French-Chinese Conference on Green Chemistry

2018 中法绿色化学 （2018-FC2GChem） 学术交流会议

A better chemistry for a better life 化学使生活更美好

French-Chinese Conference on Green Chemistry
Better Chemistry for a Better Life

FC2GChem

November 28th - 30th 2018

BOOK OF ABSTRACTS

Wednesday Nov 28

Time	chairs	Session	Talks
8:00 – 8:30			Registration
8:30 – 9:10			Opening ceremony
9:10– 10:20	J Yu / M Che	Session 1	IL1 A CORMA / IL2 D ZHAO
10:20 – 10:40			coffee break
10:40– 11:50	JM Tarascon / K Ding	Session 2	IL3 M FONTECAVE / IL4 Y TANG
11:50– 13:10			group picture and buffet lunch
13:10– 14:20	Y Tang / M Lemaire	Session 3	IL5 P MAESTRO / IL6 K DING
14:20– 15:30	D Bortzmeyer / Y Sun	Session 4	IL7 C MICHEL / IL8 S GAO
15:30– 15:50			Coffee break
15:50– 17:00	D Zhao / A Giroir-Fendler	Session 5	IL9 G ROTHENBERG / IL10 Y WANG
17:00– 18:10	P Maestro / Y Lu	Session 6	IL11 Y SUN / IL12 P MONSAN
18:30			Gala dinner
21:30			

Thursday Nov 29

Time	chairs	Session	Talks
8:00 – 9:45	W Bu / M Fontecave	Session 7	IL13 S SUN / IL14 JM TARASCON / IL15 J TANG
9:45– 10:05			coffee break
10:05– 10:40	P Monsan / S Sun	Session 8	IL16 W BU
10:40– 11:10			OC1-2 D DASSONVILLE - XQ WANG
11:10– 11:45			IL17 B SU
11:45– 12:30			Buffet lunch
12:30			Poster session
13:45–15:30	C Michel / H Liu	Session 9	IL18 F DUMEIGNIL / IL19 Y LU / IL20 J LECLAIRE
15:30– 15:50			Coffee break
15:50–17:00	J Tang / B Pora	Session 10	IL21 JF GERARD / IL22 N JACQUEL
17:10–18:10	N Naghavi / B Su	Session 11	Round Table
18:30			Conference dinner
21:30			

Friday Nov 30

Time	chairs	Session	Talks
8:00 – 9:45	F Xiao / C De Bellefon	Session 12	IL 23 X BAO / IL 24 C PINEL / IL 25 P FONGARLAND
9:45– 10:05			coffee break
10:05– 10:40	B Andrioletti / M Pera-Titus	Session 13	IL 26 F POPOWYCZ
10:40– 11:10			OC3-4 X LIU - G POMALAZA
11:10– 12:20	X Bao / E Lecomte	Session 14	IL 27 H LIU / IL 28 S PANNAKAL
12:20– 13:45			Buffet lunch
13:45– 14:55	S Paul / Y Wang	Session 15	IL 29 M JACQUIN / IL 30 W YANG
14:55– 16:05	P Wu / F Popowycz	Session 16	IL 31 F XIAO / IL32 S STREIFF-V ORDOMSKY
16:05– 16:25			coffee break
16:25– 17:35	C Pinel / W Yang	Session 17	IL 33 F JEROME / IL 34 J YU
17:35– 17:50			Closing ceremony
			FC2GChem 2020 Steering committee

> 18h Tuesday 27 Nov Registration

Table of Contents

Bienvenue / 欢迎词 / Welcome

为了传承中国上海与里昂以及所在罗纳-阿尔卑斯大区的友好传统历史，进一步发展合作、互赢的双边关系，我们精心组织召开"化学使生活更美好"为主题的 2018 中法双边绿色化学论坛 (FC2GChem)，诚挚欢迎您参会。

我们真诚感谢所有参会者对本次大会的全力支持和帮助，随后的一周请大家尽情地享受美妙的科学盛宴。

祝研讨会能够给所有参会人员留下美好的回忆。

Dans la continuité des relations historiques d'amitié et de partenariat entre Shanghai et la France, nous sommes heureux de vous souhaiter la bienvenue à l'occasion de la conférence FC2GChem 2018, Conférence Franco Chinoise sur la Chimie Verte, une Chimie Meilleure pour une Vie Meilleure.

Nous vous remercions tous de votre participation et de votre soutien qui permet de proposer un programme scientifique exceptionnel durant cette semaine.

Bonne conférence!

In the continuity of the historical friendship and partnership between Shanghai and France, we are happy to welcome you at the FC2GChem 2018 conference, French-Chinese Conference on Green Chemistry, A better Chemistry for a Better life.

We thank you all for your participation and support which allow us to propose an exceptional scientific program over the week.

Have a nice conference!

Ming-Yuan He (何鸣元), Buxing Han (韩布兴), Yves Queneau, Laurent Bonneviot, Organisateurs du FC2GChem 2018 Shanghai

Préface /（序言）主旨 / Preface

　　由华东师范大学承办的主旨为"化学使生活更美好"的中法绿色化学论坛将于 2018 年 11 月 28 至 30 日在上海举行。该系列会议每两年举办一次，2014 和 2016 年先后在中国上海和法国里昂举行。华东师范大学是第二次承办该会议。

La conférence "Franco-Chinoise sur la Chimie Verte, une Chimie Meilleure pour une Vie Meilleure" ("French-Chinese conference on Green Chemistry, a better chemistry for a better life", FC2GChem), se tient cette année à Shanghai, après l'édition de Shanghai et Wuhan en 2014 et celle de Lyon en 2016.

The "French-Chinese conference on Green Chemistry, a better chemistry for a better life", FC2GChem takes place in Shanghai, after the 2014 edition held in Shanghai and Wuhan, and the 2016 edition in Lyon.

　　本次会议由中国化学会绿色化学分会和法国化学会联合举办，会议云集中法绿色化学学术和产业界跨学科的高端专家130余人。同时会议荣幸邀请到十多位中法以及其他国家的科学院院士就绿色化学研究的最新前沿做大会邀请报告。会议围绕绿色化学研究的前沿，探讨最新的发展，内容包括有机合成、催化、新材料以及理论和计算化学等。组委会最终确定34个高水平的邀请报告、4个口头报告和30余个墙报。本次会议同时得到法国驻中国大使馆、国际著名研发公司、高校和科研院所的鼎力赞助。为了促进中法化学会绿色化学分会的深度合作，双方绿色化学分会的负责人将在本次会议期间举行"中法绿色化学分会合作框架协议"签署仪式。

Organisée sous le patronage de la Société Chimique Chinoise et de la Société Chimique de France, la conférence FC2GChem rassemble à nouveau plus de130 scientifiques Français et Chinois, issus des mondes académiques et industriels, dans un cadre interdisciplinaire impliquant spécialistes de la chimie organique, de la catalyse, de la chimie théorique, de la chimie des matériaux et des procédés. La conférence est honorée de la présence de plusieurs membres des deux académies des sciences et autres institutions prestigieuses.
Avec l'appui de l'Ambassade de France en Chine, de nombreux sponsors institutionnels et privés des deux pays, du Pôle de Compétitivité Axelera (Chimie Environnement), nous sommes heureux de proposer un programme riche d'environ 100 conférences et communications. L'East China Normal University (ECNU) et la ville de Shanghai, qui toutes deux ont tissé historiquement des liens forts d'amitié et de collaboration avec les institutions et régions françaises, sont fières d'accueillir à nouveau cet évènement prestigieux après Lyon en 2016.
La conférence sera l'occasion de sceller la volonté commune d'avancer conjointement vers une chimie meilleure pour une vie meilleure dans un accord réciproque de soutien aux initiatives collaboratives dans le domaine de la chimie verte co-signé par les divisions et groupes de chimie verte et durable de la Société Chimique Chinoise et la Société Chimique de France.

Organized under the auspices of the Chinese and the French Chemical Societies, this FC2GChem conference will again gather more than 130 Chinese and French scientists from industry and academia in an interdisciplinary environment involving, organic, catalysis, materials, process and theoretical chemists. The conference will be honored by the presence of several members of Chinese and French academies and other prestigious institutions.
With the support of the French Embassy to China, of institutions and industrial sponsors from both countries, and of the pole of Competitiveness Axelera (Chemistry and Environment), we are happy to propose a very rich programme with nearly 100 conferences and communications. East China Normal University (ECNU) and the city of Shanghai, whcih have both built strong historical relationships of friendship and collaboration with french institutions and regions, are proud to host again this prestigious event after Lyon in 2016.
The conference will be the opportunity to seal the common will to jointly advance towards a better chemistry for a better life with an offical reciprocal agrrement supporting collaborative initiatives in the field of green chemistry co-signed by the Green and Sustainable divisions and groups of Chinese Chemical Society and the French Chemical Society.

　　化学已经渗透到了生活的方方面面和其它各领域，对现代社会的可持续环境发展起着举足轻重的作用。在这个背景下，化学家有责任发展绿色化学合成方法和创新工艺，最大限度减小化学对环境污染以及对我们赖以生存的地球家园的影响。青年一代科学家代表了绿色化学的未来，本次大会为优秀青年学者提供了一个广阔的交流平台，展示各自在绿色化学各个领域取得的最新研究进展。同时组委会将评定优秀口头报告并颁发中法绿色化学论坛荣誉证书。

La chimie intervient à tous les niveaux de la vie courante (biens manufacturés, produits et matériaux) et dans tous les champs importants de notre société (énergie, construction, transport, nourriture, hygiène, santé, etc.). Dans le cadre d'un développement durable respectueux de l'environnement, cette omniprésence de la chimie dans la vie moderne pousse les chimistes à minimiser son impact sur la pollution tant en ce qui concerne les procédés chimiques que les produits eux-mêmes. C'est le rôle de la **chimie verte** qui consiste à développer des procédés innovants plus propres et des produits moins dangereux, de faible toxicité, de cycle de vie contrôlé, de faible impact autant sur les ressources naturelles que sur l'effet de serre. Cet enjeu est une des priorités des actions bilatérales Franco-Chinoises.

Chemistry intervenes in all the manufactured goods, products and materials of the everyday life and in the most important fields of our society: energy, construction, transportation, foods, hygiene, health, etc.
In the frame of a sustainable development respectful of the environment, such an omnipresence of chemistry in the modern life prompts us to minimizing pollution and hazard of the chemical processes. This is the goal of Green Chemistry that looks for innovative chemical processes and products which show lower impact, notably with respect to users and manufacturers safety, life cycle and low toxicity, natural resources preservation, low greenhouse gas emissions. This topic is a major priority among the bilateral scientific actions and partnerships involving China and France.

Après le prix (FC2GChem-Université de Lyon) qui avait été décerné en 2016 à Lyon à deux jeunes checheurs chinois, l'édition 2018 à Shanghai verra deux jeunes chercheurs Français récompensés et invités à présenter leurs travaux lors d'une communication.

After the prize (FC2GChem-Université de Lyon) awarded in 2016 to two young Chinese scientists, this 2018 edition in Shanghai will see two young French scientists who will present their work in a short communication.

　　我们诚挚感谢所有研究机构、企业和公司以及赞助商对本次大会顺利召开提供的资金资助和人力资源支持，同时也要感谢在绿色化学和催化领域对本次会议作出重要贡献的所有中法研究团体、研究人员以及个人。

Nous remercions l'ensemble des institutions et entreprises qui sont soutenu financièrement l'organisation du congrès, et les personnes qui se sont investies dans la préparation de cet évènement 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.

We thank all institutions and companies which supported the organization of this conference and summer school and all persons who have involved themselves so efficiently for preparing this exceptional event, which aims at showing the importance of the field of Green Chemistry and catalyze interactions within the Chinese and French scientific communities.

Ming-Yuan He（何鸣元）, Buxing Han（韩布兴）, Yves Queneau, Laurent Bonneviot, Organisateurs du FC2GChem 2018 Shanghai

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The FC2GChem Committees are extremely grateful to their partners and sponsors for the financial support to the organization of the conference.

Institutional partners supporting the event:

East China Normal University
Ministère de l'Europe et des Affaires Etrangères - Ambassade de France en Chine
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Laboratoire IMP
Laboratoire IC2MP
Laboratoire E2P2
Laboratoire UCCS

Programme Social / 会议外的其它社会活动 / Social Program

Wednesday November 28, 18:30   Gala dinner

The F2CGChem Gala dinner will be held thanks to the support of the company SOLVAY at the **Restaurant of the Global Harbor HYATT Hotel**.

Address: Hyatt Regency Shanghai Global Harbor
No.718, Ningxia Road, Putuo, 200063 Shanghai
（环球港凯悦酒店，上海市普陀区宁夏路718号）

Transportation from the conference site will be arranged right after the end of the last session, by 18:30 pm. Precise information will be given on site.

Dinner will end by 9:30pm. Dress code is formal casual.

During the dinner, a short informal ceremony will take place for awarding the FC2GChem Prize to two French students:
Delphine DASSONVILLE (Ecole Normale Supérieure de Lyon)
and
Guillaume POMALAZA (Université de Lille)

This follows the 2016 prizes that were awarded to two Chinese students Changhui LIU and Yulin YANG during the 2016 FC2GChem conference in Lyon.

The dinner will be also the place for the ceremony awarding the CNRS Bronze Medal to:
Vitaly V. ORDOMSKY (E2P2L, CNRS-Solvay, Shanghai)

In the presence of
Dr **Claire-Marie PRADIER**, Institut National de Chimie du CNRS,
Dr **François OZANAM**, Comité National de la Recherche Scientifique,
and Dr **Patrick MAESTRO,** Scientific Director, Solvay

Thursday November 29, 18:30   Conference Dinner

The Roundtable dedicated to industrial issues in Green Chemistry will be followed by a conference dinner organized with the support of the Shanghai Key Lab of Green Chemistry and Chemical Processes (GCCP).
The dinner will take place at the **Shunfeng restaurant** (西郊百联店金时代顺风大酒店).

