxane, BHMF is favored while in water, we observe the opening of the furan ring yielding to 1-hydroxyhexane-2,5-dione (HHD). This change of selectivity was ascribed to the increasing presence of surface hydroxyl when water is used as a solvent exploring the reaction mechanism using periodic DFT. [1]

In collaboration with P. Benito, we explore the electroreduction of HMF into BHMF using Cu cathode. The yield of the reaction is limited by the presence of two side reactions: the C-C coupling into a dimer and the formation of humins (uncontrolled polymerization). To better understand how we would limit the formation of those side products, we modelled the reaction mechanism of the main and the dimerization using periodic GC-DFT, including the electrolyte as a continuum model and the electrochemical potential. This allowed us to properly describe the desorption of the intermediate carbon radical that is found to be easy, and likely at the origin of the uncontrolled polymerization and humins formations, but also of the C-C coupling. Provided the large amount of dimer, we also considered the possible C-C coupling favored by the co-adsorption of two HMF onto the Cu(111) surface.[2]

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Design of Efficient Zeolite-Based Catalysts from Surface Sorption Equilibrium

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Catalysis is a surface phenomenon, and adsorption of reactants and desorption of products on the active sites in catalysts is critical. To enhance catalytic activity and selectivity in catalysis, it has been great efforts to modify the active sites such as adjusting composition, modulating valence state, and changing coordination environment. By optimization of these factors, it is actually achieved the active sites with rapid adsorption of reactants and desorption of products. In addition, design and modification of catalyst supports are also important for control of catalytic activity and selectivity. The suitable choice and/or right modification of catalyst supports have accelerated the adsorption of reactants and desorption of products, giving enhanced catalytic performances.

Besides catalytic activity and selectivity, the stability of active sites is of vital importance. To enhance catalyst stability, it is usually reduced the product coverage on active sites, which is obviously related to the product desorption on the active sites. In addition, the choice and modification of catalyst supports are very helpful for improving stability of active sites such as strong interactions between active sites with supports and introduction of porosity and functionalization of unique groups in catalyst supports for fast diffusion of products. Moreover, leaching and aggregation of active sites are key obstacles for catalyst stability, which are mainly due to the formation of mobile intermediates between active sites with reactants for fast migration.

As shown above discussions, catalytic performances of active sites, in essence, are influenced by adsorption of reactants and desorption of products as well as migration of reactant intermediates, where the sorption properties are strongly related to the concentrations of reactants, products, and intermediates around active sites. Therefore, it is possible to adjust these factors to design and construction of efficient catalysts.

On the catalyst surface, there could be surface sorption equilibrium for reactants and products based on Langmuir sorption and kinetic reaction when catalysis occurs ($* + A \rightleftharpoons *A$, where $*$ denotes a surface site). Because the sorption equilibrium is dynamic and the sorption species are strongly dependent on the local concentrations or partial pressures of reactants and products on and/or around the active sites, it can be changed the surface equilibrium of the reactants and products to enhance catalytic performances [1,2]. For examples, if the products are desorbed very quickly from the active sites, the active sites would be effectively exposed to reactants, giving high rate for the formation of products; If the reactants are quickly adsorbed on the active sites, it would be accelerated the conversion of reactants; If the addition of promoters on or around the active sites could simultaneously accelerate the adsorption of reactants and desorption of products, it is also enhanced the catalytic performances; If migration of the intermediates formed by active sites with reactants would be effectively hindered, it could be achieved stable catalysts.

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Catalytic Conversion of Cellulosic Biomass to Chemicals

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Cellulose and hemicellulose are naturally occurring carbohydrate polymers, and provide carbon-neutral alternatives to fossil resources for the sustainable production of fuels and chemicals. This work reports our recent progress in the reactions of cellulose and its derivatives, such as sugars and furan compounds, to diols, dicarboxylic acids and other oxygenated chemicals, with a focus on understanding the catalytic functions and reaction mechanisms for the site-selective cleavage of the C-O and C-C bonds. One such example is that tungsten-based catalysts are efficient for selectively cleaving the C-C bonds of sugars to generate C₂-C₄ oxygenate intermediates (e.g. glycolaldehyde), following a novel mechanism that is distinct from classical retro-aldol condensation. These C₂-C₄ oxygenates act as versatile platform molecules for synthesizing diverse chemicals. Such applications of the C₂-C₄ oxygenates inspire us to propose a potentially promising strategy for the production of chemicals in the future biorefinery industry, mirroring the paradigm of the current petrochemical industry that relies on C₂-C₄ olefins as core building blocks.

This work was carried out mainly by Drs. Y. Liu, C. Chen, Q. Sun, F. Wang, Z. Li, K. Liu and C. Hong under the financial support from the National Natural Science Foundation of China and National Basic Research Project of China.

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Understanding Catalysis, One Atom at a Time

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Most efficient chemical processes used in industry rely on heterogeneous catalysis. While the search for more sustainable processes and the changes in environmental policies impose the continuous development of more efficient catalysts, we have currently little understanding of the structure of the actives in these processes. Hence, due to their inherent complexity, heterogeneous catalysts have been mostly developed empirically.

Here, we will show how constructing active sites, one atom at a time on surfaces, enables molecular-level understanding and implementation of rational approaches for the improvement of catalytic processes. We will first illustrate how this approach enables to generate selective single-site catalysts. We will next show how from these isolated (single) sites, one can generate and understand far more complex systems such as supported nanoparticles, where interfaces, alloying... play a critical role. This lecture will be developed around these themes and will show how the development of advanced characterization tools augmented by computational approaches can provide useful information to bridge the gap between fundamental and applied (industrial) catalysis. In addition, this lecture will explore how data-driven high-throughput experimentation can be used to explore efficiently the chemical space

Design Synthesis of Novel Metallosilicates for Selective Oxidation

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Titanosilicates with isolated framework Ti sites, as a typical class of metallosilicates, offer great potential for developing novel catalytic technologies for liquid-phase oxidation reactions using hydrogen peroxide as the oxidant. Cyclohexanone oxime (CHO) and methyl ethyl ketoxime (MEKO) are important bulk or fine chemicals. Traditional production of ketoxime relies on the hydroxylamine method. The first-generation TS-1 titanosilicate developed a transformative technology for the one-step ammoxidation of ketone, ammonia, and hydrogen peroxide in *t*-BuOH solvent system to produce ketoximes. The new-generation titanosilicates of large-pore Ti-MWW [1] and Ti-MOR [2] not only provide new ammoxidation technology in *t*-BuOH, but also enable the development of organic solvent-free aqueous-phase technology, which has been applied and promoted on a large scale in the production of MEKO and CHO. In the future, it is expected to develop greener ammoxidation technologies using bifunctional catalysts, as well as coupling electrocatalytic oxygen reduction reaction and thermocatalysis by titanosilicates (Fig. 1). Especially, large-pore Ti-MWW and Ti-MOR titanosilicates can achieve the confined dispersion of Pd species within their channels, thereby efficiently catalyzing the ketone ammoxidation reactions using hydrogen and oxygen instead of H₂O₂.

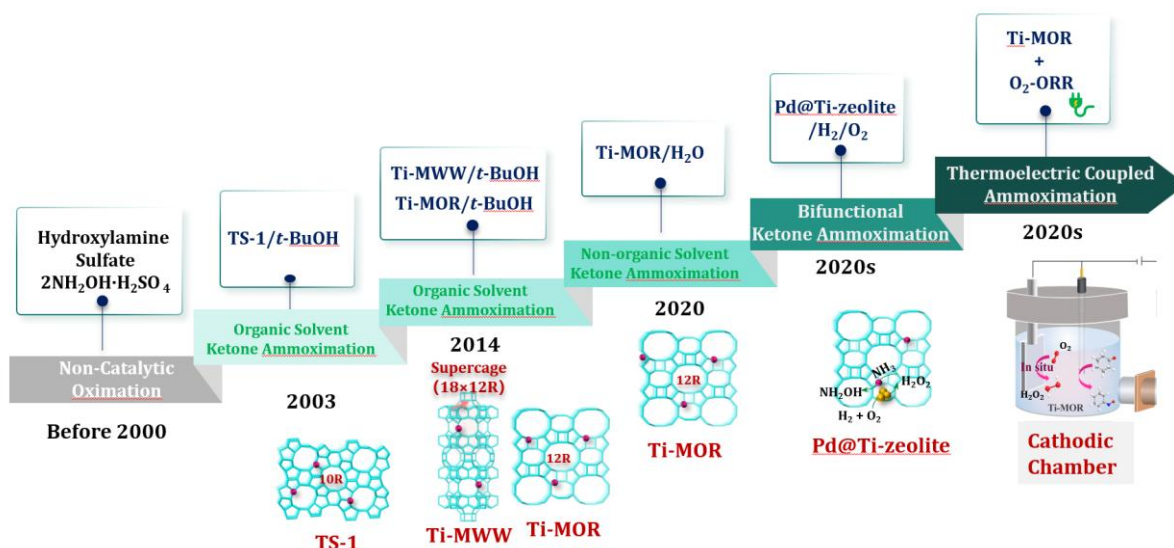


Fig. 1: Technology development roadmap for ketoxime production

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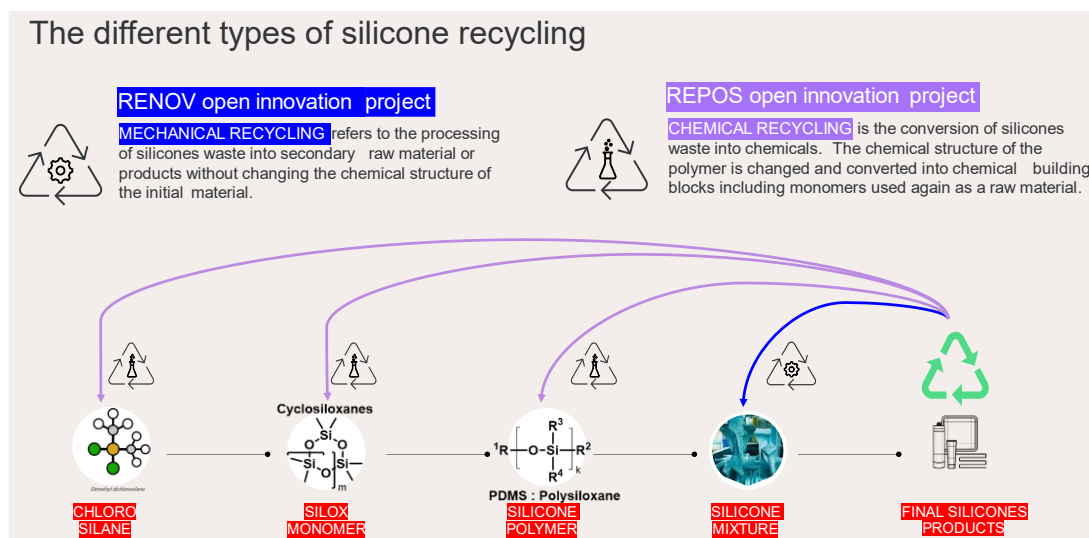
Chemical Recycling of Silicones: Back to Circularity

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Chemical recycling of silicones offers a strategic route to improve the circularity of high performance materials while reducing waste and carbon footprint. Silicones are widely used in fluids, elastomers, coatings, adhesives and advanced applications, but their diversity of formulations and end-of-life combinations makes collection and separation particularly challenging. This presentation reviews complementary chemical recycling strategies that convert silicone waste into reusable chemical building blocks or functional materials, including back-to polymers [1], back-to-cyclic monomers [2] and back-to-chlorosilanes [3] approaches. Particular attention is given to mild depolymerization and functionalization processes enabling chain scission, molecular weight reduction, chain-end modification and reshuffling of PDMS structures, including crosslinked and filled substrates. The open-innovation project highlights the close collaboration between academic laboratories and Bluestar Silicones France to scale up low-temperature silicone recycling, producing cyclic monomers and valorized oligomers from industrial waste and downgraded products.



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Photothermal Catalytic Reduction of CO₂

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Coupling photocatalysis with thermocatalysis is considered as the best way for CO₂ reduction to produce useful hydrocarbons. Particularly, photocatalytic CO₂ reduction activity could be improved via photothermal effect induced by local heat and the enhanced visible light harvesting from plasmonic effect generated by metal nanoparticles. However, the sluggish hot electron transfer between metal particles and semiconducting materials remains an unavoidable bottleneck and how to synergically combine photocatalysis and thermal catalysis to achieve an applicable CO₂ reduction. The innovative concept of paving an efficient hot electron shift bridge can act as a crucial springboard in the practical application of advanced photothermocatalyst for efficient CO₂ reduction and high-valued chemical production.

Could Carbenes and related Low-valent Carbon Species Replace Transition Metals

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Almost 20 years ago, we realized that due to their lone pair of electrons and accessible vacant orbital, singlet carbenes resemble transition metal centers, and thus can potentially mimic their chemical behavior. We will discuss recent results demonstrating that, for some catalytic reactions including those involving single electron transfers, carbenes can indeed compete with transition metal complexes.

The development of catalytic processes promoted by carbenes, which are genuine organic compounds, could address the major drawbacks of current transition metal catalysis technology that are the excessive cost of metal complexes (metal + ligands) and in many cases the toxicity of the metal.

Carbenes are 6-electron species. To push the boundaries further, we wish to undress carbon atoms even more. As an illustration we will discuss our recent results dealing with a dicoordinate carbodication and a radical-cation.

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“Early Career” Invited Lectures

Harnessing Supramolecular Confinement: Functionalities from Macrocycles to Cages

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The unique appeal of macrocycles and cages lies in their well-defined cavities, which confine guest molecules with high affinity and selectivity, enabling a wide range of applications. Our research focuses on engineering novel supramolecular architectures, mainly coordination cages, with tailored confinement effects to develop functional materials for chemical separation and supramolecular catalysis. This endeavor encompasses four key directions: (i) the design of highly stable, electron-deficient zirconium-cluster cages via an "anion-assisted dissolution" strategy, enabling efficient photocatalytic oxidation and pollutant capture[1-3]; (ii) the construction of smart biomimetic cages capable of precise steroid recognition, frustrated Lewis pair (FLP)-mediated signal-responsive guest uptake and release, and allosteric regulation of encapsulated catalysts[4-6]; (iii) the integration of coordination cages into porous solids (MOC@MOF and MOC@PIL) to harness the synergy between molecular recognition and porous supports, yielding stimuli-responsive spin-crossover materials and recyclable, high-performance adsorbents[7,8]; and (iv) the synthesis of BODIPY[3]arene, a new macrocycle that switches between two conformers in response to its environment and functions as a tunable solid-state adsorbent for either D₂/H₂ separation or rapid iodine capture[9]. By integrating molecular design with functional exploration, this body of work offers new strategies for separation and catalysis.

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Dehydrogenation of Alcohols and Polyols in Liquid Phase with Metal Catalysts

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Acceptorless dehydrogenation of linear alcohols and polyols is an atom-efficient and environmentally friendly process that can allow the production of a broad range of unsaturated products used in the pharmaceutical and fine chemical industries. Elimination of the need for external hydrogen acceptors, oxidants, or sacrificial carbonyl compounds, can make this process more economical and safer. Performing the reaction in liquid phase allows working without the need to separate the H₂ produced. Therefore, the acceptorless dehydrogenation reaction represents a viable route for the production of hydrogen or for liquid organic hydrogen carrier [1]. From the perspective of developing a potential hydrogen storage system, dehydrogenation of complex alcohols derived from biomass is an attractive approach because they can serve as high-density hydrogen substrates [2]. In addition to delivering hydrogen, AD of linear polyols can generate valuable unsaturated compounds that are used in food and beverages manufacturing as well as in the fragrance and flavor industries.

Regarding acceptorless dehydrogenation of alcohols to the corresponding carbonyl compounds, literature on the use of heterogeneous catalysts in liquid phase is limited. The main challenge with polyols is their propensity toward multiple side reactions that can lead to low selectivity and low hydrogen production. Our researches aim to develop efficient metal catalysts in order to reduce the environmental impact and improve the viability of these processes.