Address: Fourth Floor at Bailian Xijiao Shopping mall,
No. 88 Xianxia Rd., Changning District, 200335, Shanghai
（上海市长宁区仙霞西路88号百联西郊购物中心4楼）

Transportation: Bus transport at the entrance of Yifu hotel at 18:15 on Nov. 29. Precise information will be given on site.
Dinner will end by 9:30pm. Dress code is formal casual.
During the dinner, several addresses will be given by the Conference Chairs.

Scientific Program

Wednesday November 28th

8:30   Opening Ceremony

8:30   Welcome talks
Conference chair talk by Prof. **Buxing HAN**
Welcome address from Dr **Gaétan MESSIN**, Service de la Science et de la Technologie, Ambassade de France en Chine, Consulat Général de Chine à Shanghai

8:40   Welcome addresses by French Institutions representatives:
Dr **Claire-Marie PRADIER**, Institut National de Chimie du CNRS
Prof. **Anne GIROIR-FENDLER,** Deputy Vice-president for International Affairs**,** Université Lyon 1
Prof. **Marie-Christine BAIETTO**, Vice-President for research, INSA Lyon
Dr **Claude DE BELLEFON**, Vice-President for Research, CPE Lyon
Dr **Philippe MAURIN**, Director of International Affairs, ENS Lyon

9:00   Signature of the agreement between CCS and SCF on green chemistry
by Prof **Gilberte CHAMBAUD**, President of the French Chemical Society, on behalf of the board of the Sustainable Thematic Group of the French Chemical Society
and Prof **Mingyuan HE**, Chairman of the Green Chemistry Division of the Chinese Chemcial Society

9:10   Session 1 - Chairs: Jihong YU, Michel CHE

      IL1 **Avelino CORMA**, Instituto Tecnologia Quimica, University of Valencia, Spain
          Designing zeolites for catalytic applications

      IL2 **Dongyuan ZHAO**, Laboratory of Advanced Materials and Collaborative Innovation
          Center of Chemistry for Energy Materials, Fudan University, Shanghai
          Functional mesoporous nanoparticles: from symmetry to asymmetry

10:20   Group picture, Coffee break

10:40   Session 2 – Chairs: Jean-Marie TARASCON, Kuiling DING

      IL3 **Marc FONTECAVE,** Laboratoire de Chimie des Processus Biologiques
          Collège de France, Paris
          Solar fuels: green catalysts for solar-driven conversion of CO_2 to hydrocarbons/alcohols

      IL4 **Yong TANG**, State Key Laboratory of Organometallic Chemistry
          Shanghai Institute of Organic Chemistry, CAS
          Methylene manolate-based reactions and their applications

11:50   Lunch

13:10   Session 3 - Chairs: Yong TANG, Marc LEMAIRE

      IL5 **Patrick MAESTRO**, Solvay, Brussels
          The importance of academia - industry relationship illustrated through some examples

      IL6 **Kuiling DING**, State Key Laboratory of Organometallic Chemistry
          Shanghai Institute of Organic Chemistry, CAS
          Case study on catalytic conversion of CO_2 to value-added organic chemicals

14:20   Session 4 – Chairs: Denis BORTZMEYER, Yuhan SUN

    IL7 **Carine MICHEL**, Laboratoire de Chimie de l'Ecole Normale Supérieure de Lyon, Université de Lyon
Modeling reactivity at the solid/liquid interface: are we there yet?

    IL8 **Shuanhu GAO**, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University
Natural products total synthesis using photo-reactions

15:30   Coffee break

15:50   Session 5 - Chairs: Dongyuan ZHAO, Anne GIROIR-FENDLER

    IL9 **Gadi ROTHENBERG,** Van 't Hoff Institute for Molecular Sciences University of Amsterdam, The Netherlands
Designing effective green routes from biomass to chemicals

    IL10 **Ye WANG**, State Key Laboratory of Physical Chemistry of Solid Surfaces Xiamen University
Solar energy-driven coupling of C_1 molecules into ethylene glycol

17:00   Session 6 - Chairs: Patrick MAESTRO, Yong LU

    IL11 **Yuhan SUN**, CAS Key Laboratory of Low-Carbon Conversion Science and Engineering, Shanghai Advanced Research Institute, CAS
Hydrothermal catalysis to valorize biofeedstocks into high value special chemicals

    IL12 **Pierre MONSAN**, NAPA Center, Ramonville – St-Agne
Recent achievements in industrial biotechnology at TWB

18:30   Gala dinner

Thursday November 29th

8:00   Session 7 - Chairs: Wenbo BU, Marc FONTECAVE

    IL13 **Shigang SUN**, State Key Laboratory of Physical Chemistry of Solid Surfaces Xiamen University
Structure design and property control of fuel cell catalysts

    IL14 **Jean-Marie TARASCON**, Chimie du Solide-Energie, Collège de France, Paris
Materials/ synthesis approaches for better Li(Na)-ion batteries

    IL15 **Jing TANG**, East China Normal University
Precious metal excluded porous carbon-based electrocatalyst for oxygen reduction reaction

9:45   Coffee Break

10:05   Session 8 - Chairs: Pierre MONSAN, Shigang SUN

    IL16 **Wenbo BU**, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University
Inorganic theranostic agents as the tumor microenvironment-mediated nanoplatform for tumour-specific therapy

    OC1 **Delphine DASSONVILLE**, Laboratoire de Chimie, Ecole Normale Supérieure de Lyon
Biocompatible quantum dots loaded dual-color mesoporous silica nanoparticles as a green alternative for biochemical sensing

OC2   **Xu-Qing WANG**, East China Normal University
Rotaxane-branched dendrimers

IL17   **Baolian SU,** University of Namur, Belgium, and Wuhan University of Technology
Zeolite single crystals with ordered and hierarchically interconnected macro-meso-microporosity for green catalysis

11:45   Lunch

12:30   Poster session

13:45   Session 9 - Chairs: Carine MICHEL, Haichao LIU

IL18   **Franck DUMEIGNIL**, Unité de Catalyse et Chimie du Solide (UCCS), Université de Lille
Hybrid catalysis as an innovative way for upgrading biosourced substrates

IL19   **Yong LU**, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University
From nano- to macro-engineering of nanocomposites onto monolithic foam-/fiber-structures: as structured catalysts for process intensification

IL20   **Julien LECLAIRE**, Institut de Chimie et Biochimie Moléculaires et Supramoléculaires (ICBMS), Université de Lyon
Dynamic covalent chemistry of carbon dioxide: opportunities to address environmental issues

15:30   Coffee Break

15:50   Session 10 - Chairs: Jing TANG, Bernard PORA

IL21   **Jean-François GERARD**, Institut des Matériaux Polymères (IMP), Université de Lyon
Synthesis of hybrid organic-inorganic nanomaterials from sol-gel chemistry of silicon alkoxides combined with bio-based polymers, monomers, and building blocks

IL22   **Nicolas JACQUEL**, Roquette Frères, Lestrem
POLYSORB® Isosorbide and its amazing application with polyesters and polycarbonates

17:00   Short break for preparing the roundtable

17:10   Session 11 - Chairs: Negar NAGHAVI, Baolian SU

Roundtable "Sharing the Chinese and French visions on green and sustainable chemistry and on cooperation between universities and industry"

Among topics, a focus will be made notably on Environmental pollution and solutions in the fabrication of industrial catalysts

Will notably contribute to the roundtable (with short talks of 5 min max):
Dr **Xiangjun CAI**, SINOPEC CATALYST CO., LTD.
Dr **Hengli GUO**, Sinopec Shanghai Research Institute of Petrochemical Technology
Dr **Denis BORTZMEYER**, Arkema
Dr **Gary ZHAO**, Solvay
Dr **Bernard PORA**, Roquette
Dr Edith **LECOMTE NORRANT**, Legomedic

All participants will be welcome to contribute in the discussion.

18:30   Conference dinner

Friday November 30th

8:00   Session 12 - Chairs: Fengshou XIAO, Claude DE BELLEFON

    IL23   **Xinhe BAO**, University of Science and technology of China, State Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, CAS
Optimal utilization of carbon resources

    IL24   **Catherine PINEL**, Institut de recherches sur la Catalyse et l'Environnement (IRCELYON), Université de Lyon
Influence of chain length on selective hydrogenolysis of polyols

    IL25   **Pascal FONGARLAND**, Laboratoire de Génie des Procédés Catalytiques (LGPC), Université de Lyon
Compartmented reactors to optimize hybrid catalytic systems involving chemical and enzymatic catalysis

9:45   Coffee Break

10:05   Session 13 - Chairs: Bruno ANDRIOLETTI, Marc PERA-TITUS

    IL26   **Florence POPOWYCZ**, Institut de Chimie et Biochimie Moléculaires et Supramoléculaires (ICBMS), Université de Lyon
Methodological synthetic tools for biomass valorization

    OC3   **Xue LIU**, Shanghai Key Laboratory of Green Chemistry and Chemical Processes, East China Normal University
Structural diversity and functionalization of germanosilites

    OC4   **Guillaume POMALAZA**, Unité de Catalyse et Chimie du Solide (UCCS), Université de Lille
Highly active mesoporous catalyst for renewable 1,3-butadiene from ethanol

11:10   Session 14 - Chairs: Xinhe BAO, Edith LECOMTE NORRANT

    IL27   **Haichao LIU**, Beijing National Laboratory for Molecular Sciences, College of Chemistry and Molecular Engineering, Peking University, Beijing
Selective hydrogenolysis of cellulose and its derivatives to chemicals: catalytic functions and reaction pathways

    IL28   **Steve PANNAKAL**, L'Oreal Research & Innovation, Bangalore, India
L'Oréal's implementation of green chemistry & sustainable process to afford high value botanicals

12:20   Lunch

13:45   Session 15 - Chairs: Sébastien PAUL, Ye WANG

    IL29   **Marc JACQUIN**, Institut français du Pétrole et des Energies Nouvelles (IFPen), Etablissement de Lyon, Solaize
Bio-butadiene manufacture from butandiols

    IL30   **Weimin YANG**, State Key Laboratory of Green Chemical Engineering and Industrial Catalysis, Sinopec Shanghai Research Institute of Petrochemical Technology
Zeolite catalysts for the production of alkylbenzenes: from zeolite synthesis to industrial applications

14:55   Session 16 - Chairs: Peng WU, Florence POPOWYCZ

      IL31   **Fengshou XIAO**, Department of Chemistry, Zhejiang University
               Green synthesis of zeolites and examples for zeolite-based green catalysis

      IL32   **Stéphane STREIFF & Vitaly V. ORDOMSKY**, Eco-Efficient Products and Processes Laboratory (E2P2L), CNRS-Solvay, Shanghai
               E2P2L: an open innovation lab in sustainable chemistry

16:05   Coffee Break

16:25   Session 17 - Chairs: Catherine PINEL, Weimin YANG

      IL33   **François JEROME**, Institut de Chimie des Milieux et Matériaux de Poitiers, Université de Poitiers
               Synthesis of renewable meta-xylylenediamine and alkyl levulinate from biomass-derived furfural

      IL34   **Jihong YU**, State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University
               Advances in zeolite science and application

17:35   Closing ceremony

        Dinner (or transfer to airport for some attendees)

Poster Session

P1   *Bio-inspired manganese mesoporous silica hybrid material as a water compatible antioxidant*
Beltzane GARCIA-CIRERA, Montserrat CORBELLA, Laurent BONNEVIOT, **Belén ALBELA**

P2   *HMF in multicomponent reactions: straightforward routes towards novel fine chemicals*
Weigang FAN, Yves QUENEAU, Florence POPOWYCZ

P3   *OMS as catalytic support in NO and NH_3 oxidation*
Souheila ADJIMI, Jesus-Manuel GARCIA-VARGAS, Sonia GIL, Yanglong GUO, Marc PERA-TITUS, **Anne GIROIR-FENDLER**

P4   *Au-Cu bimetallic catalysts for the selective oxidation of fatty alcohol ethoxylates to alkyl ether carboxylic acids*
Qingyi GU, Yang ZHAO, Wenjuan ZHOU, Raphael WISCHERT, Carine MICHEL, Marc PERA-TITUS

P5   *Non-metallic aerobic oxidation of alcohols over anthraquinone based compounds*
Jingpeng ZHAO, Dan WU, **Willinton Y. HERNANDEZ-ENCISO**, Wenjuan ZHOU, Mickael CAPRON, Vitaly V. ORDOMSKY

P6   *Unveiling the role of choline chloride on furfural synthesis from a highly concentrated xylose*
Shi JIANG, Charlie VERRIER, Changru MA, Yves QUENEAU, Marc PERA-TITUS, François JEROME, Karine DE OLIVEIRA VIGIER

P7   *Single-site carbon-based cun₄ material as a selective electrocatalyst for CO_2 reduction to ethanol*
Dilan KARAPINAR, Huan Ngoc TRAN, Nastaran RANJBAR, David W. WAKERLEY, Nadia TOUATI, Sandrine ZANNA, Dario TAVERNA, Andrea ZITOLO, Frederic JAOUEN, Victor MOUGEL, Marc FONTECAVE

P8   *Reductive amination of biomass-based aldehydes in aqueous solution over versatile NiyAlOx catalysts*
Hangkong YUAN, Jerry-Peng LI, Fangzheng SU, Zhen YAN, **Bright T. KUSEMA**, Stéphane STREIFF, Yongji HUANG, Marc PERA-TITUS , Feng SHI

P9   *Exploring the advances and challenges for innovation in green chemistry for the pharmaceutical world of tomorrow*
Edith LECOMTE-NORRANT

P10   *One-pot synthesis of d-phenylalanine-functionalized multi-walled carbon nanotubes: a metal-free chiral catalyst for the asymmetric electroreduction of aromatic ketones*
Ying-Na YUE, Sheng ZENG, Hui WANG, Shuo WANG, Huan WANG, **Jia-Xing LU**

P11   *Metal – polyamine combined approach towards CO_2 capture and conversion*
Francesca MAROCCO STUARDI, Julien LECLAIRE

P12   *Structure-sensitive and insensitive reactions in alcohol amination over non-supported Ru nanoparticles*
Guanfeng LIANG, Yage ZHOU, Jingpeng ZHAO, Andrei Y. KHODAKOV, **Vitaly V. ORDOMSKY**

P13   *Colloidal tectonics for tandem synergistic pickering interfacial catalysis: oxidative cleavage of cyclohexene oxide into adipic acid*
Bingyu YANG, Loic LECLERCQ, Véronique SCHMITT, **Marc PERA-TITUS**, and Véronique NARDELLO-RATAJ

P14   *Merging metathesis and photochemistry: a sustainable access to heterocyclic structures*
Sophie FEUILLASTRE, Quentin GLENADEL, Youssef NASSAR, Ludovic RAFFIER, Béatrice PELOTIER, Fabienne FACHE, **Olivier PIVA**

P15   *Carbohydrate amphiphiles: resource for biobased surfactants*
Yves QUENEAU, Lianjie WANG

P16   *Electrochemical CO_2 valorization to dicarboxylic acids and propiolactones*
Renate SCHWIEDERNOCH, Mengjia WU, Stéphane STREIFF, Haosheng SHU

P17   *Carbon-based catalytic frameworks for green chemistry*
Thierry SLOT, N. Raveendran SHIJU, Gadi ROTHENBERG

P18   *Regulation of framework titanium siting in Ti-MWW by boron and aluminum incorporation and its effect on the catalytic performance in cyclohexene oxidation*
Zhimou TANG, Yunkai YU, Li LI, Zhen CHEN, Jia WANG, Yueming LIU, Mingyuan HE

P19   *Solventless conditions for the Baylis-Hillman reaction of HMF and GMF*
Lianjie WANG, Mohammed AHMAR, Yves QUENEAU

P20   *Iodization of palladium-supported catalyst for ethers production from bio-derived feedstocks*
Dan WU, Willinton Y. HERNANDEZ-ENCISO, Vitaly V. ORDOMSKY, Andrei Y. KHODAKOV

P21   *Addressing some fundamental questions in alcohol amination*
Zhen YAN, Lin FANG, Bright KUSEMA, Marc PERA-TITUS

P22   *Fluorescent metallosupramolecular functional materials*
Lin XU and **Hai-Bo YANG**

P23   *The p band intermediate state (PBIS) tailors photo-luminescence emission at the nanoscale interface*
Tai-qun YANG, **Kun ZHANG**

P24   *Reaction-induced CoO@Cu$_2$O nanocomposites in-situ onto SiC-foam for gas-phase oxidation of bioethanol to acetaldehyde*
Guofeng ZHAO, Songyu FAN, Xiaxia PAN, Pengjing CHEN, Ye LIU, Yong LU

P25   *Mild reduction of phosphine oxides by phosphites*
Peng LI, Raphael WISCHERT, **Jianxia ZHENG**, Pascal MÉTIVIER

P26   *Utilization of CO_2 as a C1 building block for the synthesis of cyclic carbonates and carbamates,*
Xiao-Tong GAO, Shi-Liang XIE, **Feng ZHOU**

P27   *Pickering-assisted catalysis for efficient solvent-Free oxidative desulfurization using H_2O_2 and polyoxometalates*
Wen-Juan ZHOU, Yichong CHENG, Fangzheng SU, Qingyuan LI, Marc PERA-TITUS

P28   *Valorization of biomass ketoses to surfactants through aldolisation,*
Biwen ZHU, Guorong CHEN, Nicolas DUGUET, Marc LEMAIRE

P29   *Natural products total synthesis and medicinal studies*
Shuanhu GAO

P30   *Interfacial interaction regulated CO oxidation over transition metal atoms on hexagonal boron nitride*
Xin LIU, Hongdan ZHU, Meng XU, Roberto LINGERRI, Changgong MENG, Gilberte CHAMBAUD

Abstracts

Invited Lectures

Designing zeolites for catalytic applications

Avelino CORMA

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Different zeolite synthesis concepts have resulted in a better understanding of the synthesis mechanisms and in the development of new structures and applications. From the point of view of the zeolitic catalysts, previous knowledge and intuition allows to select, among different structures, those that may be useful to catalyse a certain reaction. The main criteria of selection is based on pore dimensions and pore topology. Then, when a first selection has been made, further improvements can be achieved by adapting chemical composition and crystallite size.

There is no doubt that it would be desirable to directly synthesize a zeolite that fulfils the geometrical requirements for a given reaction, while locating the active sites at the required framework position, in such a way that an optimum matching between the zeolite and the reaction transition state will be stablished. This should drive into a minimization of the activation energy of the process and, specially, a maximization of the selectivity to the desired product.

Besides discussing synthesis methods for preparing new zeolites, based on former concepts, and showing their possibilities for adsorption/separation and catalysis, a methodology for the "*a priori*" synthesis of zeolites directed to specific applications will be presented. Within this methodology, a reaction mechanism for the catalytic process is first postulated, that includes a potential reaction transition state. Then, a mimic of such a transition states (TS) is synthesized as Organic Structure Directing Agent (OSDA) and the zeolite synthesis is carried out certainly using previous existing knowledge on the influence of gel composition time and temperature, for performing the synthesis. The methodology not only should be useful for directing into structures with pores and cavities adapted for reaction TS stabilization, but also should direct the location of framework charge compensation for a given catalytic reaction.

It will be shown that, following the above methodology, it is possible to prepare zeolites with improved activity and selectivity than the ones used today for chemical and petrochemical processes during alkylaromatics transformations, and for cracking processes directed to maximize olefins productions.

IL2

Functional mesoporous nanoparticles: from symmetry to asymmetry

Xiaomin LI and Dongyuan ZHAO*

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In addition to conventional symmetric structured hybrid nanomaterials such as core-shell, yolk-shell *etc.*, a new generation of anisotropic composite nanoparticles with asymmetric nanostructures on geometry and chemical properties have attracted wide concern because of their unique characteristics and potential applications. Compared with the conventional symmetric hybrid materials, the structural asymmetry is ideally suited for multiple-guests conjugation and loading at the single-particle level. The function of each component can work independently without interaction with each other to realize the truly "multifunctional entities". Here we present the development and progress for the synthesis of the asymmetric ordered mesoporous nanocomposites. A series of new synthesis approaches have been developed based on the oriented assembly strategy in our group, including the anisotropic growth of ordered mesoporous channel, anisotropic encapsulation route, surface-charge-mediated selective encapsulation approach, degradation-restructuring induced anisotropic epitaxial growth, *etc.* Series of novel multi-level architecture functional mesoporous nanocomposites with asymmetric nanostructures on geometry, chemical composition, surface property, and functionality *etc.* were developed, including Janus, Single-Hole Hollow, Diblock Janus, Triblock Janus *etc.* Most importantly, the obtained asymmetric nanocomposites possess unique multiple independent surfaces, compositions, functions *etc.*, which are ideal for selectively multiple-component conjugations, loading, and smart delivery system designing *etc.* The obtained asymmetric functional mesoporous materials with uniform and controllable pore channels, high surface area and open frameworks, showing great potential applications on catalysis, adsorption, and biomedicine.

Fig. 1: Scheme illustration of the symmetric and asymmetric functional mesoporous materials.

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Solar fuels: green catalysts for solar-driven conversion of CO_2 to hydrocarbons/alcohols

Marc FONTECAVE

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Conversion of carbon dioxide into hydrocarbons and alcohols using solar energy is an amazingly attractive strategy for storing such a renewable source of energy into the form of chemical energy (a fuel). This can be achieved in a system coupling a photovoltaic (PV) cell to an electrochemical cell (EC) for CO_2 reduction. To be beneficial and applicable, such a system should use low-cost and easily processable photovoltaic cells as well as "green" catalysts and display minimal energy losses associated with the catalysts at the anode and cathode and with the electrolyzer device. Here we describe a series of original and efficient Cu-based catalysts for water oxidation at the anode [1] and for CO_2 reduction into either ethylene (or ethane) or ethanol at the cathode [2] as well as Fe-based catalysts for the conversion of CO_2 into CO [3]. Furthermore, we report a reference low-cost PV-EC flow system for CO_2 reduction to hydrocarbons working with a large solar-to-hydrocarbon efficiency, setting a new benchmark for an inexpensive all earth-abundant PV-EC system [2] (Figure 1).
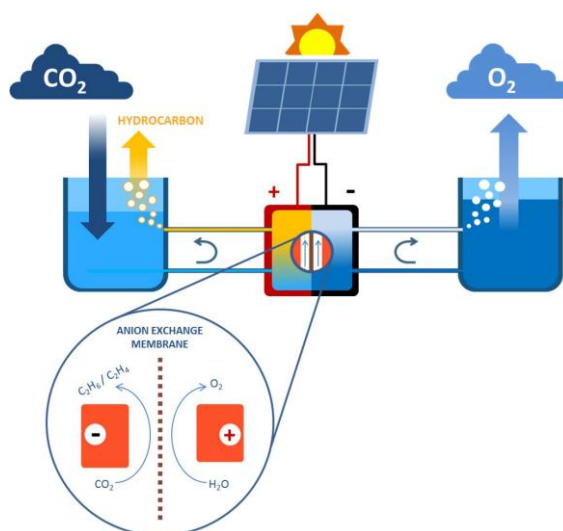
Fig. 1: a PV-EC flow system for light-driven CO$_2$ conversion to hydrocarbons

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IL4

Methylene manolate-based reactions and their applications

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Synthetic efficiency is of the most importance in modern organic synthesis, including the three key elements of a reaction: the atom economy, the step economy, and the selectivity.[1-2] One of the efficient methods in the synthesis of complex molecules is developing new reactions for the rapid construction of the molecule core from simple and readily available materials. Recently, we developed a direct and efficient method for the highly stereoselective construction of tetracyclic spiroindoline skeletons via intramolecular [3 + 2] annulations of cyclopropane-1,1-dicarboxylates with indoles.[3] In line with our interest in developing concise synthesis of polycyclic indoline motifs, we found that simple tryptamine derived-enamines could react with methylene malonate in a tandem fashion, allowing one-step and gram-scale access to the core skeleton of the malagashanine alkaloids. In addition, this new reaction is successfully applied for the synthesis of 11-demethoxy-16-epi-myrtoidine, leading to a new and concise and rapid access to malagashanine alkaloids and their analogues (Scheme 1). In this presentation, I will report this reaction and related.
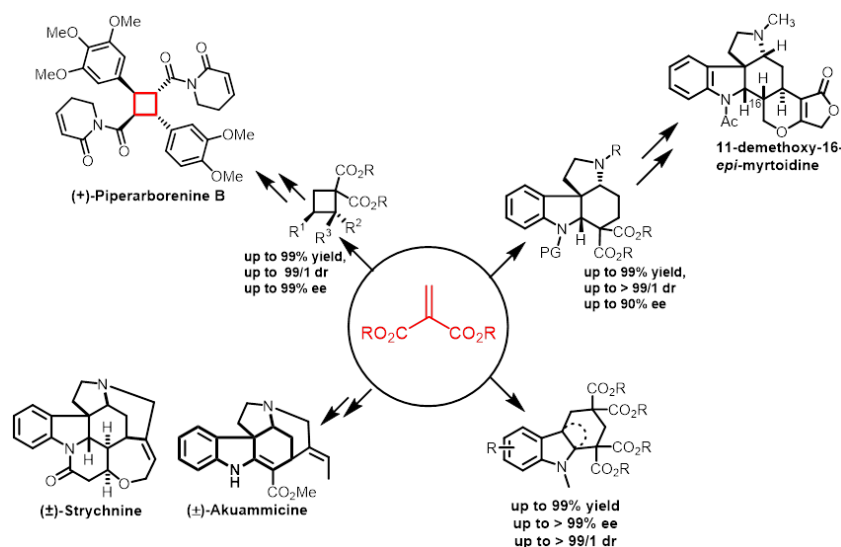
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The importance of academia - industry relationship illustrated through some examples

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A good relationship between the industrial world and academic is key for future innovation. As a matter of fact, innovation has his early roots in the development of knowledge and scientific discoveries that are mainly done in the academic world, provided that relevant and faithful exchanges are further done between industry and academia, in order to transfer this knowledge to application, both incremental and breakthrough.

The key here is to learn to work together and to respect the time scales and horizons that are significantly different between the two worlds, but that must be put in perspective together.

I will illustrate how Solvay, through its long term commitment and experience in the area, establishes a continuum from Science to Innovation, through connection with the academic world, and particularly with joint teams, through connection with start-ups, and finally with end-users

Examples will be given in the areas of materials science, soft condensed matter, chemistry and catalysis, and new technologies for research like robotics and microfluidics.