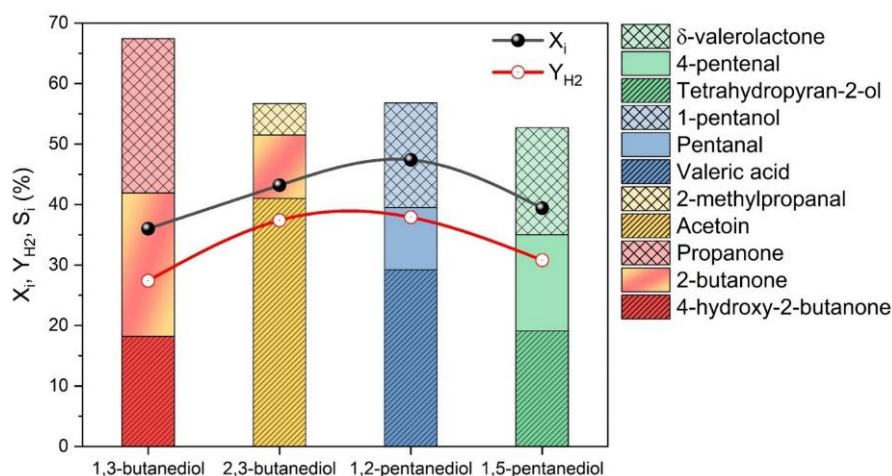


Fig. 1: Dehydrogenation of polyols over Cu/TiO₂ catalyst: conversion (X), H₂ yield (Y_{H2}) and selectivity (S).

We have demonstrated that cobalt- and copper-based catalysts can be active and selective for the dehydrogenation of alcohols. Then reactions were conducted in semi-bath reactor with constant flow of inert gases. The acceptor-less mechanism was verified by online analyses of the gas phase. We have investigated both supported metal nanoparticles and unsupported shaped nano-objects. Our work has focused in particular on the influence of preparation methods and aging of the catalysts. Theoretical and experimental approaches have been combined to gain a better understanding of the catalytic results. These systems were employed for the acceptorless dehydrogenation of various linear aliphatic C4-C8 polyols.

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The Green Synthesis of Biomass based Carbon Materials via Biomolecular Tailoring and its Application in Energy Storage

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Biomass-derived porous carbons are promising metal-free electrocatalysts for the oxygen reduction reaction (ORR) because of their tunable pore architecture and surface chemistry, renewable feedstocks, and low cost [1,2]. Lignocellulosic biomass offers intrinsic hierarchical structures and native heteroatoms; however, its limited nitrogen content and the stochastic structural evolution during pyrolysis hinder precise control over catalytic sites and mass-transfer pathways [3]. Here, microbial pretreatment was integrated with chemical activation to enable the controlled synthesis of structurally tailored, nitrogen-doped porous carbons. Selective biodeconstruction of the lignocellulosic matrix simultaneously reorganized the precursor architecture and enriched biogenic nitrogen, thereby facilitating subsequent activation and carbonization. The effects of microbial treatment, chemical activation, and pyrolysis on carbon composition, pore structure, morphology, and ORR activity were systematically elucidated, together with the synergistic roles of nitrogen speciation and pore architecture through experiments and density functional theory calculations.

A 15-day anaerobic digestion treatment doubled the nitrogen content of the solid precursor. The resulting carbon exhibited a twofold increase in specific surface area, with graphitic and pyridinic nitrogen accounting for 51.6% of the total nitrogen species. These structural and chemical advantages markedly enhanced ORR kinetics and enabled a maximum power density of $886 \text{ mW} \cdot \text{m}^{-2}$ in microbial fuel cells. Subsequent ZnCl_2 activation increased the mesopore fraction by 15.2% and raised the combined proportion of graphitic and pyridinic nitrogen to 59.0%, yielding an ORR onset potential of 0.88 V versus RHE. In a complementary route, selective enzymatic etching by *Aspergillus* sp. reconstructed the lignocellulosic framework into a mesoporous carbon network with a characteristic pore size of approximately 4.5 nm, thereby mitigating mass-transfer limitations. Fungal hyphae and nitrogen-containing biomolecules served as in situ nitrogen precursors, favoring the formation of pyrrolic-N active sites. Theoretical calculations revealed that these sites modulated the O_2 adsorption configuration, inhibited O–O bond cleavage, and reduced the $^*\text{OOH}$ formation barrier to 0.36 eV. Consequently, the catalyst achieved nearly 100% selectivity for the two-electron ORR, a Faradaic efficiency of 97.2% in an H-cell, and an H_2O_2 production rate of $26.34 \text{ mol} \cdot \text{g}_{\text{cat}}^{-1} \cdot \text{h}^{-1}$ in a continuous-flow reactor.

This project not only provides a series of novel methods for the controllable synthesis of hierarchically structured nitrogen-doped porous carbon materials with excellent catalytic activity and high stability for oxygen reduction reaction but also offers fundamental insights and theoretical guidance for nitrogen-enriched pyrolysis and efficient conversion of lignocellulosic biomass into nitrogen-doped porous carbon materials.

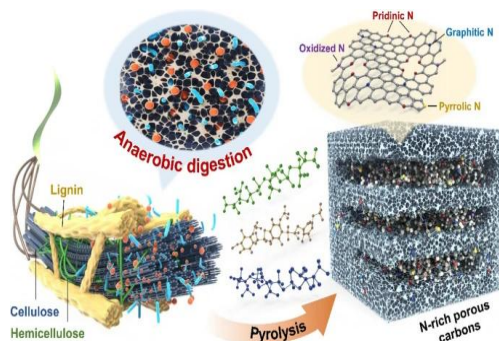


Fig. 1: Green synthesis of biomass-derived nitrogen-doped porous carbon via biomolecular tailoring

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From Residual Biomass to Value-added Products: a Systemic Green Chemistry Approach

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Agricultural and agro-industrial residues represent abundant renewable resources for the production of value-added molecules and products. However, their sustainable valorization cannot be limited to the optimization of a single extraction or conversion step. It requires a systemic approach considering biomass availability and variability, collection, pretreatment, selective fractionation, molecular stability, formulation, targeted applications and the fate of the remaining solid fractions. This presentation will illustrate this approach through the valorization of viticultural residues, particularly grape canes and vine stocks. The influence of cultivar, anatomical fraction and biomass pretreatment on the recovery of stilbenes, including resveratrol and viniferin, will be discussed. Recent work on mobile drying, grinding and pelletization shows that biomass conditioning can affect storage, transport, extraction kinetics and the composition of the resulting extracts. Further studies address the photochemical stability of these bioactive molecules and the development of protective formulations. Together, these results demonstrate how green chemistry can connect biomass management, molecular-scale understanding, process development and final applications to create coherent circular value chains.

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Conversion of Polyolefins to Fuels and Chemicals

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The valorization of waste plastics is pivotal for mitigating environmental pollution and fostering a circular economy. Polyethylene (PE), a major component of plastic waste, exhibits high chemical inertness due to its non-polar C-C backbone, posing significant hurdles for its activation and degradation.

We report a catalytic system utilizing layered self-pillared zeolites that enables the highly selective conversion of PE into gasoline-range hydrocarbons at 240 °C under solvent-free and hydrogen-free conditions, yielding up to 80% (Fig. 1a) [1]. The hierarchical porosity and high external surface area of the catalyst ensure optimal accessibility for macromolecular polyolefins, while the three-coordinated aluminum sites within the framework facilitate C-H activation and subsequent C-C scission [1]. Inelastic neutron scattering spectroscopy reveals that the process involves coupled aromatization, which serves as an in-situ hydrogen source to saturate small-molecule intermediates, thereby enabling a self-hydrogen-supplied pathway to gasoline (Fig. 1a). Moreover, tailoring the Brønsted/Lewis acidity allows for enhanced iso-alkane selectivity and improved octane number [2-3].

To further advance closed-loop polyolefin recycling, we developed a tandem strategy for the selective production of ethylene and propylene. To overcome the kinetic entanglement caused by the competition between olefin formation and hydrogen transfer/aromatization at shared active sites, a two-stage reactor configuration was implemented. This kinetic decoupling-coupling strategy allows for independent optimization of catalyst properties and thermal regimes in each stage. PE is first degraded into intermediate light olefins (butene/pentene) and subsequently cracked into ethylene and propylene (Fig. 1b). This bifurcated approach effectively suppresses undesired side reactions, achieving a combined monomer yield of 79% [4], significantly outperforming conventional pulse pyrolysis (36% propylene yield) [5].

Overall, by leveraging self-supplied hydrogen mechanisms and precise kinetic modulation, we have demonstrated the efficient upcycling of waste PE into high-value fuels and chemical building blocks, offering a robust technological framework for the sustainable management of plastic waste.

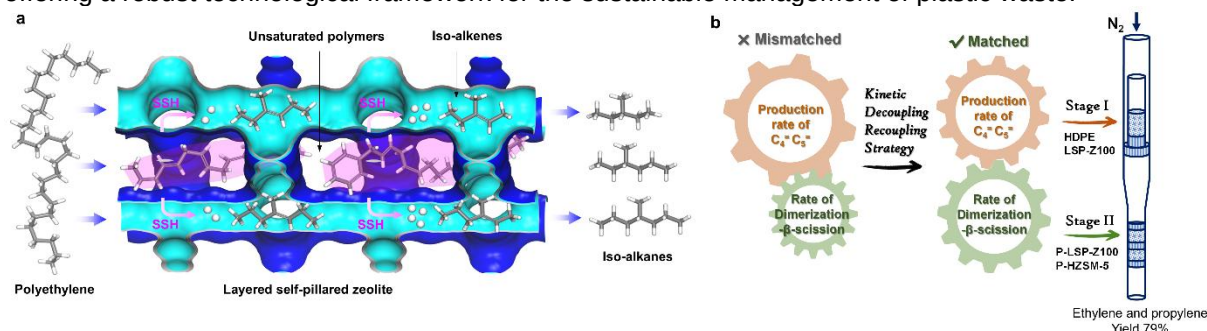


Fig. 1: Catalytic conversion of PE to gasoline (a) and ethylene and propylene (b).

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Borrowing Hydrogen Catalysis for the Sustainable Synthesis of High-Value Molecules from Alcohols and Polyols

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The synthetic valorization of biomass-derived chemicals produced from carbohydrates has received great attention from the chemistry community to extend the wide applications of these so-called bio-based platforms. In parallel with the comprehensive efforts made for increasing the efficiency and sustainability of their production, research for finding them original applications *via* the development of innovative and modern methodologies has been also intensified. In that approach, we have been involved in the development of synthetic methodologies to transform bio-based platforms such as 1,4-*D*-sorbitan and isosorbide (Fig. 1), obtained from dehydration of *D*-sorbitol, into more complex molecules with high-added value.

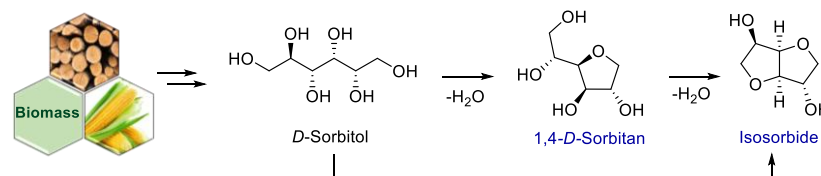


Fig. 1: Bio-based polyols from *D*-sorbitol

The advent of green chemistry has promoted innovative methodologies considering atom economy parameter. With respect to this point, borrowing hydrogen (BH) methodology has emerged as an important tool in organic chemistry for the construction of either C-N and C-C bonds.

This presentation will first highlight our efforts toward the direct functionalization of isohexide and 1,4-*D*-sorbitan derivatives toward high-value molecules using an iridium-catalyzed borrowing hydrogen strategy.³ The application of this BH approach to access functionalized saturated aza-heterocycles will then be discussed.⁴

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Electrothermal Methane Dry Reforming, beyond Rapid Heat Delivery

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Electrothermal catalysis has emerged as an effective solution to the intrinsic heat transfer limitation of endothermic reactions. Via applying electric current directly through the catalyst, the swift thermal responsiveness of internal joule heating allows precise heat supply to the active site. Here in this study, we report that the directional movement of electron through the catalyst introduces phenomena that facilitate reaction beyond rapid heat delivery. Taking electrothermal methane dry reforming (EDRM) for illustration, we present that appearance of electric current induces both structural reformation of metal sites and unique catalytic pathway. The coke formation is regulated by electric current to form ordered carbide phase which resulted in an order-of-magnitude enhancement in the intrinsic reaction rate. Meanwhile, polarization of C-H bond by electric current altered kinetics of methane activation and enabled matched reaction rate for CH₄ and CO₂ conversion. Benefiting from both efficient internal heating and non-thermal effects, EDRM achieved stable operation for over 300 h without coke formation, presenting high potential for carbon-neutral syngas production.[1]

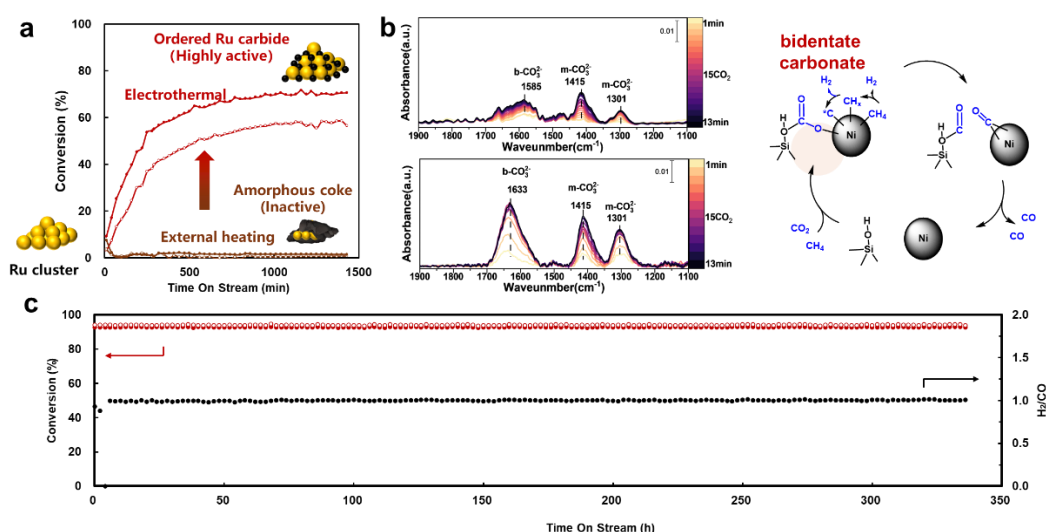


Fig. 1 Unique catalytic phenomena in EDRM including (a) structural reformation of Ru cluster and (b) bicarbonate-mediated pathway for CO₂ activation, which synergistically lead to (c) stable operation of EDRM over 300 h.

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A new generation of multifunctional and recyclable epoxy networks

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In the field of thermosetting polymers, ionic liquids and ionic liquid monomers represent a real opportunity to design new sustainable and (multi)functional-dedicated polymer materials with enhanced properties such as thermal stabilities, mechanical performances, water barrier properties, and fire retardancy. Recently, our laboratory has developed a new generation of more environmentally friendly, *i.e.* reusable, recyclable and/or degradable epoxy-amine and epoxy-anhydride networks by using IL containing cleavable bonds. Thus, several architectures have been considered in order to highlight the impact of the architecture on the physical properties of the networks [1-3].



Fig. 1: Chemical and mechanical recycling of epoxy-anhydride networks

Here, epoxy networks with glass transition temperatures including between 60 °C to 200 °C combining with good thermomechanical and mechanical properties, as well as hydrophobic behavior have been developed.

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Electrocatalytic Generation of Alkyl Radicals from Organoboron Compounds for C–C Bond Formation

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Organic electrosynthesis has emerged as a powerful strategy for sustainable redox transformations, leveraging electrons as traceless redox agents to promote electron-transfer processes and generate reactive radical intermediates without requiring external oxidants or reductants [1]. Among the reactive intermediates accessible through electrochemical activation, alkyl radicals have attracted considerable attention owing to their versatility for carbon–carbon bond formation. Despite these advantages, the large-scale implementation of electrosynthesis remains challenging because of limitations associated with mass transfer and reactor design. Continuous-flow electrochemistry offers an attractive solution by enhancing reaction efficiency, improving mass transfer, and facilitating straightforward scalability [2].

For many years, our group has been developing electrochemical methodologies based on the generation of reactive intermediates [3]. Recent efforts have focused on the anodic activation of readily available organoboron "ate" complexes to generate alkyl radicals [4]. These highly reactive intermediates can be selectively intercepted either by acetylenic sulfones to forge C(sp³)–C(sp) bonds under catalyst-free conditions or by Ni-catalyzed electrochemical C(sp³)–C(sp²) cross-coupling with aryl halides through paired electrolysis. Both oxidant-free transformations proceed under mild conditions and afford the desired products in moderate to excellent yields. Their implementation in continuous-flow electrochemical reactors significantly increases reaction rates while enhancing productivity and reducing energy consumption.