IL6

Case study on catalytic conversion of CO_2 to value-added organic chemicals

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From the viewpoint of synthetic chemistry, the utilization of CO_2 as a feedstock for the production of value-added organic chemicals might provide an option for the recycling of carbon.[1] Therefore, the development of a new reaction pathway and practical catalyst systems for the production of fine chemicals from CO_2 is highly required.[2] In this talk, two case studies on catalytic conversion of CO_2 to value-added organic chemicals will be presented, including PNP-Ru[II] catalyzed homogeneous hydrogenation of cyclic carbonates (which can be readily available from CO_2 and epoxides) for production of methanol and the corresponding diols[3] and direct transformation of CO_2 to DMF via ruthenium-catalyzed hydrogenative *N*-formylation of the corresponding amine.[4]
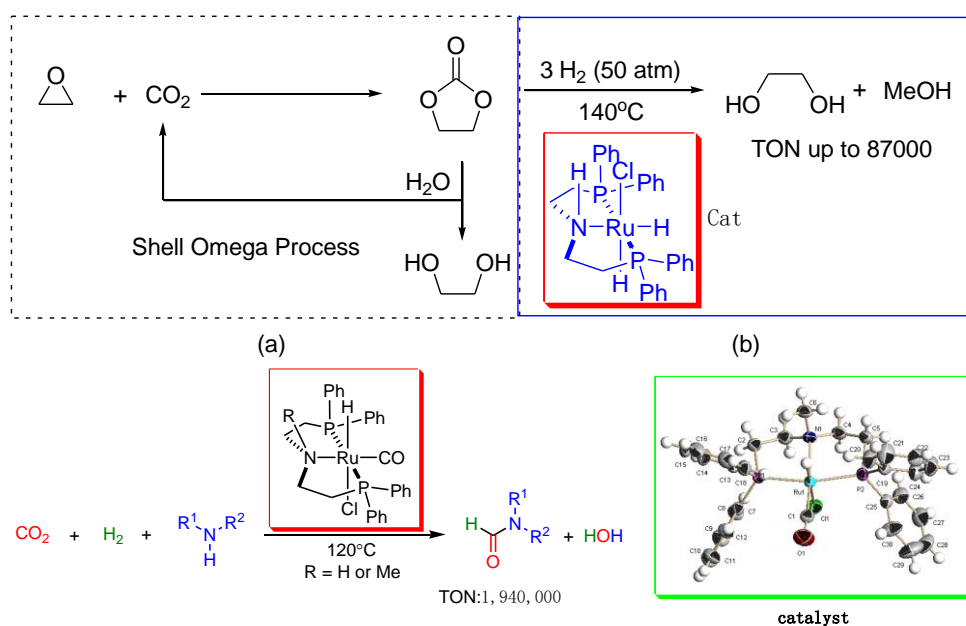
Fig. 1. Catalytic conversion of CO_2 to methanol or DMF

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Modeling reactivity at the solid/liquid interface: are we there yet?

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To describe reactions occurring at the solid/water interface is currently one of the major challenges in modeling in Heterogeneous Catalysis in particular in the context of Green Chemistry and biomass valorization where water is a natural solvent. Modeling such an interface requires a proper depiction of the water solvent together with an adequate description of the surface state. Several approaches are available nowadays in the literature, from continuum models to a full explicit description of the liquid water.[1]

We have recently shown that continuum models are key to a proper description of reactions occurring at the electrochemical interface on the formic acid oxidation into CO_2.[2] They also open the door to a proper inclusion of the effect of co-adsorbed anions in thermal heterogeneous catalysis.[3] In both cases, charges are involved and the electrostatic contribution in the major one. When H-bonding between the liquid water and the reactant or intermediate is crucial, continuum models are not sufficient and an explicit inclusion of water molecule is a necessity. As a first step, micro-solvation can be an effective approach that allowed us to interpret solvent effect in the conversion of levulinic acid into γ-valerolactone.[4] Moving to a full description of reactivity the water/metal interface is still beyond a full complete DFT approach provided the minimal size of the periodic cell that is necessary and the minimal sampling required. Nevertheless, being less demanding, inspecting transformations occurring at oxide/water interface is now reachable, as illustrated by our recent work on the stability of γ-alumina in water.[5]

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IL8

Natural products total synthesis using photo-reactions

Shuanhu GAO

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The chemical synthesis of structurally interesting and biologically relevant natural products has served as a driving force for developing new methodologies, testing the scope of existing synthetic methods. It also provides the platform for the further identification of their specific biological targets and mechanistic mode of action. Our research interests are devoted to develop synthetic useful methodologies to address natural target molecules that have novel molecular structure, potent biological activity, and the potential for mechanistic studies.

In this presentation, I will introduce our recent progress in the development of photo-induced reactions, including photoenolization/Diels–Alder (PEDA) reaction [1-2] and photo-*Nazarov* [3-4] and their synthetic applications in natural products total synthesis.
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taiwaniaquinol B

gracilamine

oncocalyxone B

BABX

R =H   Mycoleptodiscin A
R =OH Mycoleptodiscin B

benastatin J
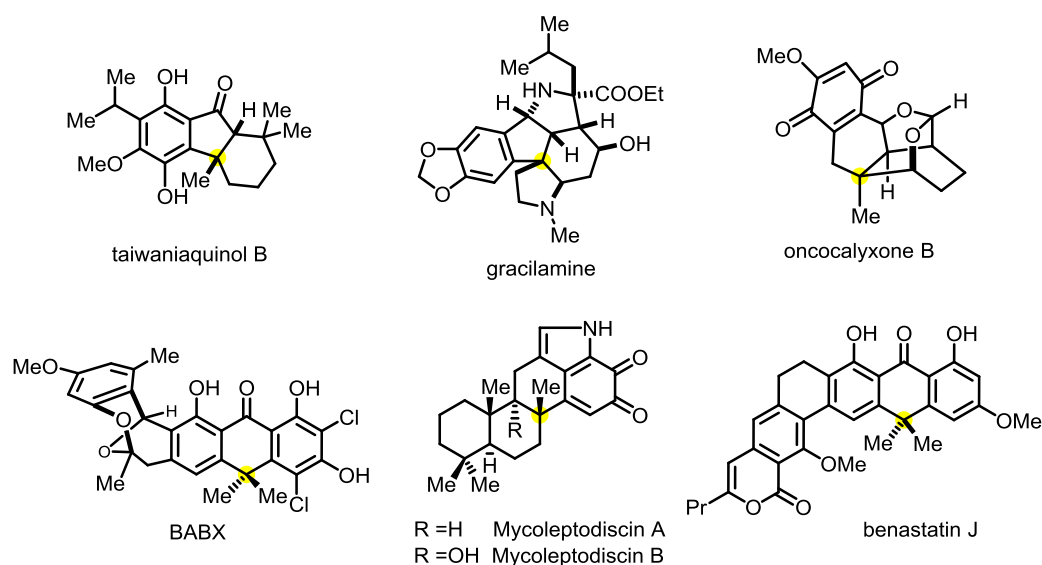
Fig. 1: Target Molecules

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IL9

Designing effective green routes from biomass to chemicals

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Converting lignocellulosic biomass to chemicals is a 'hot topic', and rightly so. Agricultural biomass is our largest source of renewable carbon, enough to make all the world's polymers, agrochemicals and fine-chemicals [1]. Yet while end-users require the same chemical products, the chemical industry faces different challenges in the switch to biomass feedstocks. Crude oil is made of alkanes, which must be functionalized to intermediates and fine-chemicals. Conversely, biomass is over-functionalized with esters, ethers, and carboxylic acids. This means that starting from biomass presents very different catalytic challenges.

In this lecture, I will present how we design catalysts for efficient conversion of biomass platform molecules, using as a hands-on example our most recent work on the catalytic conversion of lactates to pyruvates [2-4]. Focusing on practical solutions, I will show how appropriate catalytic tools can be found using fundamental insights.
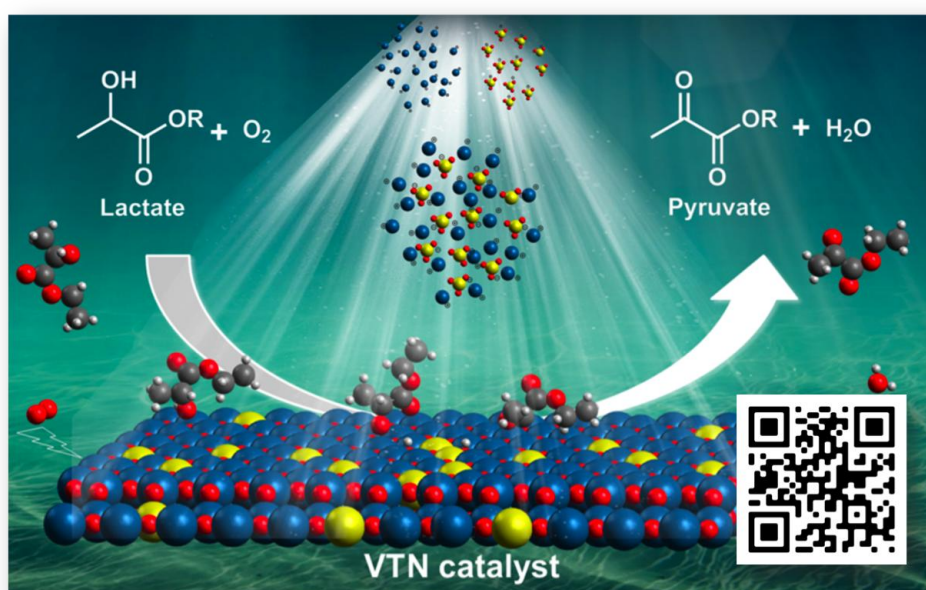
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IL10

Solar energy-driven coupling of C1 molecules into ethylene glycol

Ye WANG

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The C–C bond formation is a core reaction in synthetic chemistry. In particular, the coupling of C_1 molecules such as CH_4, CH_3OH, $HCHO$, CO and CO_2 into important C_2 compounds such as C_2H_4, CH_3CH_2OH and $HOCH_2CH_2OH$ (ethylene glycol, EG) is of high significance. Photocatalysis may provide a promising methodology for C-C coupling under mild conditions. Thus far, only a few studies have succeeded in the coupling of smaller molecules [1]. Here, I present our recent work on the development of new photocatalytic routes for green synthesis of EG by coupling of HCHO and CH_3OH.

$BiVO_4$ and Bi_2WO_6, two visible-light responsive semiconductors with conduction-band minimum higher than the redox potential of HCHO/EG but lower than that of H_2O/H_2, efficiently catalyzed the reductive coupling of HCHO to EG in aqueous solution [2]. The fabrication of $BiVO_4$ single crystals with an equal fraction of exposed {010} and {110} facets, toward which photogenerated electrons and holes migrate separately, enhanced EG formation. The loadings of $Pt@MoO_x$ and MnO_x co-catalysts onto the {010} and {110} facets, respectively, further accelerated C-C coupling (Figure 1a) [3].

We discovered that CdS is a unique photocatalyst in preferential activation of C-H bond in CH_3OH without affecting its O-H group, forming EG via $\cdot CH_2OH$ radical intermediate under visible light [4]. DFT calculations demonstrated that the preferential C-H activation is driven by photogenerated holes via a CPET (concerted proton-electron transfer) mechanism on CdS surfaces. The loading of MoS_2 nanofoams onto CdS nanorods improved EG selectivity to 90% (Figure 1b). The high EG selectivity was sustained in the long-term reaction by designing a process-intensified reactor with EG separation ability. The quantum yield of EG was >5% at wavelength ≤ 450 nm.
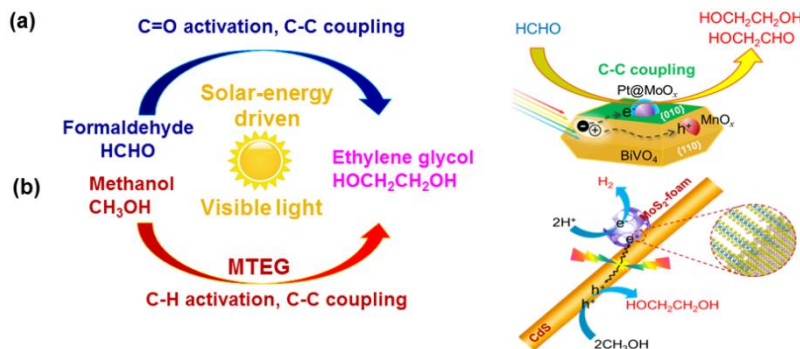
Fig. 1: Photocatalytic coupling of HCHO (a) and CH_3OH (b) into EG under visible-light.

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Hydrothermal catalysis to valorize biofeedstocks into high value special chemicals

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Hydrothermal catalysis is an important thermochemical conversion process that is used to valorize biofeedstocks into valuable platform chemicals over various heterogeneous/homogeneous catalysts [1]. Such an approach has significant potential for any type of fresh biofeedstocks with high moisture content and usually performed in water at 150-300 degrees C under pressures of 4-8 MPa. Thus, one-pot hydrothermal catalytic conversion of sugar-rich microalgae as fresh biofeedstocks to important and valuable platform chemicals, such as glycols (1,2-propanediol and ethylene glycol) 5-hydroxymethylfurfural (5-HMF) and lactic acid (LA) were carried out under mild reaction conditions over heterogeneous catalysts at SARI [2-4]. Based on the HPLC, GCMS and ^{13}C NMR analysis, complete reaction networks for hydrogenation, dehydration and hydrolysis reaction were systematically investigated to gain insights into the activation of the C-O and C-C bonds in the absence of molecular hydrogen or oxygen [5]. The roles of the active components, promoter and support of catalysts in the formation of chemicals were investigated to reveal the structure-activity relationship [6], along with the mechanism further illustrated by density functional theory (DFT) calculations. To have a deep insight into the roles of water for the hydrogenation, dehydration and hydrolysis reaction, the physicochemical properties of water and the interactions of water with biofeedstocks especially for the hydrogen transfer reaction were also discussed by isotope method. The hydrothermal catalysis sounds the prospective future, but it is necessary to establish a baseline to develop key process models and to perform a techno-economic assessment to get a better sense of the viability of the technology in future.

Key Words: Hydrothermal Catalysis; Biofeedstocks; Chemicals; Mechanism; Water
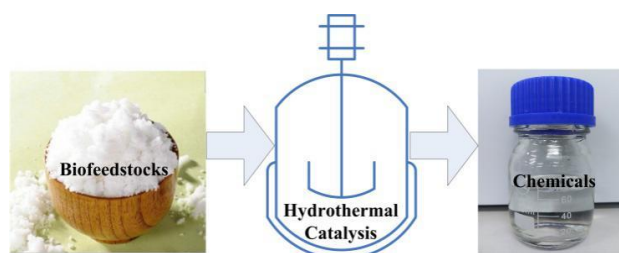

Fig.1 Hydrothermal catalysis of biofeedstocks into platform chemicals

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IL12

Recent achievements in industrial biotechnology at TWB

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Toulouse White Biotechnology (TWB) is a public Joint Service Unit managed by INRA (National Institute for Agricultural Research) under the triple supervision of INRA, CNRS (National Center for Scientific Research) and INSA (National Institute for Applied Sciences). Its mission is to help private companies to address the challenge of climate change. TWB is working hand in hand both with industry and top scientific level academics in view to develop sustainable processes based on the biotransformation of renewable resources. TWB has built a high performance interface to accelerate the transfer of innovative scientific results into efficient products and processes, as well as the offering of state of the art scientific answers to the strategic industrial issues.

Since 2012, TWB has managed 105 R&D projects, among which 45 projects with private companies for a total amount of 21 M€. Several projects developed at the industrial and/or industrial pilot scale will be described:

- Flavor ingredient production;
- Amibe liquid culture;
- Chemical intermediate production;
- Hydrophobic compound glycosylation;
- Polysaccharide enzymatic synthesis.

Twb is presently hosting four start-up companies (EnobraQ, Pili, MicroPep, BFC) and has contributed to the rising of ca. €100m venture capital funds by such SMEs.

Structure design and property control of fuel cell catalysts

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Electrocatalyst is the key in developing electrochemical energy conversion and storage, and in green chemistry of electrosynthesis using electrons as reagents. The activity, selectivity and stability of electrocatalysts depend strongly on both their bulk and surface structures. Therefore, the rational design and control-synthesis of electrocatalysts are the central subjects and are mainly focused on the structure-catalytic functionality of nanomaterials, since practical electrocatalysts often consist of nanosized particles substrated on conductive support materials. The bulk structure of nanoparticles could be tuned by changing their chemical nature and composition, while tuning their surface structure is more difficult, especially the high catalytic activity corresponding to high surface energy that leads to disappear thermodynamically the nanoparticles during their growth. This communication reports our recent progresses in three aspects of rational design and controlled synthesis of fuel cell catalysts:

(1) Tuning the surface atomic arrangement of well-defined metal nanocatalysts. Well-defined Pt, Pd, Rh and Cu nanocrystals enclosed by high-index facets have been successfully obtained by developing electrochemically shape-controlled synthesis, such as tetrahexahedral nanocrystals (THH NCs) enclosed with {hk0} high-index facets, trapezohedral nanocrystals (TPH NCs) with {hkk} high-index facets, triambic icosahedral nanocrystals (TIH NCs) with {hhl} high-index facets and hexoctahedral Pt NCs (HOH NCs) with {hkl} facets. As the high-index facets contain a high density of active centers, these NCs of high surface energy exhibit much higher electrocatalytic activity than commercial catalysts for small organic fuel oxidation reactions.

(2) Tuning the electronic structure of Pt- and Pd-based nanocatalysts. The electronic structure of NCs catalysts has been tuned either by surface decoration using foreign adatoms, or through alloying Pt and Pd with other metals. Different adatoms such as Bi, Ru and Au were used to decorate the THH Pt NCs, and both THH and TPH Pt-based alloy nanocatalysts were prepared by electrochemically shape-controlled method. The THH and TPH alloy NCs preserve the high-index facets while hold a synergy of electronic effect that enhances further the electrocatalytic activity.

(3) Synthesis of non-precious metal electrocatalysts with high ORR activity. Fe/N/C is a promising electrocatalyst for oxygen reduction reaction (ORR). By well-screening the precursors, optimizing the synthetic procedures and surface decoration, the resulted Fe/N/C exhibits high activity and stability in both acid and alkaline conditions. The results demonstrated that the Fe/N/C-SCN catalysts in a proton exchange membrane fuel cell (PEMFC) can output a maximum power density of 1.03 W cm^{-2}, and by using 2-aminothiazole as precursor the synthesized S-doped Fe/N/C catalyst with graphene nanosheets can yield a peak power density of 164 mW cm^{-2} in an anion exchange membrane fuel cell (AEMFC).

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IL14

Materials/ synthesis approaches for better Li(Na)-ion batteries

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Research's progresses in rechargeable batteries are driven by ever increasing demands for portable electronic devices as well as for powering electric vehicles and providing load-leveling for mass storage of renewable energy. Li-ion batteries are the systems of choice for the aforementioned applications. Therefore, for this to fully happen, materials with higher energy densities while being sustainable and low cost must be developed. The challenges for chemists are enormous and this calls for new sustainable materials, new concepts as well as new chemistries together with a mastering of electrochemistry. These different aspects will be addressed through this presentation.

Firstly, regarding new concepts, we will show how the discovery of a new Li reaction mechanism [1-2-3] that involves the anionic network with the reversible formation of dimers (O-O) represents a transformational approach for creating electrode materials with exacerbated capacities. Secondly, concerning new chemistry, our new findings with the Na-ion chemistry [4-5] which enlists novel materials/electrolyte designs together with the assembly of 18650 prototypes will be presented. Lastly, the implementation of electrochemical approaches towards the better understanding of alternative Li (Na) -air battery technologies will be shown. Third, some future aspects of battery research dealing with sensing-self-healing will be discussed.

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IL15

Precious metal excluded porous carbon-based electrocatalyst for oxygen reduction reaction

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Considering global warming and other environmental issues, the new-type energy devices, such as fuel cells and lithium-air batteries have been the focus of research. Porous carbons have been considered as promising electrode materials due to their excellent virtues such as low cost, designable porous framework, and good electrical conductivity. Lots of synthetic methods have been developed for fabrication of functionalized nanoporous carbon materials with high specific surface areas, tunable and accessible nanopores, high degree of graphitization, and heteroatoms doping. Meanwhile, carbon-based materials with morphologies ranging from zero to three dimensions were also elaborately controlled to achieve better properties for electrochemical applications.

In this report, I will talk on the synthesis of precious metal excluded porous carbon-based electrocatalyst for oxygen reduction reaction by integrating hard-template and soft-template methods (Fig.1). First, metal-free nitrogen-doped mesoporous carbon nanospheres with large and tunable mesopores were designed and successfully prepared.[1] The relationship between the pore size and electrochemical properties were investigated carefully. Second, hollow mesoporous nanoarchitectures composed of ultrafine metal carbide nanoparticles on N-doped carbon nanosheets were explored as an efficient oxygen reduction reaction catalyst.[2] Finally, atomically dispersed non-precious metals were introduced into the nitrogen-doped carbon frameworks to achieve a much higher activity for oxygen reduction reaction which is even close to the benchmark of Pt/C catalyst in alkaline electrolyte.[3]
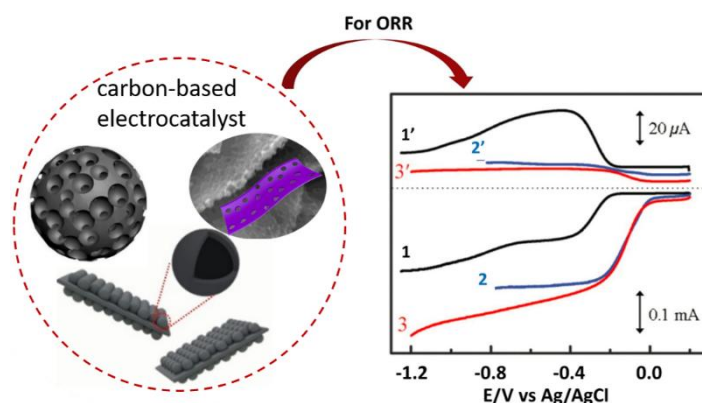
Fig. 1: Carbon-based electrocatalyst for oxygen reduction reaction. The number of 1-3 in right figure represent the pure carbon, heteroatom-doped carbon and Pt/C, respectively.

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IL16

Inorganic theranostic agents as the tumor microenvironment-mediated nanoplatform for tumour-specific therapy

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In this talk, I will focus on the latest progresses of our group on a variety of inorganic theranostic agents as the tumor microenvironment-mediated nanoplatform for the tumour-specific therapy [1]. First, I will offer a thorough description of chemodynamic therapy (CDT), which is defined as the disproportionation of hydrogen peroxide (H_2O_2) through an intratumoral Fenton reaction. Such an endogenous chemical energy to generate cytotoxic·OH could substantially surmount the limitations of penetration and nonspecificity [2-4]. Then, I will introduce the specific cancer-starving therapy. We provides a compelling proof-of-concept for the use of PVP-modified Mg_2Si nanoparticles as potential candidates for use as a tumor-targeted deoxygenating agent. This cancer-starvation therapy avoids the poisoning of normal/cancer cells by toxic drugs, and largely reduces the toxic side effects to normal cells and tissues, featuring high therapeutic biosafety [5].
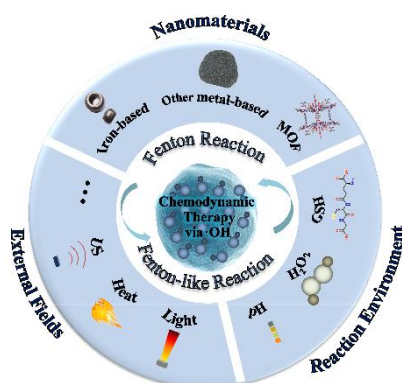
Fig. 1: Chemodynamic Therapy: Tumour Microenvironment-Mediated Fenton Reaction

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Zeolite single crystals with ordered and hierarchically interconnected macro-meso-microporosity for green catalysis

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As a size and shape selective catalyst, zeolites are widely used in petroleum and fine chemicals processing. However, their small micropores severely hinder molecular diffusion and are sensitive to coke formation. Hierarchically porous zeolite single crystals with ordered and tunable multimodal porosity at macro-, meso- and micro-length scale, full interconnectivity and high thermal and hydrothermal stability offer the ideal solution [1-7]. However, their synthesis remains challenging. We report a versatile and up-scalable, in-situ, bottom-up confined zeolite crystallization process to achieve these superior properties. The significantly improved mass diffusion properties of our zeolites with porous hierarchy, and robust single crystalline nature allow highly reduced coke formation, endowing them with enhanced catalytic activities and cycle time, and reduced deactivation rate in bulky-molecule reactions and methanol to olefins process.

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IL18

Hybrid catalysis as an innovative way for upgrading biosourced substrates

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Hybrid catalysis, a direct combination of biocatalysis and chemocatalysis could yield innovative solutions in the field of biorefineries by straightforwardly merging the advantages of both technologies, rather than sequentially carrying them out. We propose two new conceptual pathways involving hybrid catalysis to overcome limitations resulting from the enzymatic glucose isomerase thermodynamic equilibrium between glucose and fructose, which is a key step when subsequently targeting HMF as a product.[1]
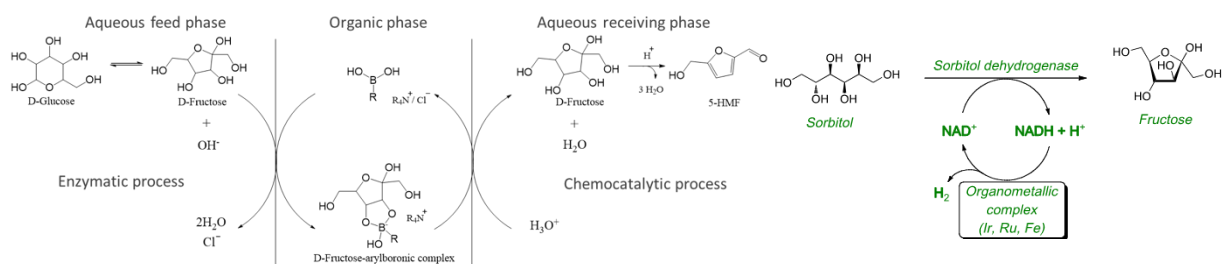
Fig. 1: Complexation/transport strategy   **Fig. 2: Hybrid isomerization**

These concepts, which will be notably described during the present lecture, are based on a complexation/transport strategy and a hybrid isomerization, respectively:

- Simultaneous implementation of glucose isomerase and of fructose to HMF dehydration chemocatalyst in a multiphasic way involving fructose complexation and transport[2] (Fig. 1);
- A route through sorbitol avoiding enzymatic isomerization, in which sorbitol - readily obtained by glucose hydrogenation - is further enzymatically converted to fructose with an *in situ* cofactor regeneration using an organometallic complex[3] (Fig. 2).