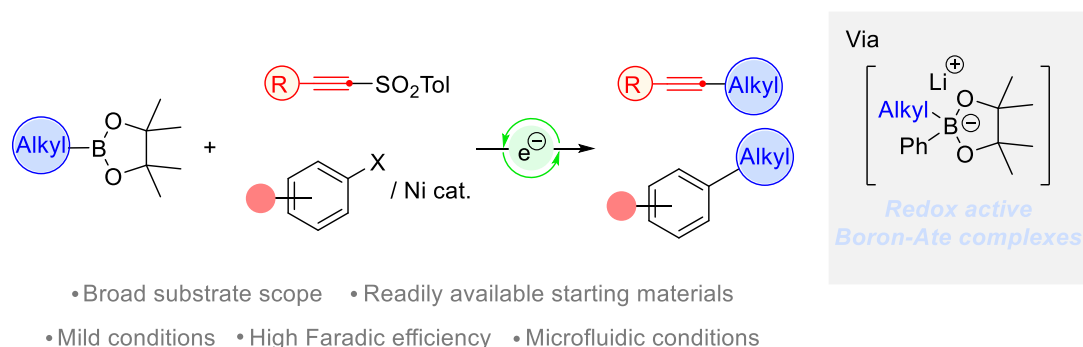


Fig. 1: Electrocatalytic Generation of Alkyl Radicals from Organoboron Compounds: Toward Sustainable Carbon–Carbon Bond Formation

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Influence of Water on the Acidity of Zeolite

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Zeolites, microporous solid acids, are widely applied in chemical industry for separation and catalysis. The recent development in the catalytic reactions in water or using reactant mixtures containing water requires exploring the catalytic activity of water-saturated zeolite. In zeolite micropores, water resides on Brønsted acid site, forming hydronium ions.[1] Confined in the space of zeolite crystalline, these hydronium ions resulting in a high local concentration in zeolite micropores while a very low concentration in the rest space of the aqueous phase. Such a heterogeneity in hydronium ion concentration brings zeolite unique properties for adsorptions and catalytic reactions.

In this presentation, we will show quantitatively the chemical composition of such hydronium ions in zeolite pores and their thermodynamic properties. In addition, the dynamics of their locations throughout the zeolite crystal and the aqueous bulk phase. With the comparison to the counterpart in gas phase, organic substrate adsorption,[1] acid-catalyzed reaction of small alcohols and cellulosic polymers, [2] and pH-dependent metal-catalyzed hydrogenation [3] will be discussed in detail to exemplify how the presence of water alters the acidity of zeolite and the related adsorption and catalytic performance.

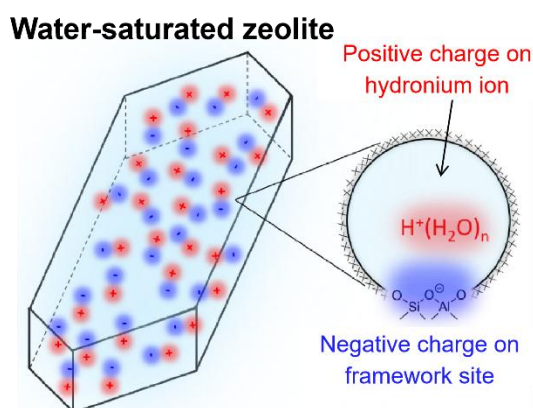


Fig. 1: Schematic illustration of water saturated zeolite crystal.

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Unlocking new Biobased Chemicals and co-Substrate in situ Production through Chemo- and Biocatalysts Combination

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Since the early 2000s, following the publication of the principles of green chemistry by Anastas and Warner, the combination of chemical and biological catalysts, also known as hybrid catalysis, has been seen as a potential means of overcoming the limitations associated with each of these two fields [1]. And although it is still, for the time being, a disciplinary field at the crossroads of two worlds that many view as opposed, the initial achievements that have marked its emergence demonstrate just how beneficial such combinations can be for both types of catalyst. Therefore, after reviewing the basic principles of combining chemical and biological catalysts, which define the backbone of hybrid catalysis, this presentation will present two examples recently carried out within our group.

The first proposes the in situ production of hydrogen peroxide combined with enzymatic halogenation reactions of phenols. Indeed, the importance of controlling H₂O₂ concentration with hydrogen peroxide dependent enzymes has been found to be a crucial element of the scale up of such routes [2,3], and while biocatalytic approaches using glucose oxidase (Gox) and formate oxidase (Fox) do exist, they require a significant amount of co-substrates forming salts and making downstream process time consuming and costly [4]. Therefore, chemical catalysts appear to be promising solutions for such applications. In this work, we explored the use of UiO-66(Zr)-NH₂ and gold supported nanoparticles on UiO-66(Zr)-NH₂ as photocatalysts for H₂O₂ production in aqueous media combined with the well-known vanadium-dependent haloperoxidase from *Curvularia inaequalis* (CiVCPO). After optimization, a one-pot/two-steps system finally allowed for phenols bromination with up to 95% conversion.

The second follows our previous work in the hybrid production of a new bio-sourced synthon, the 5-aminomethyl-2-furancarboxylic acid (AMFC) [5], by combining platinum nanoparticles and a transaminase. It turns out that this compound, which possesses two functionalisable groups, an amine and a free carboxylic acid, could be valorized in the form of amphiphilic molecules. To achieve this objective, we have chosen to carry out the amidation of the free amine of AMFC, again by hybrid catalysis, combining an acyl-coenzyme A ligase (ACL) and Au nanoparticles immobilized onto CaO. After selecting both catalyst through high-throughput screening, a one-pot/two-steps process could here again, achieve the desired products, with C4 to C8 aliphatic mono- and di-alcohols grafting onto AMFC, with yields of up to 61% in aqueous buffer at 60 °C.

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Challenges and Strategies for the Chemical Recycling of Polyester-Based Waste Plastics

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Key words: Waste plastics, Polyesters, Chemical recycling, In-situ conversion, Chemicals

Plastic waste pollution is a pressing global challenge, and waste polyesters, with their characteristic chemical structures, are particularly suitable for chemical recycling. Conventional depolymerization methods are energy-intensive, require harsh conditions, generate multiple side products, and yield low-value chemicals, making downstream purification and separation inefficient and limiting overall sustainability and profitability. To address these challenges, we have developed a framework of in situ upcycling that integrates mechanism-guided catalysis with innovative transformation pathways. The aromatic unit of polyester is directly hydrogenated using a bifunctional metal–acid PtW/MCM-48 catalyst to produce high-value p-toluic acid and p-xylene. The diol unit is selectively transformed via a carbonylolytic strategy into functionalized organic acids. An esterolysis approach simultaneously converts both terephthalic acid and diol units into multiple high-value terephthalate esters and diverse diol-derived products. These strategies substantially enhance product value while reducing separation and purification costs. Collectively, this work demonstrates that bond-selective, mechanism-guided catalysis combined with in situ product upgrading can overcome key limitations in polyester recycling. These results illustrate the potential of integrated catalytic strategies for sustainable, high-value plastic waste conversion and may inform future approaches to addressing the environmental challenges of waste plastics.

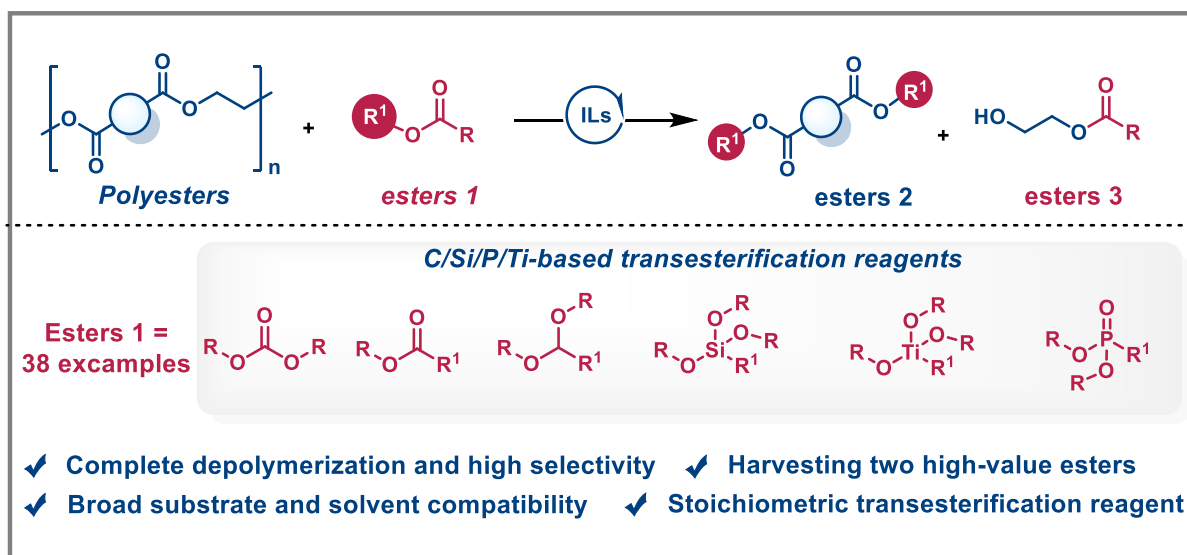


Fig. 1: Esterolysis of PET into value-added ester chemicals.

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One Solvent, Many Opportunities: 2-Methyltetrahydrofuran-3-one as a Multifunctional Solvent for Biomass Valorization

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The transition toward sustainable chemical processes requires not only renewable feedstocks but also reaction media that actively enhance biomass conversion efficiency. Bio-based solvents are key tools in this transition, going beyond simple substitution of conventional organic solvents by modulating reactivity, selectivity, and overall process performance. Among them, 2-methyltetrahydrofuran-3-one (2-MeTHF-3-one), a food-grade, readily biodegradable compound naturally found in roasted coffee aroma, has recently attracted attention as a versatile platform solvent, with growing evidence of its compatibility with enzymatic systems and supercritical processes [1-3].

In this presentation, I will discuss the potential of 2-MeTHF-3-one for the valorization of biomass fractions through three complementary applications (Fig. 1). First, in the enzymatic synthesis of glucose fatty acid esters from wheat-bran-derived glucose, 2-MeTHF-3-one significantly outperformed conventional solvents in terms of both conversion yield and lipase performance under low-water conditions.² Second, 2-MeTHF-3-one was integrated as the key component of the CoffeeCat process, an organosolv strategy enabling selective extraction of high-purity lignin from *Miscanthus × giganteus* [4]. Third, 2-MeTHF-3-one acts as a nanostructuring solvent for the preparation of lignin nanoparticles (LNPs) by nanoprecipitation, opening new opportunities for bio-based functional nanomaterials [4].

Building on these results, our ongoing ANR-funded project LANISTER aims to combine nanoparticle engineering with enzymatic catalysis: by coupling the ability of 2-MeTHF-3-one to generate lignin nanostructures while maintaining high enzyme activity, we seek to develop sustainable strategies for the transformation of recalcitrant biopolymers. Altogether, this work illustrates how a single bio-based solvent, carefully selected for its physicochemical properties, can become a powerful tool from biocatalysis to biorefinery for the valorization of lignocellulosic biomass.

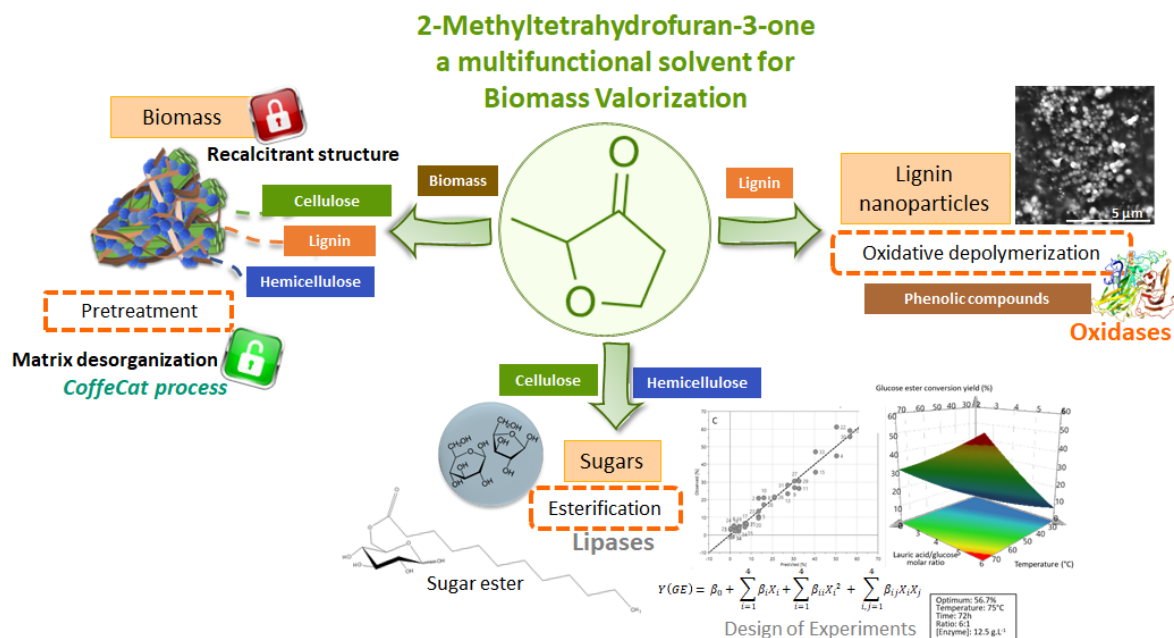


Fig. 1: 2-Methyltetrahydrofuran-3-one, a multifunctional solvent for biomass valorization

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Changes on Reaction Pathways during C-C Bond Cleavage via Metal Addition to Zeolites

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The current focus of modern petroleum refinery is to shift the gear from the production of fuel towards basic chemicals, and to allow flexible carbon resources used as refining feedstocks. Industrial practice has demonstrated that the introduction of transition metal into zeolite would benefit the product distribution in conventional catalytic cracking upon specific requests. Such benefits have been patented for long time, but the fundamental understanding lacks documentation.

In this presentation, following issues will be discussed.

1) Location, chemical environment of metal species over zeolites. The metal species could be located outside or inside the porous structure; it could be presented as metallic phase or oxide phase; it could be formed as sub-nanometer clusters or exchanged with cations. A combination of advanced characterization techniques are applied for elucidation of microscopic structures.

2) Carbocation chemistry and related reaction sequences. There are two major carbocation species competing in the C-C bond cleavage / transformation paths, i.e., 5-coordinated carbonium ion involved as transition state and 3-coordinated carbenium ion involved as reactive intermediate. It is difficult to distinguish the reaction paths with spectroscopic approaches, so detailed kinetic analysis would give important clues to understand the role of different active sites.

3) Spatial constraints for reactants / products / intermediates. It is accepted spatial constraints provide the possibility of forming late transition state which compensate the weak intrinsic acid strength of Si/Al zeolites. Zeolitic channel would naturally be considered as host for spatial constraints during the reaction. However, the species generated from the reaction is also able to limit the molecular motion in order to influence the product distribution.

Above issues were summarized from practical scenarios, including catalytic cracking of naphtha [1], light hydrocarbon utilization [2], reactive adsorption of gasoline desulfurization [3], polyolefin's circularity [4]. A perspective will be given for an oriented more complex system.

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Catalyst Design for Diesel Hydrotreating towards Low Carbon Production

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Diesel oil is an important tradition energy source to support the development of social economy. Under “dual-carbon” strategy, it is urgent to develop highly efficient diesel hydrotreating catalyst to promote energy and carbon emission reduction in clean diesel production unit. In order to make clear the strategies for catalyst design towards low carbon production, the investigations were carried out to understand the key scientific issues including kinetic models, deactivation mechanisms and the relationship between active phase structure and catalytic performance, and so on.

The adiabatic reaction kinetic model was developed by considering cross-inhibition of reactants and products, and large heat release in diesel hydrotreating. According to the model, the variation of feedstock properties along the axial direction during the reaction process was revealed. The reactor exhibits a lower efficient zone where the degree of reactions is lower. The model also suggested that CoMo type catalyst is less affected by the reduction of pressure and the hydrogen-oil ratio than NiMo type catalyst. The influence of reaction environment in the reactor was compared. The deactivation rate of the catalyst at high temperatures is much higher than that under low-temperature reaction conditions suggesting that the high temperature condition accelerates the deactivation of the catalyst. The carbon deposit amount and the growth degree of the active phase in the catalyst in higher temperature reactor is relatively high than that in the low-temperature reactor.

On the other hand, the deactivation kinetic model was constructed and it reveals that the low reduction of pressure and the hydrogen-oil ratio substantially accelerate the deactivation of hydrodesulfurization. Combined with structural characterization of fresh and spent catalysts, the results reveal the catalyst deactivation induced by a decrease in hydrogen-to-oil ratio mainly originates from the reduction in the number of active sites, whereas coke deposition plays only a secondary role.

The influence of the active phase structure on the stability and selectivity was studied. The stability can be increased by modifying the slab stacking of CoMoS phase. With the increase of the number of active phase stacking layers, the selectivity of HDS and polyaromatics can be tuned. On the other hand, the hydrogenation selectivity of mono-aromatics/polyaromatics in diesel HDS are also related to the morphology of active phase. Additionally, the support pore structure has important influence on the hydrodesulfurization activity and stability.

Based on the findings, a catalyst technology construction strategy towards the low-carbon demand has been formed (Fig.1). The CoMo type diesel hydrotreating catalyst was developed with increased performance in low energy operation model. The catalyst combination technology was proposed to adjust the selectivity of hydrodesulfurization and polyaromatics saturation to save hydrogen consumption in diesel hydrotreating.

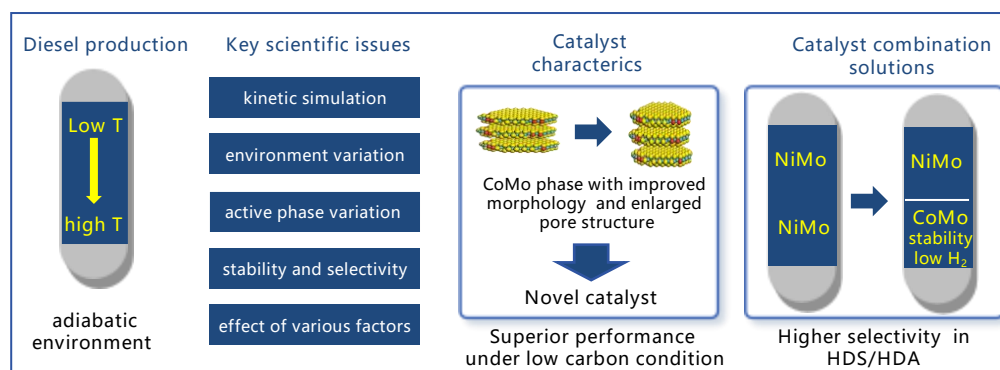


Fig. 1: Catalyst design strategies for diesel hydrotreating in low energy operation model

Engineering Heterobimetallic Catalysts for C-H Activation: from H/D Exchange to Methane Valorization

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The selective activation of C-H bonds remains a key challenge in catalysis, with direct relevance to greener chemical processes and more sustainable use of hydrocarbon resources. Heterobimetallic catalysts combining an electron-rich late transition metal (eg. Ir or Co) with an early Lewis-acidic metal (eg. Al, Hf, Ta or Nb) generate polar metal-metal pairs,[1-2] that can enable cooperative C-H activation pathways beyond the reach of monometallic systems.[3-5] Using a Surface Organometallic Chemistry approach, we have developed well-defined silica-supported MM' catalysts and evaluated them in two distinct but mechanistically related applications: hydrogen isotope exchange and methane valorization.

In the context of hydrogen isotope exchange (H/D exchange), we reported the design of a TaIr/SiO₂ supported catalyst which is several orders of magnitude more active than both monometallic analogs and homogeneous systems for the late-stage labelling of C_{sp2}-H bonds in arenes.[6] More recently, we found that HfIr/SiO₂ and TaCo/SiO₂ materials catalyze the highly challenging deuteration of C_{sp3}-H bonds of unactivated alkanes using D₂ under solvent-free mild conditions while strongly suppressing undesired hydrogenolysis side reactions leading to C-C bond cleavage and substrate degradation.[7-8] This represents a significant advance toward more atom-economical and efficient routes for producing deuterated molecules, which are increasingly important in pharmaceuticals and analytical standards.

In a second application, we developed a NbIr/SiO₂ catalyst which demonstrates exceptional activity and stability in methane-ammonia reforming, enabling efficient conversion of methane into valuable HCN and H₂ at "mild" temperature. These results represent a significant advance over existing catalysts due to the atomic-scale synergy between Ir and Nb sites, enabling access to activity and selectivity regimes inaccessible to monometallic analogs. Furthermore, the bimetallic synergy increases catalyst stability by reducing sintering and coke formation. These results highlight the potential of heterobimetallic systems for energy-efficient and more sustainable methane valorization [9].

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Development and Application of PEM Water Electrolysis for Hydrogen Production

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Energy is not only the foundation of social development but also a key support for national security and public well-being. The large-scale use of fossil fuels has led to major carbon emissions, aggravating global issues such as resource depletion, environmental degradation, and climate change. In this context, transitioning energy systems toward decarbonization and ultimately carbon neutrality has become a global priority.

Hydrogen energy, especially when produced via renewable-powered water electrolysis, is emerging as a key solution for low-carbon chemical processes. Among the available technologies, proton exchange membrane water electrolysis (PEMWE) offers advantages like high current density, fast response, and flexible integration, making it one of the most promising routes for future green energy systems. However, scaling up PEMWE faces challenges such as the need for original innovation in electrochemical platforms, reducing costs, ensuring operational safety, and achieving stable hydrogen production under fluctuating renewable inputs. At the same time, AI-driven optimization of materials, reactor design, and system operation is becoming increasingly important.

To address these issues, our team is carrying out systematic research focused on:

- Developing key materials and components (e.g., catalysts, MEAs, membranes, and bipolar plates) to ensure domestic production and large-scale application;
- Enhancing electrochemical efficiency by minimizing polarization losses;
- Establishing multi-scale reactor design methods from materials to system integration;
- Leveraging AI and high-throughput approaches to accelerate materials discovery and system optimization

In conclusion, PEMWE is a vital technology for green hydrogen production and energy decarbonization. Breakthroughs in materials, integration, and intelligent design are essential. By combining deep electrochemical understanding with AI-driven research, we aim to accelerate the industrialization of PEMWE and support the development of a hydrogen-based clean energy system[1].

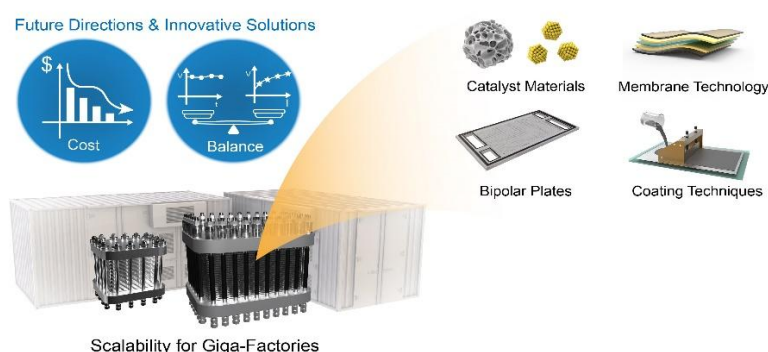


Fig. 1: Directions and innovative solutions for advancing PEMWE technology

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Innovative Catalytic Processes for Black Liquor Valorisation

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Black liquor is an aqueous effluent produced in large quantities in the pulp and paper industry. It originates from wood processed in the kraft pulping process, where cellulose is converted to paper pulp and lignin and hemicelluloses are solubilized and degraded in black liquor. Although today it is primarily burnt to recover energy and inorganic compounds, black liquor could be an interesting feedstock for the production of bio-based compounds.

In this work, two different catalytic processes were designed for the conversion of black liquor into biosourced compounds.

- 1) In the first process, phenolic compounds and aliphatic acids were produced by catalytic oxidation of lignin directly in black liquor with a copper catalyst. This process yielded a large range of molecules, including vanillin, phenol, formic and acetic acids [1,2]. A multi-technique analytical approach was developed to characterize the reaction products (HPLC-DAD, IC-MS/MS, NMR, TGA, etc.). A parametric study was performed to understand the reaction mechanism and to determine the role of the catalyst. It was established that lignin reacts first homogeneously with the alkaline medium to produce oligomers that interact with the solid catalyst to form phenolic and aliphatic compounds. The use of a continuous fixed bed reactor led to an increased space time yield in bioproducts.
- 2) In a second process, aliphatic acids present in black liquor were esterified into ethyl carboxylates over a solid catalytic acid in a continuous catalytic reactive distillation column. Reactive distillation combines catalytic reaction and separation in a single unit and is particularly suitable for shifting the thermodynamic equilibrium of reaction such as esterification. After designing new catalytic packing for reactive distillation, the process was implemented with model feed (glycolic acid and ethanol). The reaction was followed by offline analysis of distillate and residue products by HPLC-RID-DAD and Karl-Fisher.

These results provide an incentive for the design of new processes for the chemical valorization of black liquor.

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Low-temperature Catalytic Upcycling of Mixed Polyolefins via Tandem Catalysis

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Polyolefins and their chlorinated derivatives such as polyvinyl chloride (PVC) are among the most prevalent plastics in global production and waste streams. Traditional waste-to-energy methods such as incineration and pyrolysis, as well as most chemical upcycling methods for PVC utilization, require thorough, high-temperature dechlorination to prevent the release of toxic chlorinated compounds [1].

We present here a strategy for upgrading discarded polyolefins and PVC into chlorine-free fuel range hydrocarbons and hydrogen chloride in a single-stage process catalyzed by chloroaluminate ionic liquids [2]. This approach offsets endothermic dechlorination and carbon-carbon bond cleavage with exothermic alkylation and hydrogen transfer by isobutane or isopentane in a low-temperature tandem process (<100°C) [3]. The light isoalkanes are available from refinery processes and partly from recycling of the product stream. This process efficiently treats real-world mixed and contaminated PVC and polyolefin waste streams by reducing energy input, equipment complexity, and intermediate steps, thereby lowering costs and environmental impact.

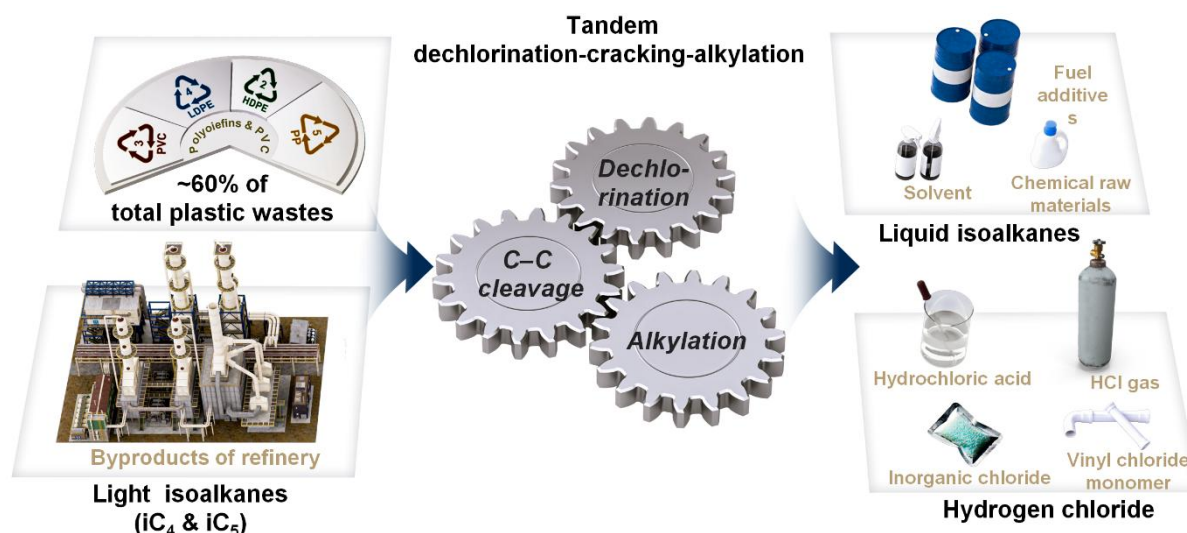


Fig. 1: Coupling of mixed PVC and polyolefin waste plastics with light isoalkanes through a tandem dechlorination, alkylation, and cracking process, producing liquid isoalkanes and HCl in a single stage.

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From Rationalization to Prediction of Reactivity and Selectivity through DFT Simulations : The Case of Diels-Alder Reactions of Biobased Furanic Derivatives

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Predicting and rationalizing chemical reactivity and selectivity is a central problem in all branches of chemistry, which has a particular resonance in green chemistry since a deeper understanding may help in designing more efficient transformations; In this respect, numerical simulations relying on DFT are of certain interest – although one must also keep in mind the pros and cons of resorting to numerical simulations.[1]

However, these are mostly used *a posteriori* of potentially intensive experimental works.[2] In this presentation, I propose to illustrate on a series of Diels-Alder reactions between furanic compounds derived from furfural and various dienophiles how, by building on a first set of experimental data (involving alkene reagents),[3] we could then move to a predictive approach for alkyne reagents, potentially affording a direct entrance to substituted phenolic derivatives from the cellulosic biomass. [4] I will then show how experiments supported most of the DFT predictions, the principal deviation being in fact associated with an unplanned side-reaction.

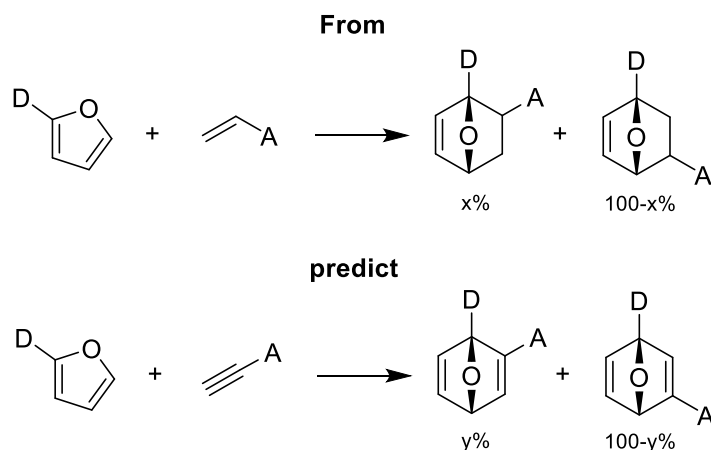


Fig. 1: Studied reactions; top: Diels-Alder reactions between biobased furanic derivatives and alkenes (experimental work by the group of Dr. F. Jérôme and K. De Oliveira Vigier, followed by DFT calculations); bottom: predicted Diels-Alder reactions with alkyne derivatives.

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Posters

How do Alkali Cations Affect Alkaline HER Activity of Nickel and Platinum?

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Large-scale green hydrogen production requires not only the development of efficient and earth-abundant electrode materials, but also strategies to enhance electrocatalytic performance without a significant increase in material complexity or cost. In this context, electrolyte engineering provides a complementary approach by tuning the electrochemical interface and reaction kinetics through electrolyte composition.[1] Alkali cations are known to substantially affect the kinetics of electrocatalytic reactions, including the CO₂ reduction and the alkaline hydrogen evolution reaction (HER)[2], yet the microscopic origin of this effect and its dependence on the electrode material remain unclear. Here, we investigate the influence of Li⁺, Na⁺, K⁺, and Cs⁺ on alkaline HER over Ni, a commercially relevant catalyst for alkaline electrolysis, and Pt, a benchmark HER catalyst. Grand-canonical Density Functional Theory (DFT) is combined with Quantum Mechanics/ Molecular Mechanics (QM/MM) simulations[3] to account for both electrode potential and the explicit aqueous electrolyte environment, and the computational results are compared with electrochemical measurements. We find distinct cation-dependent HER trends on Ni and Pt. These experimental trends correlate with the calculated activation barriers for water dissociation, considered here as a proxy for the Volmer step, whereas the adsorption free energies of *H and *OH show comparatively weak cation dependence.

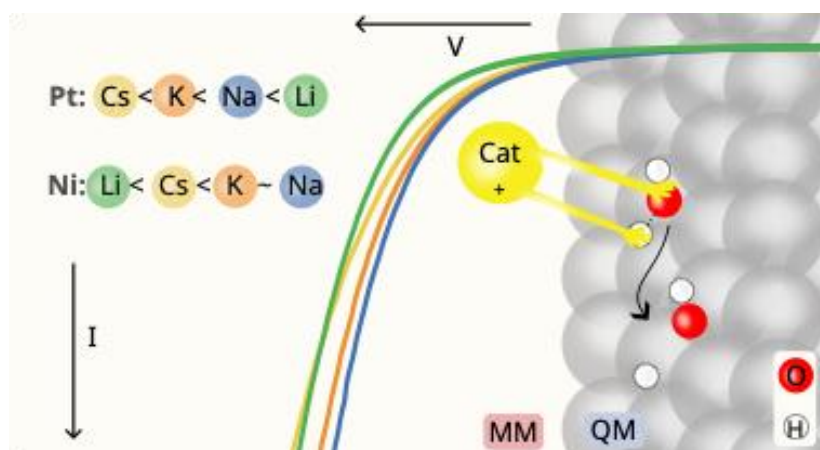


Fig. 1: Schematic illustration of the alkali cation effect on HER over Pt and Ni. The experimentally observed cation-dependent activity trends differ between Pt and Ni. The explicit electrolyte environment is described using molecular mechanics (MM), while the electrode and reaction intermediates are treated quantum mechanically (QM), enabling the cation-dependent interfacial environment and water dissociation involved in the Volmer step to be investigated.