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IL19

From nano- to macro-engineering of nanocomposites onto monolithic foam-/fiber-structures: as structured catalysts for process intensification

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Structured catalysts and reactors (SCRs) technology is an inviting avenue for process intensification. Great efforts and intensive studies have been devoted to the regular-void-pattern SCRs on the basis of ceramic honeycomb and micro-channel reactors. However, on the one hand, honeycomb and micro-channel reactors suffer from the radial transfer restriction and channel blocking, and on the other hand, the washcoating technique costs highly and is difficult to implement. In contrast, emerging foam-/fiber-structures, with irregular 3D open network, exhibit great advantages over the traditional micro-channels/honeycombs, including free radial diffusion, eddy-mixing, large area-to-volume ratio , high contacting efficiency and high flexibility in geometry design. However, effective catalytic functionalization of such foam-/fiber-structured is particularly desirable but represents a grand challenge, because the traditional washcoating easily causes non-uniformity and exfoliation of coatings. In past few years, we made significant efforts on the nano- to macro-engineering of nanocomposites onto the foam-/fiber-structures and their applications in the strongly exo-/endo-thermic and/or high-throughput catalytic reaction processes. The latest progress in foam-/fiber-based SCRs development for applications in strongly exo-/endo-thermic reaction processes such as methanation of syngas, oxidative coupling of CO to dimethyl oxalate (DMO) and DMO hydrogenation to ethylene glycol (Fig. 1) has been discussed.
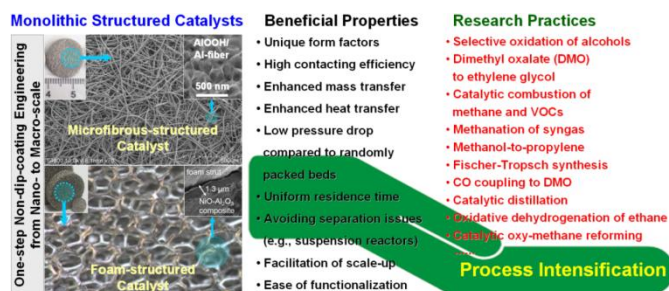

Fig. 1 Fiber-/foam-structured catalysts engineered from nano- to macro-scales: non-dip-coating preparation, beneficial properties and research practices in heterogeneous catalysis.

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IL20

Dynamic covalent chemistry of carbon dioxide: opportunities to address environmental issues

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Carbon capture, utilization or storage has been studied and developed for decades as the most promising strategy to reduce the atmospheric emissions of CO_2 and fight global warming. Yet, despite a remarkable thermodynamic efficiency, the current capture process based on chemical absorption – desorption suffers from prohibitive energetic and infrastructural cost which prevents large-scale industrial deployment. Current analyzes confirm that no substantial cost reduction is to be expected if the current scheme of process is conserved as such.

In our recent work[1], we have explored the potential contribution of self-assembling phenomena to the issue of carbon capture and/or utilization. By considering the possibility to couple the capture equilibrium relying on carbamation chemistry with either a competing or subsequent reversible reaction, we have shown that it is possible to displace on demand toward the CO_2 capture or release direction. Replacing additive/eliminative by substitutive molecular scenario through the sole addition of a molecular additive provides an access to disruptive thermodynamic paradigms. An additional chemical equilibrium involving the covalent and/or non-covalent bond formation with either the unloaded capture agent or the CO_2-loaded product[2,3] leads to efficient absorption from dilute emission and cost-effective release.[4] More recently, we have shown that capture solutions are unprecedented libraries of metal ligands, which can be valorized for the sustainable separation of metals from primary or secondary resources[5] This convergent extraction/purification strategy has been implemented in continuous flow[6] and in solvent free conditions.[7] It allows to envisage game-changing integrated processes, pooling CAPEX and OPEX to simultaneously address the entire chain value: capture from flue gas, utilization for valuable metal extraction and chemical storage.

Fig. 1: Integrated CO2 capture, utilization and storage

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Synthesis of hybrid organic-inorganic nanomaterials from sol-gel chemistry of silicon alkoxides combined with bio-based polymers, monomers, and building blocks

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Hybrid organic-inorganic nanomaterials (O/I) could be easily synthesized by combining biobased polymers or bio-based building-blocks (monomers or blocks) and sol-gel chemistry of metal alkoxides such as silicon-based ones (alkoxysilanes). From such a synthesis which denoted as 'chimie douce' as it considers low temperature conditions (inorganic phase could be prepared at room temperature) and environmentally-friendly medium (water-based), O/I nanomaterials based on biomass-sourced species which could be sensitive to high temperatures and conditions, could be designed. These ones can display physical behaviors combining the properties from the polymer and the ones from the inorganic (ceramic-like) phase. By such a way, nanofilled biobased polymers (nanocomposites) could be processed with overcoming of processing difficulties such as a large increase of viscosity in the molten state. In this lecture, the synthesis of different types of O/I nanomaterials from bio-based organic components will be described.

The first type of O/I nanomaterials considers a synthesis route considering silicon alkoxides (organosilanes) or precondensates leading to the *in-situ* generation of silicon-rich nanoparticles which are combined with a biobased monomer or building block, i.e. L-lactide or tannic acid, respectively. Hydrolytic and non-hydrolytic sol-gel reactions of tetraethoxysilane (TEOS) and □-aminopropyltriethoxysilane (APTES) were carried out in molten L-Lactide which is polymerized in a second step by ring opening polymerization (ROP) using an environmentally friendly route, i.e. without solvent (reactive extrusion). For tannin-based systems, a solution route was considered in order to process high performances hybrid organic-inorganic coatings having a silica-like inorganic continuous phase.

The second type of O/I nanomaterials deals with the *in situ* generation of silica-like nanofillers in a bio-based polymer, i.e. polylactic acid, PLA. Again, the synthesis of these O/I nanomaterials was done by using the reactive extrusion which allows to design nanocomposites without a large increase of viscosity of the filled molten polymer as preformed nanoparticles are considered. The morphologies of the PLA-based O/I nanomaterials were compared to those of nanocomposites processed by introducing functionalized fumed silica. For both types of O/I nanomaterials, tailoring of the organic phase (matrix)/inorganic-rich phase interfaces is a key issue.
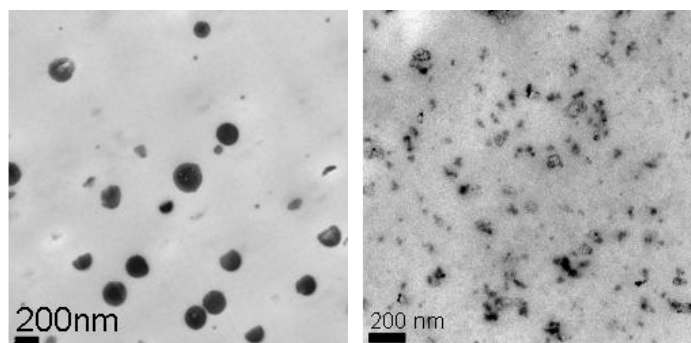

Fig. 1 – Transmission Electron Microscopy micrographs of hybrid organic-inorganic nanomaterials based on a polylactic acid (PLA) matrix synthesized from different routes: (a) *in situ* generation of inorganic-rich nanophase from polydiethoxysiloxane precondensate (PDEOS) and □-methacrylopropyltrimethoxysilane (TMSP) (1:6) in molten PLA (5% wt. eq; SiO₂); (b) combination of ring opening polymerization (ROP) of L-Lactide and sol-gel reactions of tetraethoxysilane (TEOS) and □-aminopropyltriethoxysilane (APTES) (18:1).

IL22

POLYSORB® Isosorbide and its amazing application with polyesters and polycarbonates

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Isosorbide or 1,4-3,6 dianhydrohexitol, derived from starch and more precisely from sorbitol, is one of the chemical intermediates of interest in the field of thermoplastic materials and for curable resins application. Hence, isosorbide found its place as a monomer suitable for polycondensates synthesis [1] like polyesters, polycarbonates and thermoplastic polyurethanes.

In aliphatic [2] or semi-aromatic polyesters [3], the addition of isosorbide allows a large increase of the glass transition temperature, opening to this new copolyester several usual applications of amorphous polymers. The preparation of poly (ethylene-co-isosorbide) terephthalate with different ratios of isosorbide will be particularly detailed in this presentation. The structure – properties relationship will permit a focus on the synthesis of polyesters with semi-crystalline or amorphous structures. The influence of isosorbide on the polymerization, on the processing of the resulting polyester as well as the modification of the final properties will be enlightened. The developments made on isosorbide-based polyester for making bottles suitable for hot filling applications will be presented.

In polycarbonate, isosorbide is much more than just a solution for Bisphenol A replacement. Hence, Isosorbide containing polycarbonates present significantly increased properties like mechanical strength, UV stability and optical properties with resulting properties between usual Polycarbonate and PMMA [4].

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IL23

Optimal utilization of carbon resources

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Catalysis, as a key and enabling technology, plays an increasingly important role in fields ranging from energy, environment and agriculture to health care. Rational design and synthesis of highly efficient catalysts has become the ultimate goal of catalysis research. In the present talk, I will discuss with you on the effects of nano confined catalysis, with an emphasis on the development of nano-composite catalysts for the utilization of carbon molecules, such as CH_4 and CO.

In the first example [1], I will show some new results on the direct and selective conversion of methane to valuable chemicals by the invention and development of lattice-confined single-site iron catalyst will be illustrated. As been confirmed, the C-H bond of methane could be cleaved over the single-site iron center embedded in the lattice of SiO_2 and SiC, which leads to the formation of •CH_3 radicals to leave the surface and couple in the gas phase. The controlled activation of C-H bond by the single-site catalyst prevents the complete dehydrogenation of methane to form coke on the catalyst surface.

As the second example [2], I will discuss the innovation of nano-composite catalysts for the selective conversion of coal-based syngas to lower olefins, which circumvents the surface polymerization problem confronting the conventional Fischer-Tropsch synthesis and has been recognized as "a milestone in the direct synthesis of light olefins". The well-known Fischer-Tropsch synthesis (FTS) was first developed by two German scientists, Fischer and Tropsch, in the 1920s and has now become the core technology for Gas-to-Liquid (GTL) and Coal-to-Liquid (CTL) in industry. Chemicals produced via FTS have also gone beyond liquid fuels, including other high-value hydrocarbons, such as light olefins, wax and oxygenates. Despite significant advances in both fundamental understandings and commercial applications, there are two major drawbacks in FTS technology, for instance, CO_2 emission and water consumption. In our process, the partially reduced oxide surface (ZnCrOx) was used to activate CO and H_2, while C−C coupling is subsequently manipulated within the confined acidic pores of zeolites. Particularly, oxygen from CO dissociation is removed by the reaction with CO to form CO_2, which thus may allow the direct use of coal- and biomass-derived syngas with a low H_2/CO ratio and remove the additional process of water-gas-shift (WGS) reaction. As such, both water and energy consumption could be reduced tremendously.

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IL24

Influence of chain length on selective hydrogenolysis of polyols

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The US Department of Energy listed sorbitol and xylitol among the top-12 plateform molecules. These polyols are industrially obtained at large scales via catalytic hydrogenation of glucose and xylose, respectively, whereas the microbial fermentation of glucose or glycerol was involved in the standard production of erythritol.[1] They are highly functionalized and contain an O/C ratio higher than that of most of the commodity chemicals. Thus, their transformation to more-valuable compounds requires lowering of the oxygen content. For this objective, bimetallic catalysts, in particular $Rh\text{-}ReO_x/TiO_2$ and $Rh\text{-}ReO_x/ZrO_2$ prepared by successive impregnation and reduction, were chosen to investigate the selective C-O bond hydrogenolysis of these polyols. Characterization techniques such as CO-chemisorption, TGA-MS, TEM, and XPS were carried out. The influence of several reaction parameters on activity and selectivity have been studied.

Regardless the substrate, very good mass balance was observed, and few gas products were obtained (Fig. 1). During erythritol hydrogenolysis, the highest selectivity to BTO and BDO reached 37 and 34%, respectively, at 80% conversion in the presence of $Rh\text{–}ReO_x/ZrO_2$ catalyst at 200°C under 120 bar (Fig. 1a).[2] During hydrogenolysis of xylitol and sorbitol, different types of reactions also took place, which yielded several families of products: isomers, cyclic compounds, C-C cleavage products, and deoxygenated products. The highest selectivity to linear deoxygenated C5 and C6 products from xylitol and sorbitol attained 66 and 54%, respectively, at 80% conversion at 200°C in the presence of $Rh\text{–}ReO_x/TiO_2$ (120 bar, Fig. 1b) and $Rh\text{–}ReO_x/ZrO_2$ (80 bar, Fig. 1a) catalysts, respectively.[3]
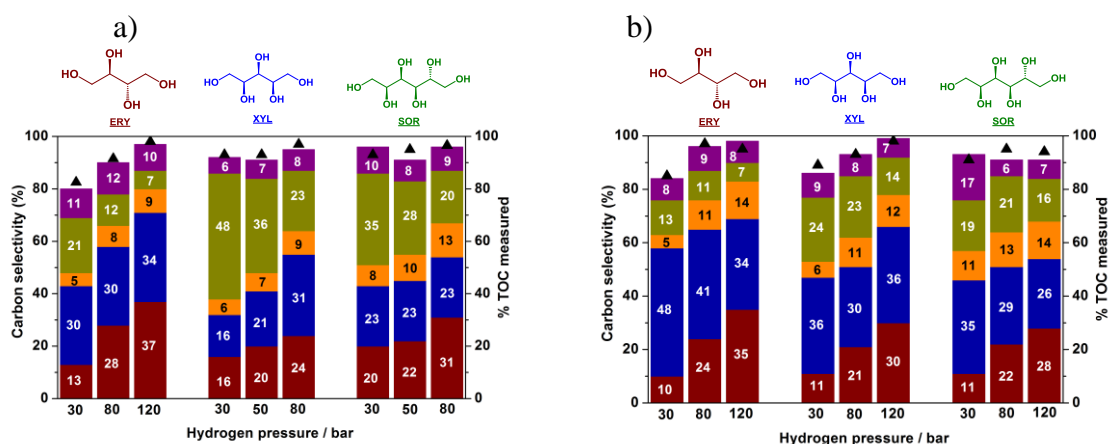

Fig. 1 Effect of H$_2$ pressure on selectivity to the reaction products and %TOC measured at 80-86% conversion. (▲) % TOC measured; (■) C-C cleavage products; (■) Cyclic compounds; (■) Isomers; (■) C4 without BTO, C5 without PTeO, or C6 without HPO; (■) BTO, PTeO, or HPO. Reaction conditions: 120 ml H$_2$O, 200 °C, a) Rh-ReO$_x$/ZrO$_2$ catalyst; b) Rh-ReO$_x$/TiO$_2$ catalyst; n$_{Sub}$/n$_{Rh}$ = 200-450.