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Design and Development of a Tandem Photoelectrochemical Device for the Solar Valorization of Biomass-Derived Furanic Compounds

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Decarbonizing the chemical sector requires replacing fossil-based feedstocks and energy with renewable carbon sources and clean energy. Lignocellulosic biomass provides an abundant source of renewable carbon, but efficiently converting its platform molecules into valuable chemicals remains challenging¹.

Photoelectrochemical (PEC) systems offer a compelling route to couple solar energy with targeted chemical transformations². In this work, we investigate the solar-driven conversion of two biomass-derived platform molecules: furfural, converted into furfuryl alcohol for resins and adhesives and 2-methylfuran as a potential bio-based fuel; and 5-hydroxymethylfurfural (HMF), converted into 2,5-furandicarboxylic acid (FDCA), a key building block for bio-based polymers such as polyethylene furanoate (PEF), a potential alternative to PET³.

Our approach combines III–V photocathodes and BiVO₄ based photoanodes with electrocatalysts⁴, with the aim of coupling the reduction and oxidation of furanic compounds in a tandem PEC configuration. Initial photoelectrochemical characterization in aqueous electrolytes shows promising photocurrent responses for P–I–N GaAs nanowires (NWs) photocathodes and BiVO₄ photoanodes, suggesting their potential for tandem integration. Ongoing work will focus on biomass-derived substrates under varying operating conditions (pH, concentration, illumination intensity) to assess activity, selectivity, and stability toward the development of an unassisted solar-driven PEC system for biomass valorization.

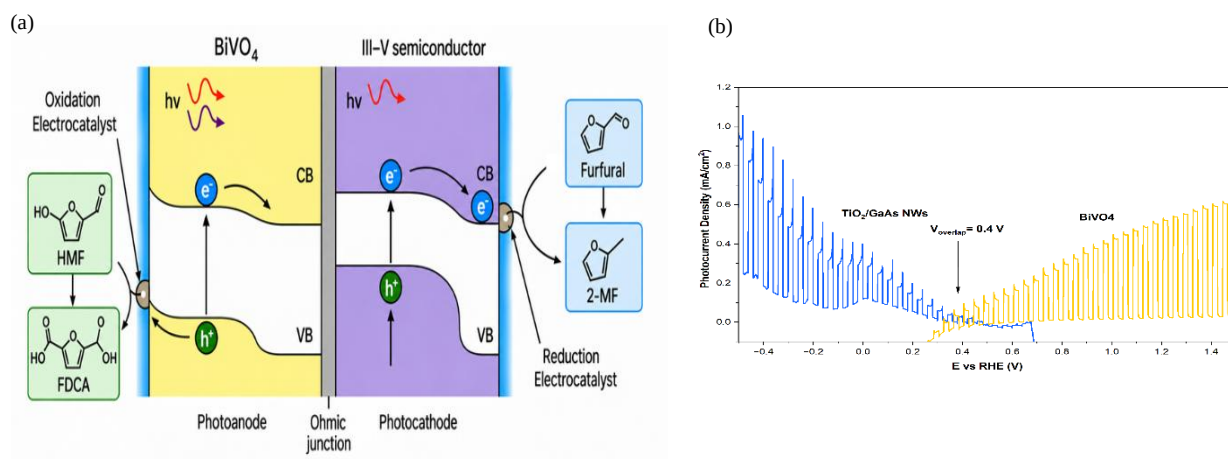


Fig. 1: (a) Tandem photoelectrochemical concept for biomass valorization. (b) Photocurrent matching of GaAs NWs with TiO₂ protection and BiVO₄ for tandem operation.

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Thermodynamic modeling of CO₂ absorption with aqueous potassium lysinate and organocatalyzed mineralization

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As the second-largest global CO₂ emitter, the cement industry requires new approaches to reduce its impact on global warming. Conventional CO₂ capture processes rely on multiple operations to produce CO₂-sourced products which are both energy- and cost-intensive. Therefore, Integrated Carbon Capture Utilization and Storage (iCCUS) is the most promising approach to effectively mitigate their impact [1].

Since the slow kinetics of CO₂ mineralization hampers its deployment [2], aqueous alkaline amino acid such as lysinate (KLys), can be used to dramatically accelerate the process. After absorbing CO₂, it both accelerates the dissolution of alkaline earth-containing industrial wastes, and their conversion into thermodynamically stable inorganic carbonates. Here, we bring an unprecedented level of understanding on the complex molecular system at work during mineralization. The system KLys-H₂O-CO₂ under thermodynamic control was fully described at 25 °C by adapting and upgrading a model described in the literature [3]. It brings a more accurate prediction of CO₂ absorption by KLys including minor species such as dicarbamate [3,4].

The next phase focused on using this knowledge to guide the optimization of mineralization which consists in catalyzing the conversion of calcium or magnesium oxides into carbonates through a two steps process (**Figure 1**). CO₂ loading levels on KLys resulting from absorption and Ca or Mg to CO₂ molar ratios were screened onto two classes of industrial wastes containing and compared to other CO₂ carriers. This knowledge guided approach delivered optimal conditions for catalyzed mineralization of industrial demolition waste, which recently achieved 96 % conversion by coupling with mechanical activation, and 99% recovery of the amino acid.

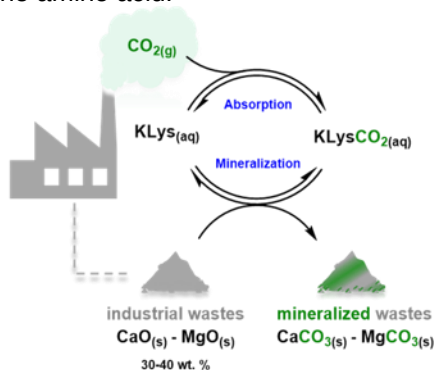


Fig. 1: Absorption and mineralization process organocatalyzed by potassium lysinate.

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Total Synthesis of Miyabeacin B Is Ansarane a potential 3D Bioisostere of Naphthyl group?

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Willows consist of more than 1,500 distinct species and are a significant source of bioactive compounds, including salicylic acid and its derivatives. More complex structures have also been reported as (+)-Grandifloracin **1**, isolated in 2012 from the species *Uvaria dac* [1] and Miyabeacin B **2**, isolated in 2007 from *Salix Miyabeana* [2] (Fig. 1). They both exhibit biological properties; in particular (+)-Grandifloracin which targets pancreatic cancer cell lines. Despite a modest activity ($PC_{50} = 14.5 \mu M$) [3], it nevertheless warrants particular attention, notably due to the marked resistance of pancreatic tumors to most currently available chemotherapeutic agents.

Thus, we set out to explore the potential of one of the precursors of (+)-Grandifloracin, possessing a spiroepoxycyclohexadienone **I** moiety which lends itself to numerous transformations and above all, offers a rapid access to ansarane structure using photochemistry. This caged compound exhibits a highly symmetric skeleton with intriguing chirality. Its properties are comparable to those of a naphthyl group and may be considered as a potential bioisostere.

Accordingly, we accomplished the total synthesis of Miyabeacin B and investigated a new 3D chemical space toward the preparation of novel constrained scaffolds inspired by this natural product.

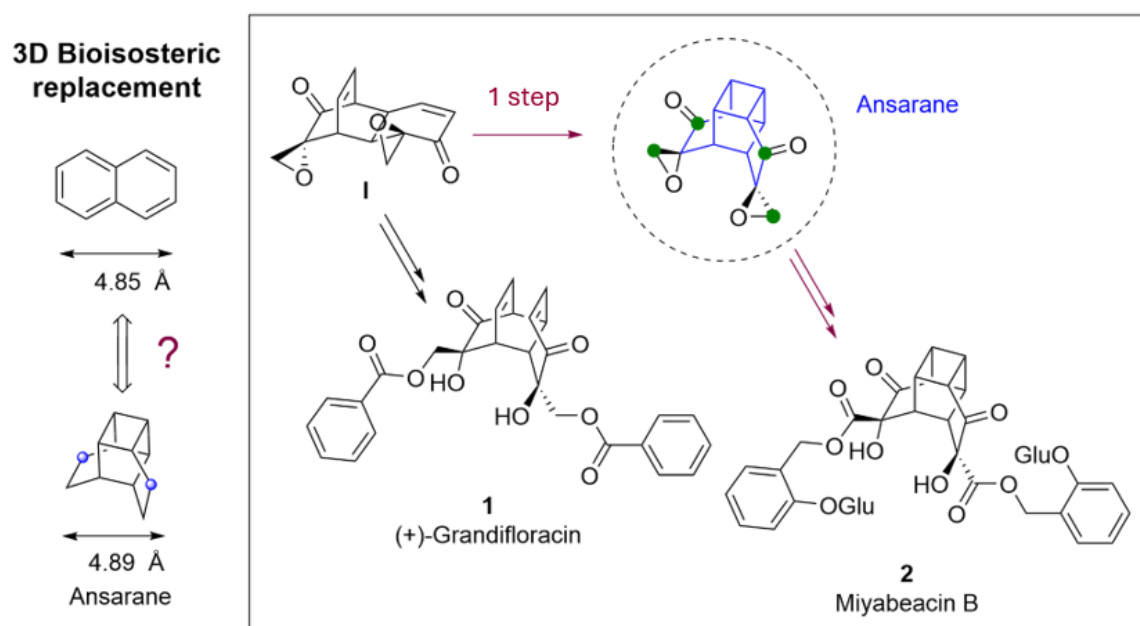


Fig. 1: Synthetic strategy toward miyabeacin B from a polyfunctionalized ansarane platform

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Molecular and Macromolecular Heterocyclic Compounds formed during the Transformation of Sugars into Caramel

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Caramel is obtained by heating carbohydrates (glucose, fructose, sucrose) and water at high temperature, sometimes with the addition of a promoter such as ammonium bisulfite (NH₄HSO₃) or citric acid. Although studied since the 19th century, with Péligot's characterization of caramel acidity [1] and Gélis separation of caramel in three fractions (caramelan, caramelen and caramelin) [2], the chemistry of caramel remains poorly understood. Since, it is now accepted to consider two main fractions in caramel [3-6]. The volatile fraction is responsible for its aroma, and the non-volatile fraction contains small oxygenated heterocycles such as 5-hydroxymethylfurfural (5-HMF) and 4-hydroxy-2,5-dimethyl-3(2H)-furanone (HDMF), as well as oligomers including difructose dianhydride, which benefit the gut microbiota, and polymers.

Building on this research, we started to explore in more details the non-volatile fraction of caramel, notably focusing on the involvement of 5-HMF and other heterocycles in the formation of hybrid systems, possibly precursors of higher-molecular-weight compounds. 5-HMF, an interesting biobased platform molecule [7], [8] is formed during the caramelization process. Our goal was to characterize some carbohydrate-HMF hybrids which can be formed under acidic conditions. Among possible reactions, we studied the condensation of 5-HMF and D-glucose by their reaction involving the aldehyde group of HMF with the C4 and C6 hydroxyl groups of D-glucose through an acetalization reaction (Fig. 1), and found that HMF specific reactivity makes such a normally easy reaction more complex in this case, due to the instability of HMF under acidic conditions.

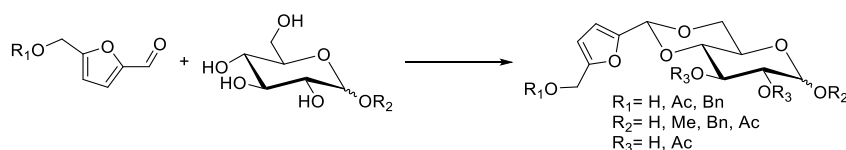


Fig. 2 : Condensation of HMF and its derivatives on D-Glucose and its analogues

Some first results of the investigation of size-exclusion chromatography performed on various types of caramels and related products will be also disclosed.

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Boranil-based Molecular Emitters for the Development of Responsive Supramolecular Materials with Enhanced Chiroptical Properties

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Constructing sophisticated luminescent dyes around a tetrahedral boron (III) center is a particular approach that has fueled the creativity of chemists motivated by their use in organic electronics and applied photonics or as molecular probes in biomedical analysis, sensors and materials science [1].

We have recently described a very simple and efficient gram-scale synthetic pathway towards Boranils substituted directly on the boron center by 1,1'-bi-2-naphthol derivatives (BINOL) [2]. These chiral dyes typically feature high molar absorption coefficient in the range of 35,000 to 90,000 M⁻¹.cm⁻¹, absorption dissymmetry factor (g_{abs}) in the range of 2.5–5.5 × 10⁻⁴ at the maximum wavelength of absorption of Boranils and CPL brightness up to BCPL = 5.4 M⁻¹.cm⁻¹. Based on this new family of CPL emitters, we are currently developing supramolecular chiral soft-materials such as stimuli-responsive gels and liquid crystals [3],[4].

As an illustration, we have developed molecular switches taking advantage of the control of energy transfer to a photochromic diarylethene (DAE) core to modulate chiroptical properties in liquid crystals thin films with enhanced g_{abs} and g_{lum} . The second strategy consist in doping a chiral stimuli-responsive gels with achiral Boranil emitters to seek for chirality induction in its emission. The gel response to electron transfer should allow modulation in the CPL emission.

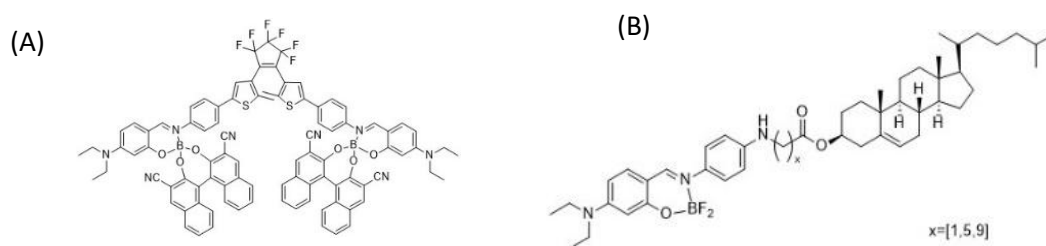


Fig. 1: (A) DAE Boranil Bis BINOL, (B) Cholesterol functionalized Boranil

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Electrochemically-Driven Auto-Tandem Nickel Catalysis for the Production of Butafulvenes

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Butafulvenes (3,4-bis(methylene)cyclobutenes) are a unique class of highly strained, anti-aromatic cyclic compounds that hold great promise for advanced applications such as the design of highly unsaturated materials, solid state luminescent materials, as well as the construction of complex cyclobutene-containing natural product-like molecules. However, the synthetically challenging structural features of these compounds still hamper their broad investigation and application. A classical synthetic approach relies on the preparation, or in situ generation, of a bisallenic (1,2,4,5-tetraene) intermediate followed by its electrocyclization, a process that requires relatively high temperatures (Fig. 1 A).^[1] Over the years, transition metals (Ni, Cu, Pd) have been shown to facilitate the conversion of bisallenes into butafulvenes, allowing milder reaction conditions.^[2-5] In this context, we have successfully developed an efficient catalytic method relying on the combination of nickel catalysis and electrochemistry for the synthesis of butafulvenes from propargyl electrophiles operable under mild conditions. Our approach exploits the capacity of nickel to catalyze in tandem the generation of bisallenes directly through dimerization of propargyl electrophiles, and their subsequent cycloisomerization to butafulvenes (Fig. 1 B). Overall, this study presents a robust, and sustainable methodology, setting the stage for new advancements in the exploration of the reactivity and properties of butafulvenes.

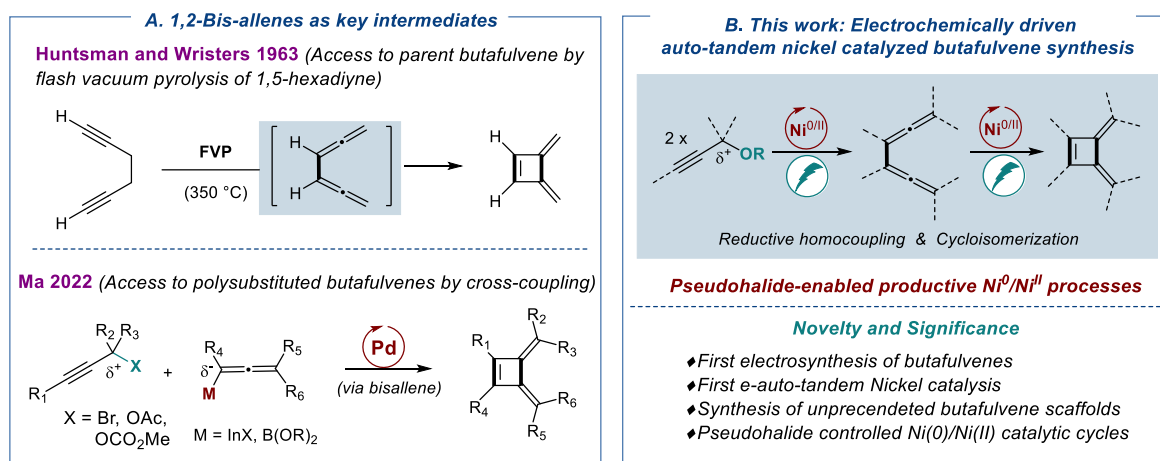


Fig. 1: Nickel-Catalyzed Electrosynthesis of Butafulvenes

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Valorization of 5-HMF for the Synthesis of Novel Spirocycles using aza-Piancatelli Reaction

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Over the last century, the world has relied on fossil fuels as its main source of energy and industrial production of goods. However, reserves are diminishing whilst the demand is growing. New strategies involving biobased chemicals have emerged to replace petrochemicals. Amongst various molecules, 5-hydroxymethylfurfural (5-HMF), obtained from the dehydration of hexoses, is considered as one of the promising platforms.¹

Besides its conversion in high-valued platforms (furan dicarboxylic acid, levulinic acid...) and its applications in polymer synthesis, 5-HMF reactive structure makes it an interesting starting material in fine chemistry. In this respect, our group was the first to investigate the use of 5-HMF in various multi-component reactions.²⁻⁴ Still dedicated to the upgrading of 5-HMF, our group grew curiosity in broadening its use in fine chemistry through synthetic sequences including the Piancatelli reaction. Discovered in the 1970's, it directly converts 2-furylcarbinols to 4-hydroxycyclopentenones under acidic conditions. Since then, several studies have focused on the development and mechanism of the reaction. More recently, the aza-Piancatelli reaction with nitrogen nucleophiles has been extensively studied, from inter- and intramolecular versions to enantioselective and cascade cyclisations.⁵ Having developed the preparations of adequate furylcarbinols precursors starting from 5-HMF or chloromethylfurfural (CMF), we developed the synthesis of spiromorpholines and spirobenzoxazines thanks to an aza-Piancatelli key step. Two libraries of spirocyclopentenones were reported, with moderate to high diastereoselectivity and isolated yields.⁶

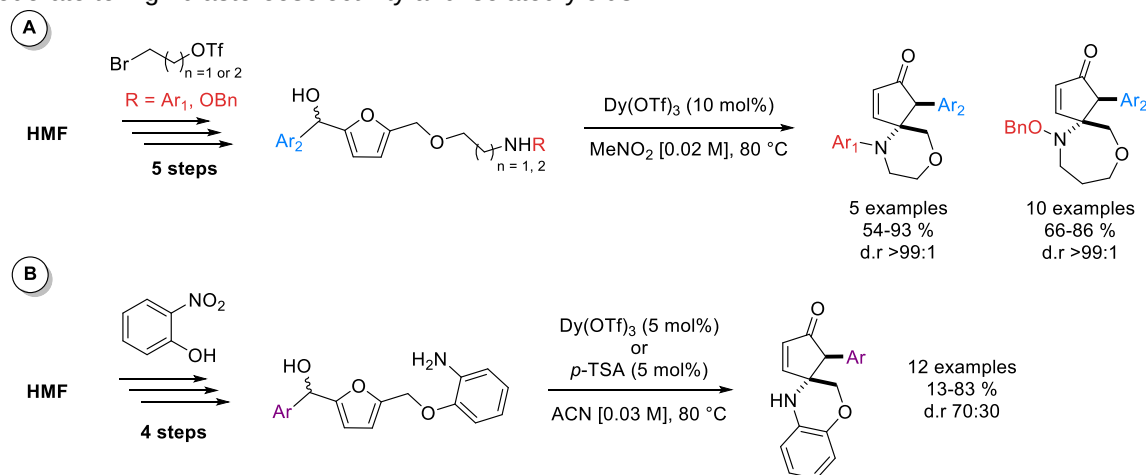


Fig. 2 : **A** Synthesis of morpholine or oxazepine-fused spirocycles and **B** Synthesis of spirobenzoxazines.

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Efficient and Sustained Electrocatalytic Methanol Production from CO₂ on Heterogenized Butoxy-substituted Cobalt Phthalocyanines

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Electrochemical CO₂ reduction (CO₂RR) powered by renewable electricity offers a promising route for converting CO₂ into value-added chemicals and fuels. Among the possible products, methanol is particularly attractive as both a liquid fuel and a versatile chemical feedstock [1]. Cobalt phthalocyanine (CoPc)-based molecular catalysts have shown promise for the multi-electron reduction of CO₂ to methanol [2–4]; however, further improving methanol Faradaic efficiency while maintaining stable performance during prolonged electrolysis remains a key challenge.

Here, we investigate peripheral functionalization of CoPc as a strategy to improve methanol selectivity and operational stability. Introduction of four *n*-butoxy substituents affords (nBuO)₄CoPc/CNT, which enhances methanol production without imposing a penalty in overpotential. The resulting catalyst reaches a maximum initial Faradaic efficiency for methanol of 39 ± 5% at –0.95 V vs RHE and retains a Faradaic efficiency of ca. 30% after 6 h of electrolysis, in marked contrast to the rapid deactivation observed for CoPc/CNT under the same conditions.

These results demonstrate that peripheral molecular functionalization can enhance methanol selectivity and operational stability during prolonged CO₂ electroreduction, highlighting molecular substitution as a promising strategy for the development of durable CoPc-based electrocatalysts.

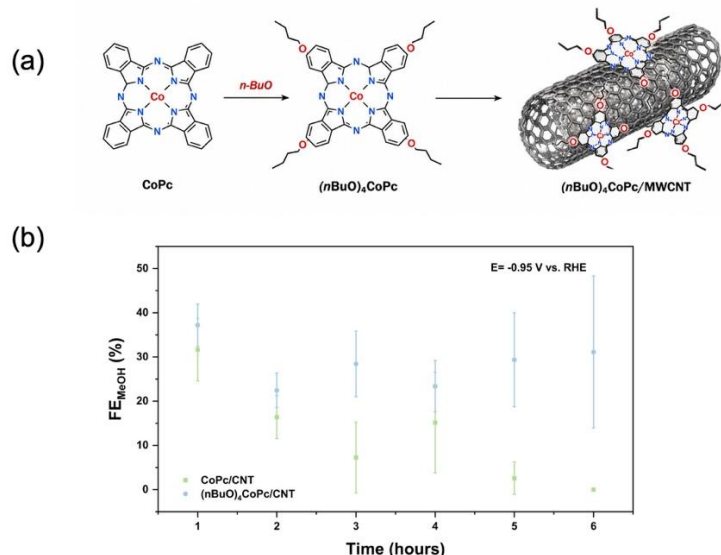


Fig. 1: (a) Schematic illustration of CoPc, (nBuO)₄CoPc, and its immobilization on MWCNTs. (b) Methanol Faradaic efficiency during 6 h electrolysis at –0.95 V vs RHE.

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Stable Electrothermal Methane Dry Reforming Using Structured Ni/CHA Zeolite

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Highly endothermic methane reforming requires substantial energy input to maintain reaction performance. In conventional reactors, energy is supplied by external heat sources and transferred driven by temperature differences. This creates cold spots within the catalytic bed, which compromises catalytic performance and triggers side reactions such as coke formation.

To address the mismatch between reaction heat demand and heat supply spatially and temporally, this presentation introduces electrothermal catalytic reaction technology. Electrically heated catalysts act as heat sources to deliver energy in situ to catalytic active sites, which markedly improves energy utilization efficiency and suppresses side reactions. The embedment of Ni particles within cavities of CHA zeolite prevents metal sintering and thus avoids coke formation by methane pyrolysis. Altogether, the electrothermal methane dry reforming achieves 300 h stable conversion at high space velocity.

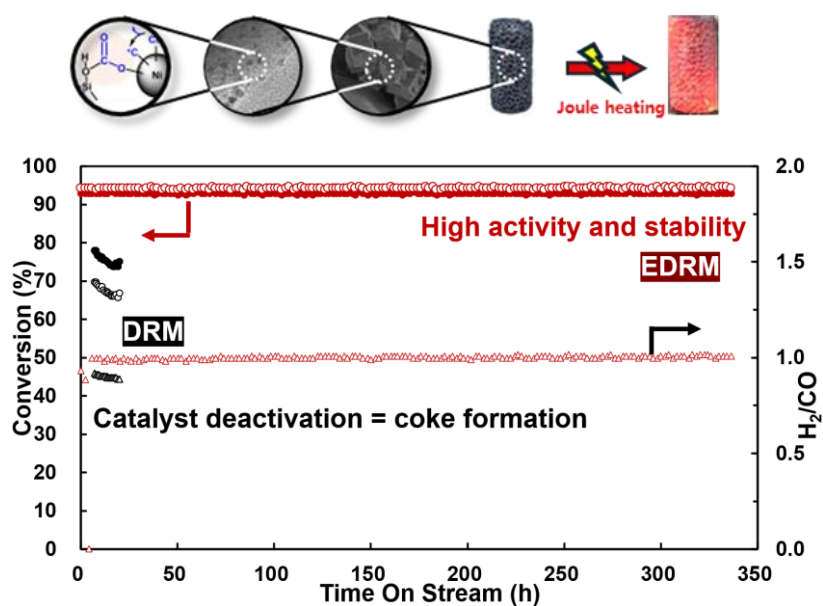


Fig. 1 Stable operation of electrothermal methane dry reforming for over 300 h using Ni-embedded CHA zeolite.

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Screening of Catalysts for the Heterogeneous Fenton Process for Plastics Degradation

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1. Introduction

Since their invention in the early 1900s, plastics have gradually become indispensable due to their durability, low cost and malleability, with global production reaching 430.9 million tons in 2024 [1]. However, extensive plastics use has raised environmental concerns, notably the accumulation of microplastics (MPs) in aquatic environments and their potential human health impacts [2]. Among methods for degrading MPs, heterogeneous Fenton reaction has attracted attention due to its strong oxidation ability and wider pH range [3]. Therefore, the objective of this work is to study the oxidation of polyethylene glycol (PEG), as a model polymer, to advance heterogeneous Fenton for eliminating MPs and polymeric wastes. For this purpose, four commercial materials (Fe-ZVI, Fe₃O₄, FeS₂ and FeOOH) were firstly screened as catalysts for degradation of the monomer ethylene glycol (EG), providing a basis for subsequent PEG study.

2. Main Results and Discussion

After confirming that the decrease in EG concentration due to adsorption on all four catalysts was negligible, their catalytic performances for EG degradation were evaluated at initial pH 9 (Fig. 1a), pure water and pH 3. Only FeS₂ exhibited effective EG mineralization performance. Fe-ZVI, Fe₃O₄ and FeOOH only possessed 2.5%, 2.1% and 2.1% of EG conversion towards liquid organic products, respectively. It can be considered as negligible because it is of the same order of magnitude than the chemical degradation of EG in the presence of H₂O₂ (without any catalyst). In contrast, FeS₂ achieved 100% EG conversion within 60 min at initial pH 9, indicating its potential for degrading EG by heterogeneous Fenton reaction. The effect of initial pH on EG degradation was further investigated over FeS₂. This catalyst displayed comparable mineralization rates in the range of pH 3–9 (Fig. 1b), while the pH decreased to around 3 regardless of the initial pH value. These results indicate that FeS₂ catalyst can maintain a high mineralization efficiency and possess the strong pH self-adjusting ability in a wide range of pH (3 to 9). Moreover, the Fe leaching of FeS₂ was 63 mg/L after 120 min at initial pH 9, corresponding to around 2.26 wt% of the total Fe content. To assess the contribution of these dissolved ions, a homogeneous Fenton reaction was conducted using 63 mg/L Fe²⁺ at initial pH 3 (Fig. 1c). The homogeneous reaction achieved 16.2% mineralization after 120 min, accounting for only 22% of the total mineralization observed in the FeS₂ system (74.9%), indicating that the heterogeneous reaction played the dominant role.

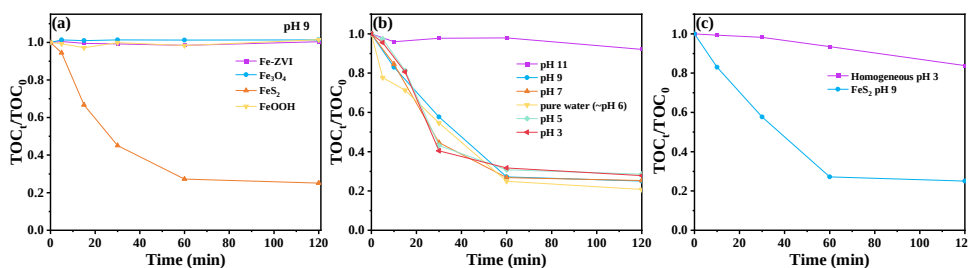


Fig. 1: (a) EG mineralization over Fe-ZVI, Fe₃O₄, FeS₂ and FeOOH catalysts during reaction at initial pH 9; (b) EG mineralization over FeS₂ catalyst at different initial pH; (c) EG mineralization comparison between homogeneous reaction at initial pH 3 and FeS₂-catalyzed Fenton reaction at initial pH 9 (Conditions: 100 mL of solution containing 0.2 g/L EG, 6.0 g/L of catalyst, 63 mg/L of Fe²⁺ from FeSO₄ in homogeneous, 50 mM of H₂O₂, RT)

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Conversion of Polyesters and CO₂ to Monomers and Carbonates

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The valorization of waste polyester plastics is crucial for advancing a circular carbon economy. Polyethylene terephthalate (PET), produced globally at over 70 million tonnes annually, is difficult to recycle because its stable structure typically requires high temperatures and additional solvents.

We report an ethylene oxide-mediated one-pot cycloaddition–transesterification–glycolysis (CTG) process that converts PET, CO₂, and glycerol into PET monomers and glycerol carbonate at ≤110 °C without additional cosolvents, achieving yields of 92% and 99%, respectively. Ethylene oxide plays a dual role: it swells the PET matrix to overcome mass-transfer limitations and reacts with CO₂ to generate ethylene glycol in situ for PET glycolysis. Kinetic studies demonstrate that the synchronized cycloaddition, transesterification, and glycolysis steps are essential for exploiting this dual functionality. Furthermore, C¹⁸O₂ isotope-labeling experiments combined with theoretical calculations elucidate the reaction pathway from ethylene oxide and CO₂ to ethylene glycol intermediates and subsequent PET depolymerization. The process is applicable to various waste polyesters and real-world plastic products and remains effective at temperatures as low as 60 °C.

Overall, this strategy integrates enhanced mass transfer and cascade reaction engineering to enable the mild, solvent-free co-valorization of waste PET and CO₂, offering a promising route toward sustainable carbon-resource recycling.

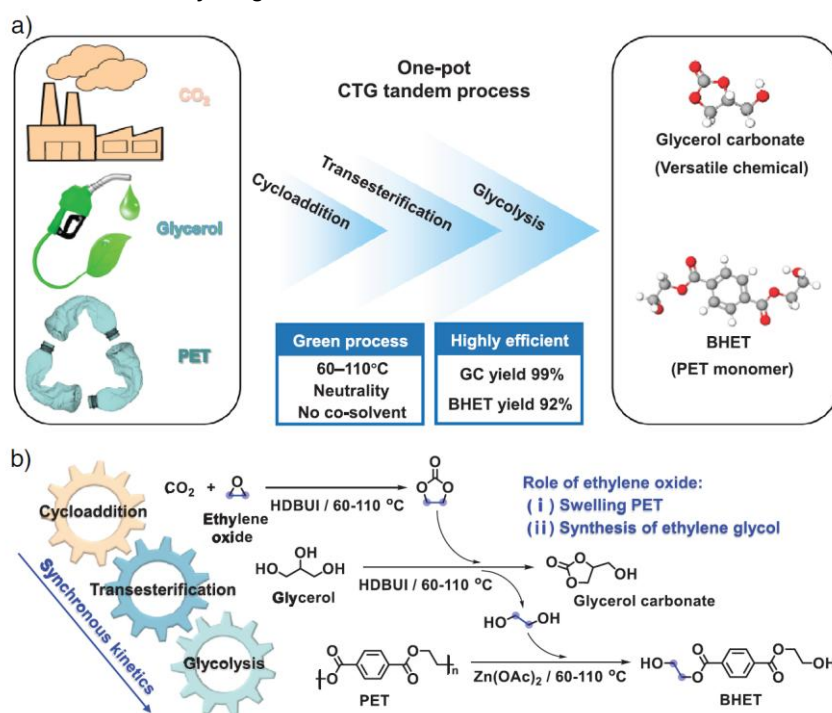


Fig. 1: Scheme 1. One-pot CTG conversion of PET, CO₂, and glycerol under mild conditions (a) and the dual role of ethylene oxide in the synchronized tandem reactions (b).