Rhodium-based bimetallic catalysts are clearly efficient in C-O hydrogenolysis reaction. Deoxygenated linear polyols are obtained in good yields after optimization of the reaction conditions. Application to more complex media are under development.

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IL25

Compartmented reactors to optimize hybrid catalytic systems involving chemical and enzymatic catalysis

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Combining different type of catalytic systems has been addressed recently with the idea to take the "best" of each system and develop a synergic process. Different approaches are reported coupling two chemical steps, either organic chemistry or homogeneous catalysis or heterogeneous catalysis, or coupling one of this chemical step with supported or free enzymatic catalysis[1-2]. Such hybrid catalysis has been applied to kinetic resolution, dynamic kinetic resolution and non-stereoselective reactions.

Whereas the concept of hybrid catalysis is well accepted, real "one-pot" hybrid systems in which chemical and enzymatic reactions are simultaneously performed locally, are facing several drawbacks due to the specificities of each catalytic system.
Two new reactor concepts based on a compartmentation approach are being developed to answer these drawbacks

- One concept is based on a traditional stirred tank reactor in which two zones are created with their specific agitation (aerated and non-aerated zone), heating or cooling exchanger and dedicated catalytic baskets.
- The other based on segmented flow, also named "Taylor flow", inspired from microfluidic concepts where fluids are flowing trough a capillary tube allowing a wide variety of possibilities (gas-liquid, liquid-liquid …) and where a solid phase can be present as a slurry system or immobilized on the capillary walls via a dedicated coatings.

The aim of the project is to evaluate the advantages and drawbacks of each concept with the help of a model reaction where an reversible reaction (fructose enzymatic isomerization) is pushed to completion by an irreversible chemical oxidation reaction. Experimental and modeling methodologies including kinetics, reactor performances characterization and experimental validation will be commented.
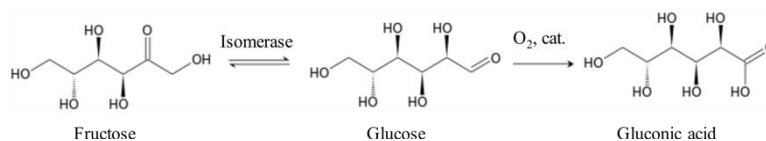

Fig. 1: Model hybrid catalytic system for one-pot set-up

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IL26

Methodological synthetic tools for biomass valorization

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Biomass is a widely available carbon source apart from oil and coal in nature, which has been an important resource for the production of chemicals and fuels. The conversion of biomass platforms into high-added values compounds appears to be of increasing interest, both in the realm of fine chemical synthesis targeting highly functionalized molecules.

Projects developed in our group focused in the promotion of **5-hydroxymethylfurfural** (HMF) and **isosorbide** platforms.

5-Hydroxymethylfurfural (HMF) is regarded as one of the most promising biomass derived platform chemicals due to its rich chemistry and ready availability from carbohydrates. Multicomponent reactions (MCR) using HMF offer straightforward access to novel fine chemicals, though the peculiar reactivity and lower stability of HMF compared to furfural and other simple aromatic aldehydes has limited its use in such strategies. Recently, we reported our results on the use of HMF in the 3-component Biginelli reaction, leading in one single step to a series of functionalized dihydropyrimidinones [1]. As part of our on-going interest on the application of HMF towards fine chemicals and on green and sustainable chemistry, we also explored the possibility to synthesize furan-based α-amino phosphonates via the one-pot Kabachnik-Fields condensation, directly from HMF [2].

Isosorbide is a chiral dianhydrohexitol produced by Roquette Frères (Lestrem, France) that expanded its production to several thousand tons in 2011. Over the last decades, functionalization of biosourced isosorbide has also attracted considerable interest for polymer applications and for asymmetric induction in organic synthesis (auxiliaries, ligands and organocatalysts) [3]. Reported synthesis of isohexide-based amines involved the use of highly reactive leaving groups, such as tosylates. Although effective, this process has low atom efficiency and high amount of waste is generated. 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 C-C and C-N bonds [4].
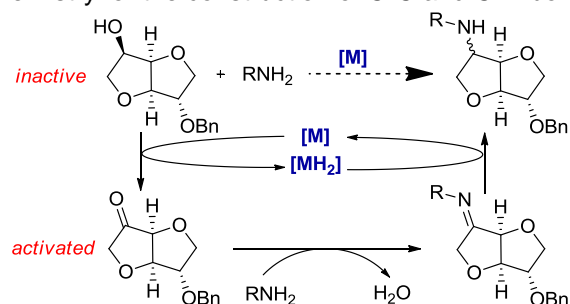

Fig. 1: Catalytic amination using borrowing hydrogen methodology

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IL27

Selective hydrogenolysis of cellulose and its derivatives to chemicals: catalytic functions and reaction pathways

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Cellulose is the most abundant source of biomass on earth. Cellulose and its derivatives, such as glucose, sorbitol and 5-hydroxymethyl furfural, provide renewable alternatives to fossil fuels for synthesis of fuels and chemicals. In this work, we report our recent progress in catalytic conversion of cellulose and especially its derivatives into alcohols and carboxylic acids, such as propylene glycol and adipic acid, focusing on our understanding on the requirements for catalytic functions and reaction pathways.

Supported Ru clusters efficiently catalyzed the selective hydrogenolysis of sorbitol to ethylene glycol and propylene glycol. The sorbitol hydrogenolysis requires bi-functional requirements and involves the competitive Ru- and base-catalyzed reactions of ketose or aldose intermediates, derived primarily from kinetically-relevant sorbitol dehydrogenation. This dehydrogenation step most likely proceeds by preferential activation of its C(5)-H bond on the Ru surfaces. Glycerol hydrogenolysis turnover rates (normalized per surface Pd atom measured by H_2 chemisorption) and propylene glycol selectivity on the PdZn/m-ZrO$_2$ catalysts depend sensitively on their Zn/Pd molar ratios. The kinetically-relevant step of glycerol hydrogenolysis involves the *α*-C-H cleavage in 2,3-dihydroxypropanoxide intermediate to glyceraldehyde on PdZn alloys and Pd. The transition state of *α*-C-H cleavage is more stable on PdZn alloys than on Pd, due to the stronger oxophilicity of Zn, which thus facilitates *α*-C-H cleavage of the Zn-bound intermediate by adjacent Pd on PdZn alloys.

IL28

L'Oréal's   implementation of green chemistry & sustainable process to afford high value botanicals

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Botanical extracts from Traditional Chinese Medicine (TCM) and Traditional Indian Medicine (TIM) are a rich treasure house for bioactive substances as they are extensively used in several industry sectors, such as cosmetics, phytomedicines, nutraceuticals, spice and food industry to support primary health care, but also for innovation and discovery. The Botanical Extract market is rapidly growing over the years owing to factors like shift in consumer demand towards botanical cosmetic products, various schemes launched by the governments, key investment & expansions being made in the TCM & TIM medicinal plant/botanical extract industry, among others. Today, there is a pressing need to produce high value botanical extracts more sustainably through the implementation of green chemistry principles as applied to the protocols for botanical extract processing [1]. Processing is a critical aspect of botanical extract production, especially due to the low yield and also due to several down-streaming steps for generating high purity enriched botanical extracts [2]. During the presentation, you will hear about some of the initiatives of L'Oréal Research & Innovation to develop innovative, green by design extraction strategies commencing from the pre-development design phase of bio-mass waste transformation to a fully Industrial process implementation that is in line with our sustainability commitment. Examples spanning from one pot extraction at relatively low temperatures in a remarkably short time, recycling and re-use of solvents/by products targeted at zero discharge will be shared [3].

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Bio-butadiene manufacture from butandiols

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Butadiene is one the main components of synthetic rubber, and is today almost exclusively produce by steam cracking of naphta. Main purpose of steam cracking is to produce ethylene, and prices of the co-products like butadiene have always been erratic due to drift between offer and demand.

This has been particularly true since 2010, with the beginning of production of shales gas. Large quantities of natural gas liquids (and particularly ethane in US) have been produced at low price, driven investment on natural gas liquids steam cracker, instead of naphta steam cracker. In this context, on-purpose technologies to produce butadiene are needed.

IFP Energies Nouvelles and Michelin started in 2011 a collaborative project, co-founded by ADEME, in order to produce butadiene from renewable resources. In this work, we focus on the pioneer studies made by a group of American laboratories [1-9] during World War II, in order to produce butadiene from sugar in a three step process : 1) fermentation of sugar into 2,3-butandiol, 2) esterification of the 2,3-butandiol and finally 3) pyrolysis of the diester. This process was known to produce a butadiene of high purity, but was never industrialized because the only micro-organism capable of producing 2,3-butanediol from sugar was pathogenic.

Recent progress in fermentation makes this process much more attractive. To quote examples, Genomatica produces today 1,4-butandiol form sugar, and Lanzatech produces 2,3-butandiol (and ethanol) form sugar or syngas, both with non-pathogenic micro-organism.

Using modern chemical engineering tools, we propose some improvements of the two last steps of this process.

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IL30

Zeolite catalysts for the production of alkylbenzenes: from zeolite synthesis to industrial applications

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Zeolites, an important type of microporous crystalline materials, are widely used in industrial catalysis for the production of chemicals. The R&D and industrialization of novel zeolites have played key roles in the major catalytic technology breakthroughs of oil refining, petrochemical, and coal chemical. Great efforts have been devoted to synthesize novel zeolites and 239 types of frameworks have been approved by the Structure Commission of the International Zeolite Association (IZA-SC) [1]. Currently, zeolites of about 20 of the overall 239 types of frameworks have been commercialized.

Sinopec Shanghai Research Institute of Petrochemical Technology (SRIPT) has gained progress in the R&D and industrialization of zeolite. A series of SCM-n (n=1~25) zeolites (Sinopec Composite Material) were synthesized, and zeolites with framework types of **MFI**, **MWW**, ***BEA**, **MOR**, **FAU**, **CHA** were put into industrial use [2-4].

For the productions of alkylbenzenes, like ethylbenzene and cumene, SRIPT has commercialized several zeolite-based catalysts using zeolites as active components. Herein, the R&D and industrialization of catalysts based on **MFI**- and **MWW**-type zeolites are introduced, including the direct syntheses of **MFI**- and **MWW**-type zoelites with novel morphologies, post synthesis of mesoporous **MFI**-type zeolite, preparation of binderless **MFI**-type zeolite catalyst, and the industrial uses of these zeolitic materials [5-9].

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Green synthesis of zeolites and examples for zeolite-based green catalysis

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Green Synthesis of Zeolites. Zeolites have been widely used as heterogeneous catalysts in petrochemical and fine chemical industry, but their syntheses are not sustainable because of using costly and toxic organic templates in the presence of a large amount of water under hydrothermal conditions. The use of organic templates and water solvents produce a huge amount of wastes, which is environmentally unfriendly. For the synthesis of special zeolites, the use of F^- species are necessary. The fluoride-free containing wastes are also harmful for the environments. In this talk, it is briefly summarized our recent green and generalized routes for synthesis of zeolites, including (i) organotemplate-free, (ii) solvent-free, (iii) F^--free, (iv) combing organotemplate-free and solvent-free routes, and (v) fast crystallization of zeolites at higher temperatures [1].

Examples for Zeolite-Based Green Catalysis. The goals of green catalysis are to increase activity, selectivity, and catalyst life, along with reduction of by-products and energy consumption. In our cases, when the metal nanoparticles are fixed with zeolite crystals (metal@ zeolite) by means of a controllable seed-directed growth technique, it is exhibited long reaction lifetimes, outperforming conventional supported metal catalysts and commercial catalysts consisting of metal nanoparticles on the surfaces of solid supports during the catalytic conversion of C_1 molecules, including the water-gas shift reaction, CO oxidation, oxidative reforming of methane and CO_2 hydrogenation [2]. When the Pt nanoparticles are loaded on hydrophobic zeolite supports, the full combustion of HCHO could be realized at even much lower room temperature, which is potentially important for pollutant removal in indoor air. When the metal nanoparticles are matched with zeolites very well, the synergistic catalysts could convert more CO_2 molecules to produce more CO in the reforming of methane with CO_2, which is potentially significant for reduction of global CO_2.

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IL32

E2P2L: an open innovation lab in sustainable chemistry

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The production of chemicals and fuels using biobased reagents is critical for a real transformation of the chemical industry towards sustainability and for warranting a transition into a circular economy [1-3]. In this view, a main scientific challenge is how to design heterogeneous catalysts able to convert intermediate platform molecules issued from biorefineries into valuable chemicals (Figure 1). This encompasses not only the engineering of advanced materials and organic complexes, but also the eco-design of intensified processes (*e.g.*, microreactors, electrocatalysis) with low energy consumption, low greenhouse gas emissions and ideally no-byproducts.