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Chemical Recycling of Polyolefin Plastics under Mild Conditions via GaCl₃-based Molten Catalysts

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Polyolefins (polyethylene PE, polypropylene PP) constitute over 65% of global plastic production, yet their chemical stability of C–C backbones poses a significant challenge for recycling. Herein, we report a molten-salt Lewis acid catalytic system based on GaCl₃ (MgCl₂-4GaCl₃, denoted Mg-Ga), enabling efficient conversion of PE, PP, and PS either individually or in blends under mild conditions (≤ 170 °C). With a low melting point (~ 75 °C), the liquid catalyst enhances mass transfer and contact efficiency. At 130 °C, PS was fully converted within 30 minutes, while PE and PP showed over 60% conversion. Compared to AlCl₃-based catalysts, the GaCl₃-based catalysts combine strong Lewis acidity with low melting points, ensuring optimal liquid-solid or liquid-liquid contact and superior activity, highlighting the crucial role of catalyst phase state. For co-conversion of PE/PP and PS blends, Friedel-Crafts alkylation between aromatics from PS and olefins from polyolefin cleavage synergistically increased total conversion to $\sim 85\%$ and raised mono-aromatics selectivity in C₆–C₁₅ aromatics to 33.5%. Kinetic studies demonstrated that PP and PS exhibited low apparent activation energies of 42 and 76 kJ·mol⁻¹ under Mg-Ga catalysis, respectively. Raman spectra revealed the formation of active species like [GaCl₄]⁻ and [Ga₂Cl₇]⁻, with the strongly acidic [Ga₂Cl₇]⁻ dynamically dissociating to regenerate GaCl₃ and activate C–C bonds efficiently.[1] The system also effectively degraded real waste plastics and their mixtures, achieving nearly 90% conversion and $\sim 70\%$ liquid yield under optimized conditions, with tunable product distribution based on feed composition. In summary, this study presents a low-temperature, solvent-free strategy for chemical recycling of mixed plastics by coupling C–C bond cleavage with Friedel-Crafts alkylation, offering a promising solution for plastic waste valorization.

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Yuan, L.; Gao, Z.; Shi, L. et al. *Chinese J. Catal.* **2026**, 86, 137-148.

Selective and Synergistic Upcycling of Mixed Plastic Waste

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Key words: Waste plastics; Mixed waste; Chemical recycling; Selective conversion; Synergistic upcycling

Moving from the efficient conversion of individual polymers toward the selective treatment of complex mixed waste streams is a key challenge for practical plastic chemical recycling. Real-world wastes contain multiple polymers and other components, making selective conversion and product separation particularly difficult. Here, we developed three complementary strategies: mild depolymerization, staged conversion, and synergistic upcycling. First, mild depolymerization was developed for PET/natural-fiber blends. Stabilization of the key tetrahedral intermediate and suppression of the reverse reaction enabled selective PET depolymerization under mild conditions, recovering dimethyl terephthalate and ethylene glycol while preserving cotton and wool fibers. Second, staged conversion was established for mixed aromatic oxygenated plastics including PC, PET, and PPO. Differences in oxygen-containing bond reactivity enabled stepwise hydrodeoxygenation, sequential polymer conversion, and fractionated enrichment of distinct hydrocarbon products, thereby reducing product complexity and downstream separation requirements. Third, synergistic upcycling was demonstrated for mixed plastic–biomass wastes. Oxygenated plastics served as an internal hydrogen source, while in situ hydrogen transfer from plastic conversion was coupled with reductive biomass upgrading, enabling simultaneous plastic recycling and biomass valorization without external hydrogen or reducing agents. Together, these strategies show that compositional complexity can be exploited through selective bond activation and cross-component coupling to enable selective conversion, fractionated recovery, and synergistic valorization while reducing presorting and downstream separation requirements.

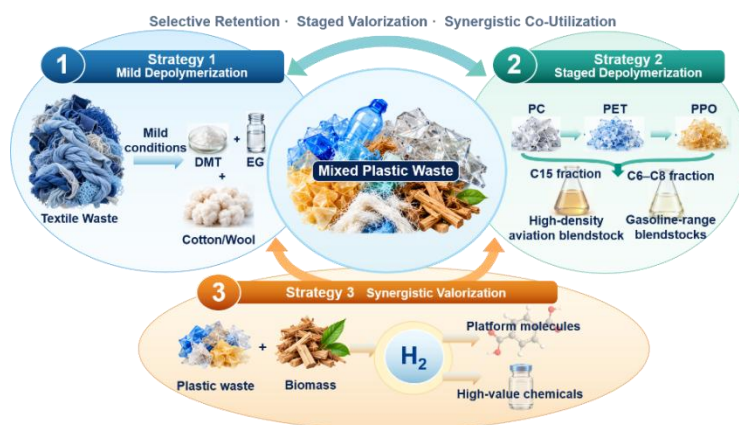


Fig. 1: Three Complementary Strategies for Precision Valorization of Mixed Plastic Waste

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Efforts for paradigm shift of basic research with industrial orientation - examples at Basic Research Department @ RIPP

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The downstream petroleum industry relies on catalyzed chemical reactions, including cracking, hydrogenation, reforming, etc. The complexity of the entire technological chain creates specialized domain segments that lead to the process of observing and solving common problems in catalysis. For example, the FCC process widely uses FAU and MFI zeolites as the primary active components. A common problem that goes beyond different classes of processes is the well-known C-C cleavage over acid sites, a finding typically overlooked by industry. In addition, the segmentation of specific fields makes it challenging to understand the logical origin of the integrated design and related applications. It has less impact on optimizing well-established technologies since the trial-and-fail paradigm would still be valid and efficient. However, for a scenario that fits the sustainable requirement, the catalytic reactions involved and their catalyst design are worth revisiting and sorting out.

For an enterprise that benefits from fuel production, it is natural to consider alternative feedstock, such as biomass and organic waste, with minor modifications of the existing plants. A biomass feedstock contains oxygen as the major heteroatom besides carbon and hydrogen, which shows a distinct difference from feedstock from fossil origin. Consequently, designing a suitable catalyst that is valid for operation at the current plant is the main task of the R&D efforts. Ideally, experience derived from Hydrodesulfurization (HDS)/Hydrodenitrogenation (HDN) processes should aid in developing a new catalyst. Because HDS / HDN are operated with fixed-bed reactors, the deactivation mechanism of biomass hydrodeoxygenation (HDO) must be fully understood before undertaking process optimization efforts.

Research Institute of Petroleum Processing (RIPP) is the technology provider to the refining and petrochemical businesses, not limited to the SINOPEC (China Petroleum and Chemical Corp.) group. The fact that the business of fuel production will decline in the foreseeable future, coupled with the inability of an enterprise to afford the high cost of a trial-and-fail paradigm for the development of technologies, the importance of fundamental research must be emphasized. The re-established Basic Research Department will ultimately bring about a paradigm shift to reduce the trial cost.

Several examples of current activities representative for the required competence of such application-oriented basic research will be presented.

Engineering Catalytic Sites and Reaction Pathways for CO₂ Electroreduction to Value-Added Chemicals

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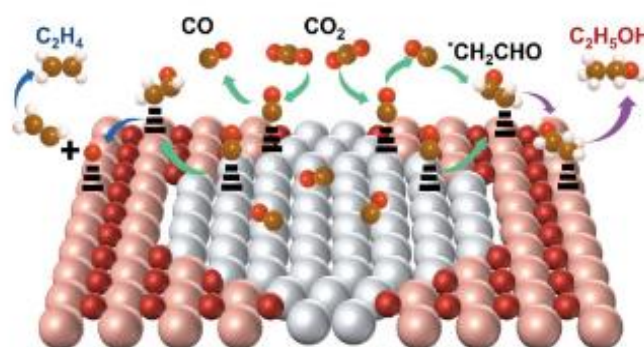
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Electrocatalytic CO₂ reduction can produce formate, methane, ethylene, and ethanol using renewable electricity, linking carbon recycling with chemical manufacturing. Selectivity remains difficult to control because multielectron and multiproton transfer, catalyst reconstruction, and local reaction conditions determine the evolution of key intermediates. We investigated how directed precursor reconstruction, grain-boundary engineering, interfacial electronic structure, and pH regulation govern active sites and reaction pathways.

Four complementary catalyst designs yielded distinct products and performance:

- NO₃⁻-mediated in situ reconstruction of Bi₂O₂CO₃ created ordered Bi facets that stabilized *OCHO, achieving 97% formate Faradaic efficiency and a partial current density of 329 mA cm⁻² on a gas-diffusion electrode.
- Tuning Cu₂O grain size and grain-boundary density produced Cu catalysts rich in concave grain boundaries, delivering >80% C₂+ Faradaic efficiency and approximately 100 h of stable operation at 200 mA cm⁻².
- An Ag/Cu₂O heterointerface, identified by theoretical screening and constructed experimentally, increased *CO coverage and lowered the *CO-*CO coupling barrier, yielding 77.8% C₂+ Faradaic efficiency at -300 mA cm⁻².
- pH-controlled reconstruction of Cu precursors regulated Ostwald ripening, surface roughness, and Cu valence, switching selectivity between CH₄ and C₂H₄. CH₄ Faradaic efficiency reached 60.5%, while the C₂H₄/CH₄ ratio reached 10.0.

These results establish dynamic reconstruction as a route to generating active sites rather than simply a deactivation process. Integrating in situ characterization and theoretical calculations links site structure, intermediate adsorption, and product selectivity, informing catalyst design for CO₂ electroreduction.



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Computational Investigation of the Glucose-Fructose Isomerization Catalyzed by a Base

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Hydroxymethylfurfural (HMF), a promising chemical intermediate, is used in the production of renewable polymers from biomass. However, the conversion yield of glucose to HMF is significantly lower than that of fructose. The latter is obtained through the enzymatic isomerization of glucose; however, glucose isomerase has limitations in its catalytic activity. Therefore, chemical catalysis appears to be a more attractive alternative. Lewis acids and Brønsted bases exhibit strong catalytic activity for this reaction, with bases being less expensive and easier to synthesize than Lewis acids.^[1]

The aim is to understand the role of homogeneous basic catalysts in glucose-fructose isomerization using advanced *ab initio* computational approaches. To start, a benchmark of several *Density Functional Theory* (DFT) functionals, including recently developed 3c functionals by M. Müller, A. Hansen, and S. Grimme^[2], was conducted and compared against the CCSD(T) reference method. Then, all reaction pathways were investigated using the SMD implicit solvation model with water as solvent and the ω B97X-3c functional.^[2] The theoretical approach provides deeper insight into the reaction mechanism and new plausible pathways. Understanding this concept serves as the starting point for the next stages of the research, particularly the study of the effect of the base and the explicit solvent on the reaction.

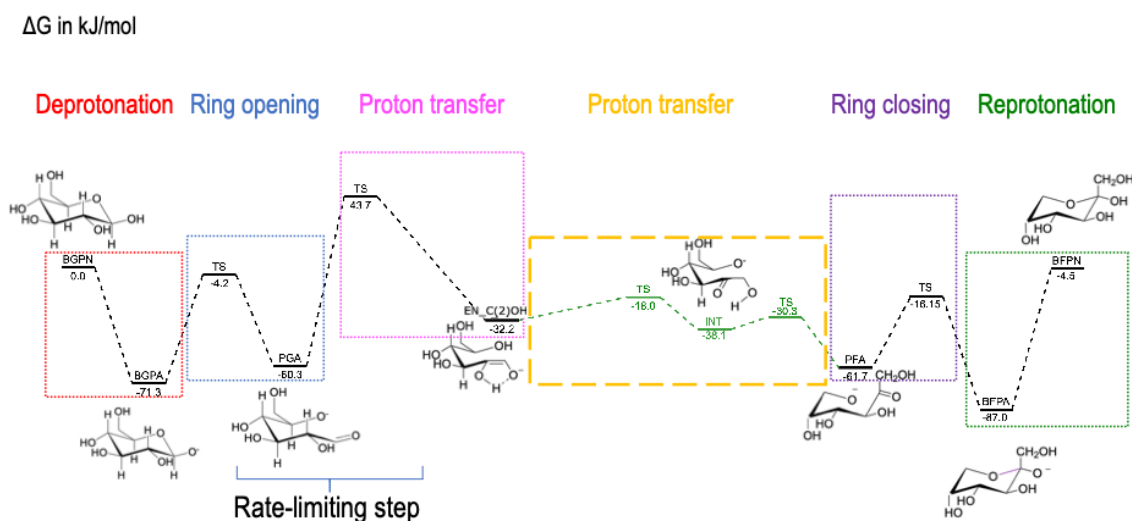


Figure 1 – Reaction profile of glucose-fructose isomerization

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Photoredox-Catalyzed Synthesis of Aromatic Difluoroacyl Spirocycles

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Spirocycles are important motifs in natural products^[1] and drug discovery^[2], yet (hetero)aromatic difluoroacyl spirocycles remain scarce^[3] despite the bioactivity of difluoroacyl derivatives^[4]. Traditional syntheses of such spirocycles are lengthy and low-yielding^[5-7], while radical cascades offer a more efficient route. Building on previous SET-based cyclizations^[8-9], we report a photoredox-catalyzed synthesis of difluoroacyl heteroarene spirocycles, with broad substrate scope, scalability, and versatile post-functionalization.

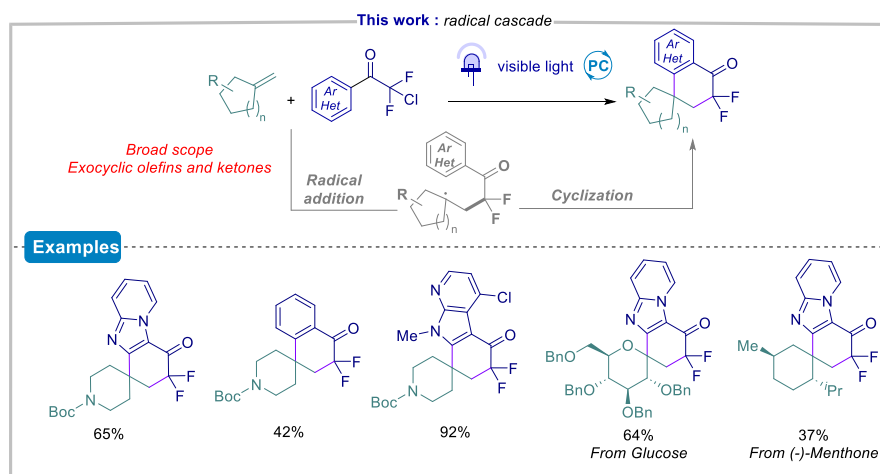


Fig. 1: Cyclic gem-difluoroacyl scaffolds synthesis

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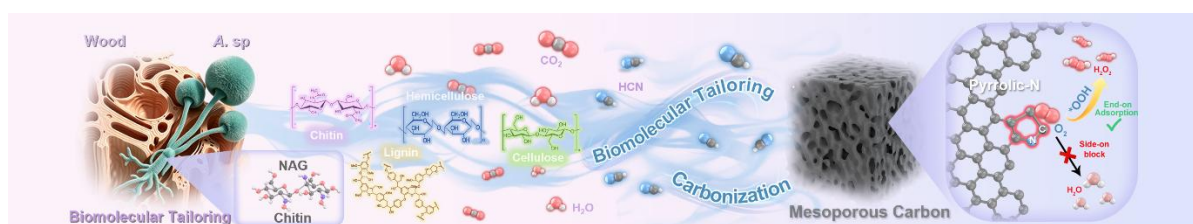
The Green Synthesis of Biomass based Carbon Materials via Biomolecular Tailoring and its Application in Energy Storage

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Biomass-derived carbon materials have attracted extensive attention in the fields of energy and environmental protection due to their advantages such as sources, renewable and low cost. Especially the biomass is rich in various heteroatoms can achieve self-doping during the preparation process, thereby providing sufficient active sites for the reaction. In addition, the regulation of pore structure is also a key to improve the performance of carbon materials. During the high-temperature pyrolysis and carbonization process, it is inevitable to cause the collapse of pore structure, and the accessibility of some pore structures is insufficient, making it difficult to precisely control the structure. Based on this, this study focuses on the controllable preparation of nitrogen-doped porous carbon via microbial pretreatment and its electrocatalytic application. Using biomass such as agricultural and forestry waste as raw materials, through a series of methods such as microbial pretreatment, regulating the pyrolysis process, and chemical activation, the controllable preparation of nitrogen-doped porous carbon is achieved, and the properties such as specific surface area, pore size distribution, nitrogen species, and surface functional groups of carbon materials are precisely regulated. The electrocatalytic performance of the resulting nitrogen-doped porous carbon materials for the oxygen reduction reaction (ORR) was further explored. This work not only provides novel strategies for the controllable synthesis of hierarchically structured nitrogen-doped porous carbons with excellent ORR activity and stability, but also offers fundamental insights and theoretical guidance for the nitrogen-enriched conversion of lignocellulosic biomass into nitrogen-doped porous carbon materials.

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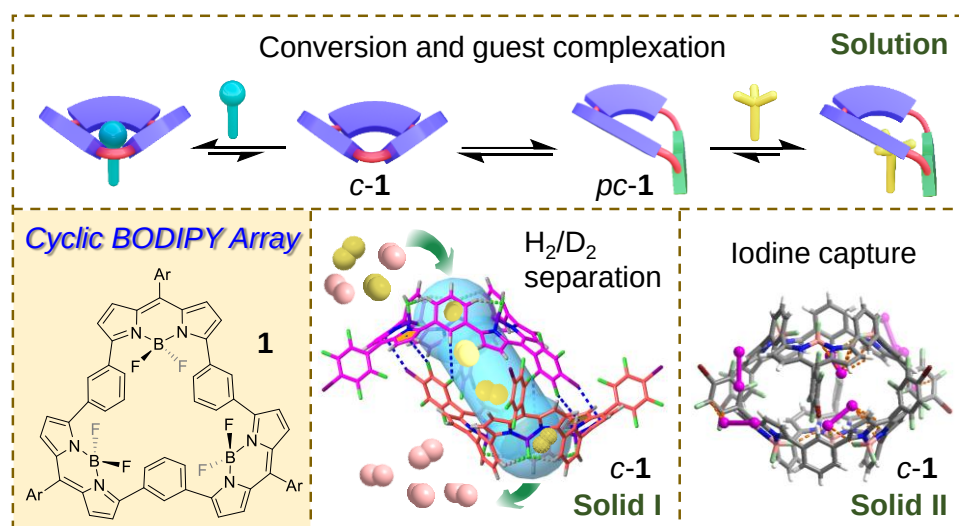
Fungal-driven biomolecular tailoring reconstructs lignocellulosic precursors through enzymatic deconstruction and hyphal integration, generating hierarchical mesoporous carbon architectures with regulated nitrogen configurations.

Cyclic BODIPY Arrays: A Class of Macrocycle-Based Molecular Solids for Hydrogen Isotope Separation and Iodine Capture

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Macrocyclic hosts play a central role in supramolecular chemistry, yet synthetically scalable platforms that combine adaptive guest binding, facile crystallization, and solid-state function remain scarce. Herein, we report a new cyclic BODIPY trimer **1**, composed of three BODIPY units linked by *m*-phenylene spacers. Trimer **1** exists as two interconvertible conformers: cone-shaped *c*-**1** and partial-cone-shaped *pc*-**1**, whose interconversion responds to solvents and guests. *c*-**1** selectively binds neutral guests bearing electron-deficient methyl groups through cooperative C–H···F interactions, while *pc*-**1** preferentially hosts ammonium cations. Gram-scale crystallization affords *c*-**1a** and *c*-**1b** with distinct packing arrangements. Activation of *c*-**1a** produces crystalline *c*-**1a'** with permanent ultramicroporosity, enabling excellent H₂/D₂ separation (IAST selectivity ~1.6 at 1 bar) and effective dynamic breakthrough of D₂/H₂ mixtures. In contrast, amorphous *c*-**1b'** is an efficient iodine adsorbent, with a capacity of 0.75 g/g (8.6 I atoms per macrocycle) and >90% removal of aqueous iodine within 60 min. Single-crystal analysis of the I₂ complex *c*-**1e** reveals iodine binding within capsule-based channels. These results establish cyclic BODIPY arrays as a tunable platform for adaptive molecular solids for separation science.



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Enzymatic Depolymerization of Lignin as Nanoparticles

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Lignin is the second most abundant natural biopolymer on Earth and the largest renewable source of aromatic compounds. Owing to its inherent properties, lignin can be valorized into a wide range of products, including antioxidants, biofuels and aroma compounds such as vanillin¹. However, lignin valorization remains challenging because of its poorly understood solubility in conventional aqueous and organic solvents². Oxidative depolymerization catalyzed by enzymes represents a sustainable alternative to conventional chemical treatments for producing valuable phenolic compounds³. Nevertheless, its efficiency is generally limited by the low accessibility of the lignin to enzymes, enzyme inactivation in organic solvents required for lignin solubilization and condensation of the generated phenolic products.

This work aims to address these problems by transforming polymeric lignin into lignin nanoparticles (LNPs) in hybrid aqueous/green solvent systems to ensure both lignin dispersion and enzyme compatibility.

Preliminary turbidimetry results already demonstrated that kraft lignin nanoparticles can be formed and that the activity of oxidative enzymes such as laccase, manganese peroxidase and horseradish peroxidase is maintained in water/2-methyltetrahydrofuran-3-one mixtures, highlighting the potential of this green, food-grade solvent system for enzymatic lignin depolymerization.

Overall, this project aims to develop a transferable platform for the valorization of diverse lignins, and contribute to the sustainable production of renewable aromatic building blocks for future bio-based industries.

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Iron-Promoted Sulfided NiW Catalysts with Synergistic Ni-Fe-W Interaction for Boosting Hydrodeoxygenation of Lipids

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Lipid-based feedstocks are attractive renewable resources for sustainable fuel production because their effective H/C ratio (~1.8) is close to that of fossil fuels, and selective hydrodeoxygenation (HDO) can convert their long carbon chains into high-value fuel components. Noble metal catalysts exhibit excellent low-temperature activity and alkane selectivity but are costly and easily poisoned. Sulfided NiW/ γ -Al₂O₃ catalysts are cheaper and more S/N-tolerant, but rising Ni prices are increasingly undermining this cost advantage. Iron, an inexpensive and abundant metal, has been explored in HDO such as lignin and phenol [1]. Notably, sulfided Fe-based catalysts combined with Zn can exhibit high hydrodesulfurization activity due to abundant sulfur vacancies and electron-rich Fe species [2], suggesting that Fe plays a beneficial role in sulfided systems. However, whether and how Fe promotes sulfided Ni-W catalysts in lipid HDO remains unclear. This study therefore investigates Fe promotion in sulfided NiW catalysts and the effect of Ni/Fe atomic ratio on catalyst structure and lipid HDO performance [3].

This work develops trimetallic sulfided NiW/ γ -Al₂O₃ catalysts with tunable Ni/Fe ratios. The optimized N1F1W catalyst achieves 99.7% conversion at 340 °C and full conversion at 360 °C with a decarboxylation/decarbonylation (DCO_x) selectivity of 86.2%, significantly outperforming the bimetallic NiW and FeW counterparts. The key advance lies in using Fe to weaken the metal-support interaction, promoting W sulfidation and forming highly stacked WS₂ slabs with abundant edge sites. Fe incorporation also modifies the electronic properties of WS₂. A Ni/Fe ratio of 1:1 creates optimal Ni-Fe-W synergy, enhancing Ni-to-W electron transfer, increasing fully promoted NiWS sites, and facilitating H₂ dissociation and H⁺ spillover. These results demonstrate that the Ni/Fe ratio is critical in balancing reducibility, sulfidation degree, and active phase dispersion to maximize WS₂ edge sites. Iron promotion is therefore a viable, cost-effective strategy for high-performance HDO catalysts, enabling sulfided catalysts with reduced Ni content for sustainable aviation fuel production. Future mechanistic studies combining in situ/operando spectroscopy with theoretical calculations are needed to elucidate the electronic origin of the Ni-Fe-W synergy and provide a molecular level basis for rational catalyst design.

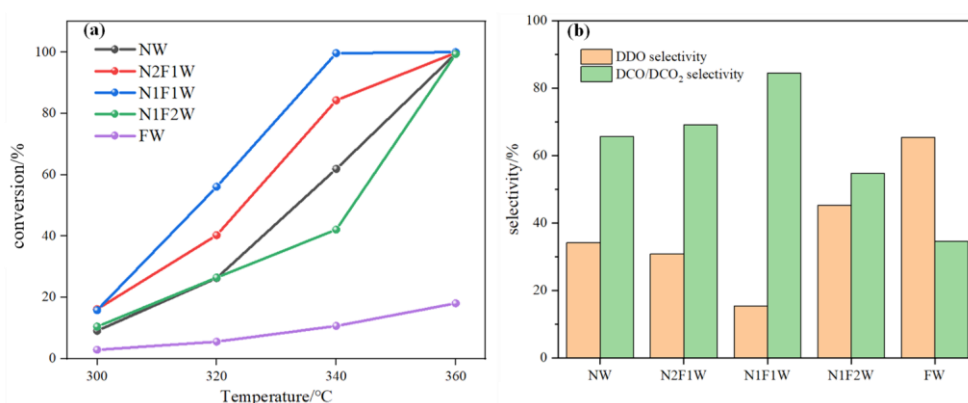


Fig. 1: Evaluation of hydrodeoxygenation activity of the sulfided catalysts for methyl decanoate. (a) Deoxygenation conversion under different catalyst temperatures, (b) Selectivity at 360 °C.

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Photocatalytic β -C-H Functionalization of Alcohol Derivatives via 1,5-HAT

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β -C-H functionalization of alcohols is an attractive transformation to convert abundant substrates into valuable building blocks.^[1] Nagib and coworkers have reported an efficient strategy to achieve the photoinduced β -C-H amination of alcohol based on the conversion of the hydroxyl group into imidate acting as a directing group.^[2] Meanwhile, Hari and coworkers also further developed this strategy by introducing olefins into the substrates, enabling the cycloalkylation of unactivated β -C-H bond.^[3] However, the development of distal C-H bond activation in alcohols is extremely challenging due to the kinetic and thermodynamic inertness of the β -C-H bond toward hydrogen atom transfer (HAT). Herein, we have developed a novel strategy for remote C(sp³)-H functionalization based on oxime carbonates. We synthesized alkyl oxime carbonates as radical precursors 1,5-HAT of the carbonate occurs via energy transfer catalysis, thus generating a new carbon radical and enabling diverse functionalization. Notably, the 1,5-hydrogen atom transfer (1,5-HAT) process of carbonate radicals represents an unprecedented discovery. This protocol provides a novel and effective path to overcome longstanding challenges in site-selective C(sp³)-H functionalization.

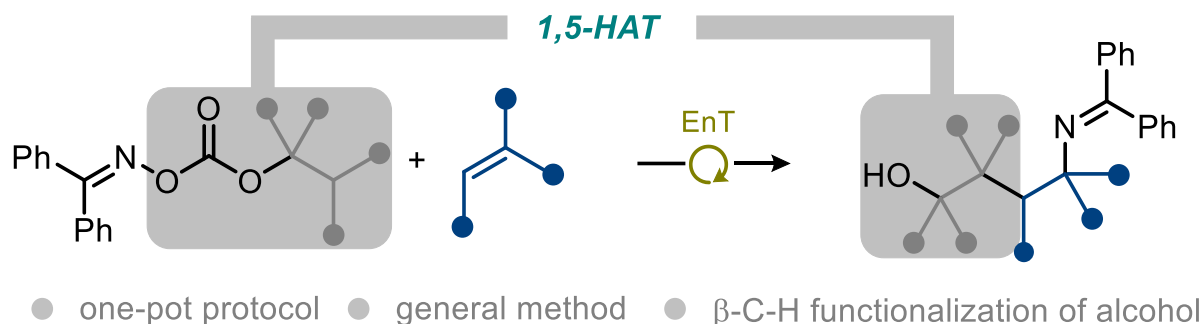


Figure 1. The β -C-H alkylation of alcohols via EnT.

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AI-Driven Design of SrTiO₃:Al Photocatalysts for Overall Water Splitting

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Particulate photocatalysis offers a scalable route to solar hydrogen production through overall water splitting (OWS). Al-doped SrTiO₃ (SrTiO₃:Al) is among the most efficient particulate photocatalysts reported for OWS, with a benchmark solar-to-hydrogen (STH) efficiency of 0.76%. However, its performance is governed by a complex interplay of bulk properties, surface chemistry, cocatalyst interactions, and thermal processing, making conventional trial-and-error optimisation inefficient.

Here, we demonstrate an AI-driven approach for the design and optimisation of SrTiO₃:Al photocatalysts for overall water splitting. By integrating high-throughput experimentation with Bayesian optimisation and data-driven modelling, we systematically explore a multidimensional synthesis and modification space encompassing photocatalyst processing, cocatalyst loading, surface treatment, and thermal conditions. The AI-guided workflow rapidly focuses experimental efforts on promising regions of the design space while continuously learning from experimental outcomes. Beyond performance optimisation, the data-driven approach provides insights into the coupled effects of synthesis and surface modification on photocatalytic activity. This work highlights how AI-guided experimentation can accelerate the discovery and optimisation of particulate photocatalysts and establish a more efficient pathway towards high-performance materials for solar-driven water splitting.

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Characterization of an Antiviral Malagasy Plant Extract for Viral Infection Control

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Virus-borne disease remain a major global public health threat and have caused numerous epidemics throughout human history. The recent COVID-19 pandemic was among the deadliest. As of march 2026, 48,173 COVID-19 cases and 1458 deaths were still reported [1], while only three antiviral treatments are available [2] highlighting the necessity for effective antiviral therapies research. Natural products represent a promising source of antiviral candidates [3–5]. However, their development is often hindered by limited compound availability, plant composition variability, and the high cost of isolation. These constraints recurrently bottleneck research from progressing beyond crude extracts and preliminary in vitro assays. An Initial study on plants from Madagascar led to discovery of a plant extract showing high in vitro activity against SARS-CoV-2. Ongoing work focuses on the chemical and biological characterization of this active extract in order to overcome the recurrent limitation encountered by plant extract. High-resolution mass spectrometry (HRMS) coupled with ultrahigh performance liquid chromatography (UHPLC) and gas chromatography (GC) were used for comprehensive metabolite annotation, while conventional high-pressure column chromatography and nuclear magnetic resonance (NMR) enable compound isolation and structural identification. To date, up to 33 molecules have been isolated and characterized. Fractionated extracts, purified compounds, and commercial analogues are evaluated for antiviral activity against SARS-CoV-2, and other viruses using MTS and luciferase-based assays. Molecular networking workflow based on mass spectral data are investigated. These integrated analyses establish a chemical profile associated with the extract's antiviral potential.

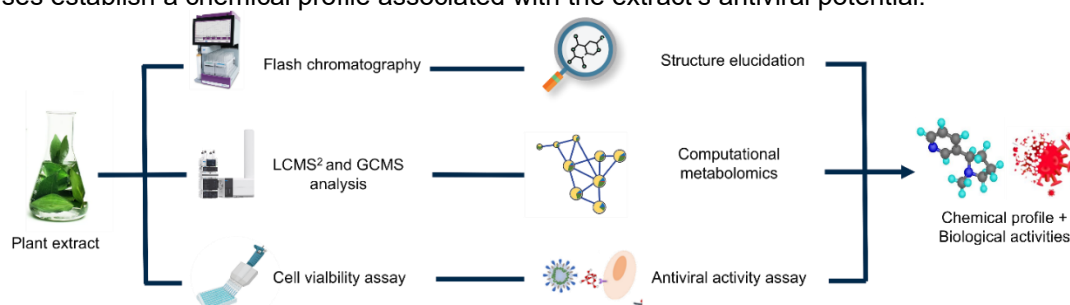


Fig. 1: General methodology

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Informations

Registration / Welcome Desk

Amphitheater I. Joliot Curie, starting Monday October 26, 7:30

Working Language

The working language of the conference is English.
No interpretation is provided in any other language.

Presentations

PPT presentations (only the ppt format, no pdf) must be provided to the chairs in due time before the lecture, preferably the day before or by email to the chairs.
Information will be sent to speakers a few days in advance.

Poster Area

The poster session will take place on Wednesday in the area located near the entrance of the amphitheater. Format A0 posters. Grids will be installed. Pins will be provided.

Certificate of attendance

All registered participants can be delivered a certificate of attendance. Please ask to the desk.

Insurance

The organizers do not accept responsibility for individual medical or personal insurance.

Lunches

Midday buffet lunches will be served near the amphitheater.

Contacts

Invoicing : Mrs Angela Rea Boutrois, email: contact@cpe-formation.fr
Other matters, please contact the conference chairs



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