In this lecture, we will illustrate the current research projects at the Eco-Efficient Products and Processes Laboratory (E2P2L) targeting the synthesis of specialty chemicals (e.g., biosurfactants, biosolvents, additives) from renewable raw materials such as biomass and CO_2. E2P2L aims at providing breakthrough innovations in the field of Catalysis for Sustainable Chemistry using a holistic approach by integrating catalyst design, chemistry, modeling and process engineering in a single site.
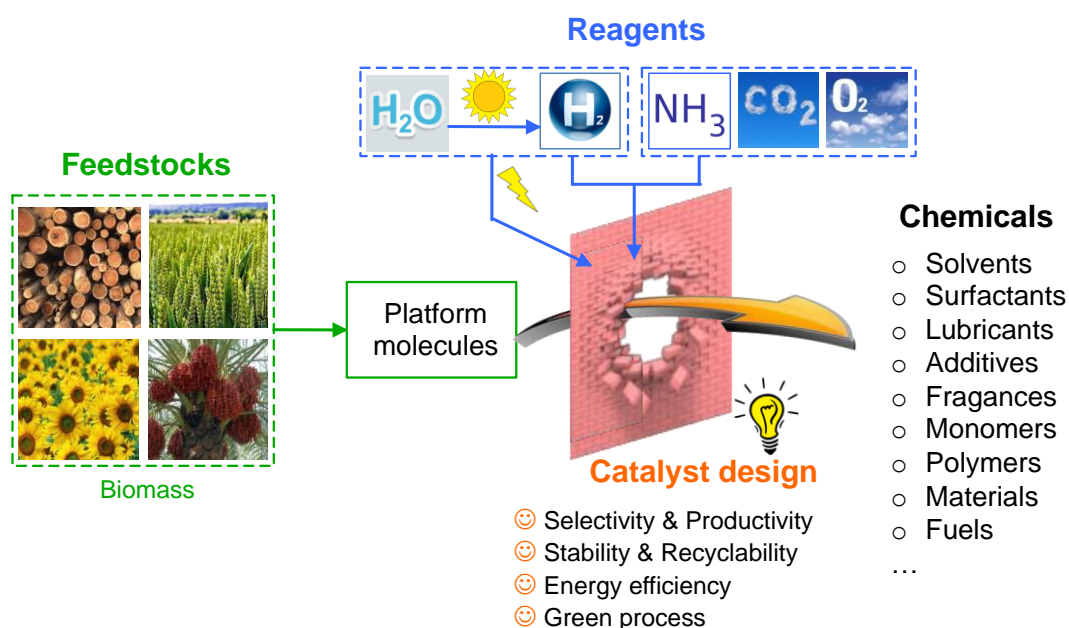
Fig. 1: Synthesis of high added value chemicals from renewable feedstocks and reagents.

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Synthesis of renewable meta-xylylenediamine and alkyl levulinate from biomass-derived furfural

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The catalytic conversion of renewable feedstocks to fuels, fine or specialty chemicals is now the subject of intense research efforts. Although a myriad of reports published daily on this topic, the emergence of bio-based fuels and chemicals in our society is unfortunately facing important hurdles such as catalyst deactivation and high dilution (often required to better control the selectivity of reactions), thus leading to unacceptable space time yields for industrial implementation, although high yields are often achieved.

As a case in point, we will discuss on the catalytic conversion of furfural to specialty chemicals, a cheap bio-based building block (1.0-1.2 €/kg) available in large scale from biomass (>200 kT/year). In particular, two important reactions will be discussed:

(1) **The catalytic conversion of furfuryl alcohol (FA) to alkyl levulinate (AL),**[1] that are industrially relevant solvents or intermediates for the manufacture of chemicals. In this part, we will show that bismuth triflate was capable of catalyzing the conversion of FA to AL with up to 91% yield from a concentration of FA in alcohol as high as 30 wt. %, which corresponds to an unprecedented space time yield of 182 kg/m^3/h. A catalytic amount of water in the alcoholic solution of FA plays an important role on the activity and selectivity of Bi(OTf)$_3$ and a so-called Lewis-assisted Brønsted mechanism was postulated to rationalize these results. A comparison with the commercialized SFOS process, operated by a subsidiary of the former Rhône-Poulenc group and running until the beginning of the 90's, shows that this novel catalytic route is compatible with industrial requirements in terms of yield, productivity and capacity,

(2) **The catalytic conversion of furfural to meta-xylylene diamine,**[2] an important target widely used in the polymer industry as curing agent for epoxy resins and coatings, and in the production of polyamide, and polyurethane. The investigated pathway involves a Diels-Alder/aromatization sequence as a key step. Guided by DFT calculations, we discovered that (1) the aromatization step could be catalyzed at low temperature by superbases instead of acids, thus avoiding the usually observed retro-Diels-Alder reaction, and (2) by playing with the rate of the reactions, it was possible to selectively drive the reaction to the meta aromatics.
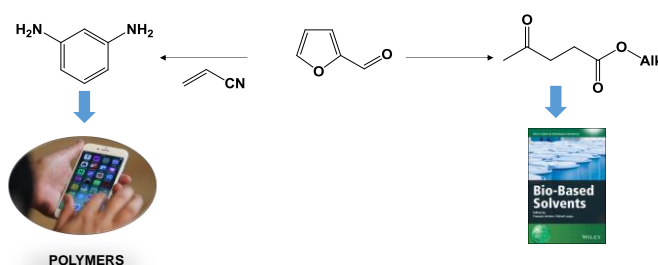

Fig. 1: Conversion of furfural to specialty chemicals

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IL34

Advances in zeolite science and application

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Zeolitic materials are widely used as catalysts, adsorbents, and ion-exchangers in many traditional chemical industries, and are playing more and more important role in the fields of sustainable chemistry [1]. In recent decade, zeolite science has witnessed significant advances in the aspects of synthesis, mechanistic study, theoretical prediction and application. For instance, we have discovered that the zeolite nucleation can be promoted through free radicals, which sheds a new light on zeolite crystallization [2]. In addition, we have developed some effective strategies for the synthesis of nanosized zeolites and hierarchically single-crystalline nanosized zeolites that are highly desirable for many important catalytic reactions. Strikingly, thanks to their intrinsic characteristics integrated with other functions, zeolites are acting a platform for many new applications in some emerging fields. For instance, utilizing zeolites as a host matrix, we have successfully embedded ultrasmall metal nanoclusters in the nanopores of zeolites, which can act as highly-efficient nanocatalysts for hydrogen generation [3]. Taking advantage of the nano-confinement effect, we have developed a "dots-in-zeolites" strategy to in-situ confine carbon dots (CDs) in zeolitic matrices during hydrothermal/solvothermal crystallization to generate ultralong-lifetime room temperature thermally activated delayed fluorescence (TADF) and phosphorescence materials. Thanks to the excellent chemical, thermal, and mechanical stability of zeolites, we have fabricated zeolite-coated mesh films for gravity-driven oil-water separation. Furthermore, we have introduced a polarity-based protocol to regulate the wetting behavior of the superamphiphilic porous nanofibrous membranes by infusing the high polar-component-of-surface-energy (PSE) liquid into the membranes to repel the immiscible low PSE liquid. It is believed that zeolites as a new paradigm may boost many new applications in the future.

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Oral Communications

Biocompatible quantum dots loaded dual-color mesoporous silica nanoparticles as a green alternative for biochemical sensing

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Developing sensors to continuously monitor biochemicals has become a priority for improving diagnosis and management of conditions related to chemical imbalances. Optical techniques are preferred because they are very sensitive and provide the ability to follow several sensors at the same time. However, they are currently based on organic fluorophores, which require a lot of synthesis steps and lack the stability for continuous monitoring. Recently, sensors based on semiconductor nanoparticles called quantum dots (QDs) started to be developed. They are good candidates for sensing and imaging because of their impressive optical properties that can be precisely tuned by changing either their size or their composition [1]. However, they are currently made of toxic elements like lead, cadmium or selenium, have poor biocompatibility and are usually made through high temperature synthesis using organic solvents. Greener sensors based on new semiconductor materials with only non or mildly toxic elements, such as ZnS:Mn or $AgInS_2$ quantum dots, ideally synthesized in water, are developed and encapsulated in mesoporous silica nanoparticles.

Indeed, mesoporous silica is a good carrier for *in vivo* applications, being sparsely cytotoxic, stable in water, easy to functionalise while presenting high cellular uptakes [2]. The mesoporous structure also allows us to encapsulate multiple types of guests at the same time, ranging from drugs to nanoparticles. Encapsulating QDs inside mesoporous silica is also useful to enhance the luminescence detection limit by spatially confining the optical signal of QDs encapsulated inside one nanoparticle, reducing the amount of nanoparticles needed to get a sufficient signal.

Moreover, by embedding quantum dots with different optical properties as a core-shell like structure inside mesoporous silica, a new type of dual-color sensor can be obtained. Indeed, thanks to the mesoporous structure of the nanoparticle, the "shell" quantum dots encapsulated near the surface can interact and be quenched by the environment, while the luminescence of "core" QDs will remain unchanged and be used as a reference. This dual-color type of sensor offers many advantages over intensity measurements from sensors made with only one indicator dye. For example, intensity measurements of luminescent sensors consisting of a single luminophore are susceptible to error due to variation in the number of sensors excited (absence of signal can be due to absence of sensor or quenched sensors), fluctuations in light source intensity, instrumental drift or photobleaching.
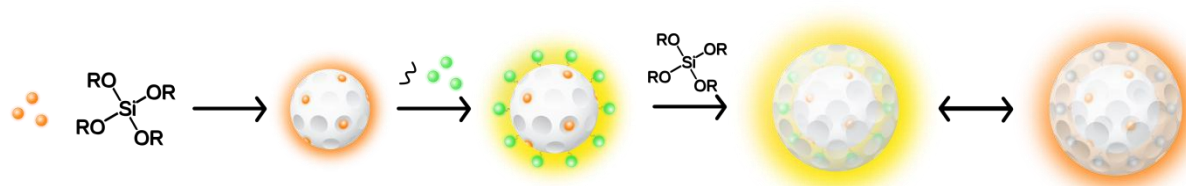

Fig. 1: Principle scheme of a dual-color probe based on non-toxic quantum dots and mesoporous silica nanoparticles

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OC2

Rotaxane-branched dendrimers

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   Rotaxane dendrimers, which are defined as "*the dendritic molecules containing rotaxane-like mechanical bonds to link their components*" by Kim, have evolved to be a hot topic within the field of mechanically interlocked molecules (MIMs) and dendrimer chemistry. The alliance between rotaxane and dendrimer endows the resultant rotaxane dendrimers not only intriguing topology but also wide applications in the field of molecular nanoreactors, gene delivery, and light-harvesting system, etc[1]. Over the past few years, the research mainly focused on rotaxane dendrimers with rotaxane cores or (pseudo)rotaxane termini. However, the construction of rotaxane dendrimers with rotaxane branches has been rarely explored due to the intrinsic complexity and steric hindrance with hyperbranched mechanical bonds. Based on our continuous interests on linear neutral platinum-acetylide chemistry, we have successfully realized the construction of type III-A [46]rotaxane dendrimers up to fourth-generation via a divergent strategy[2]. Moreover, functional rotaxane-branched dendrimers substituted with ferrocenes as termini were future prepared through the surface chemical transformations. Recently, starting from a switchable [2]rotaxane precursor, the use of a controllable divergent approach allowed for the successful synthesis of rotaxane-branched dendrimers up to the third-generation with 21 switchable rotaxane moieties dispersed on each branch[3]. More importantly, upon the addition and removal of dimethylsulfoxide (DMSO) molecule or acetate anion as the external stimulus, the amplified responsiveness of the individual switchable rotaxane units endowed the integrated rotaxane-branched dendrimers a three-dimensional switching feature, allowing for the remarkable and reversible size modulation, which might be applied in the reversible uptake and release applications, or even switchable organocatalysis in the future.
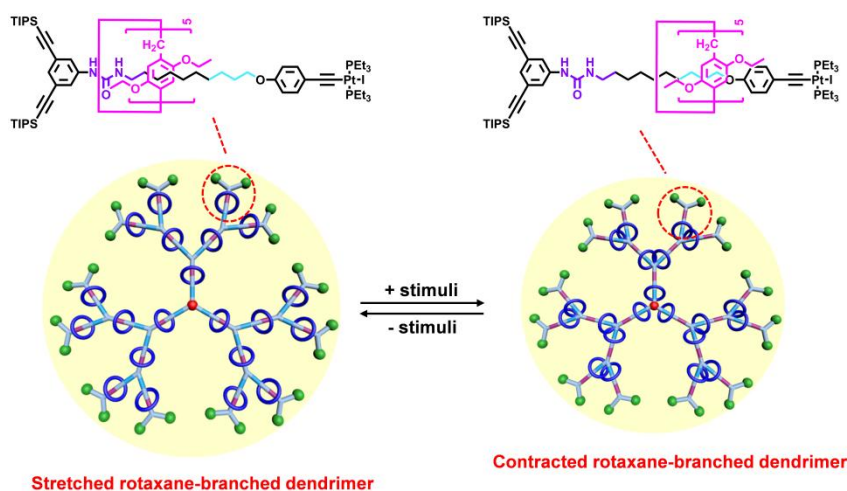

Fig. 1: Schematic representation of the dimensional modulation of rotaxane-branched dendrimer upon the addition or removal of external stimuli

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Structural diversity and functionalization of germanosilites

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Germanosilicates, a rapidly increasing number of topological structures with secondary double four ring (D4R) building units and large or extra-large pore systems, are becoming an important zeolite family. Benefiting from the structural instability and modifiability of Ge-rich D4R units, germanosilicate UTL experienced an unusual orientated collapse and reconstruction within an extremely narrow time window during the structural stabilization process by nitric acid treatment at elevated temperature. Taking full advantage of this unique structural change, extra-large pore Sn-UTL zeolites were postsynthesized [1]. In addition, several structural derivatives with continuously tunable pore sizes were also obtained by precisely controlling the acid treatment process [2].

Interestingly, the unexpected conversion of intergrowth germanosilicate CIT-13 into single crystalline high-silica ECNU-21 zeolite with a new topology has been realized via a creative top-down strategy. The polymorph phenomenon in CIT-13 was eliminated completely by selectively removing the intergrowth structure composed of unstable Ge-rich D4R units via alkaline-assisted hydrolysis, which was capable to cleave not only chemically weak Ge(Si)-O-Ge bonds but more importantly the metastable Si-O-Si bonds. Furthermore, structurally ordered ECNU-21 served as a stable solid-acid catalyst for the shape-selective hydration of ethylene oxide to ethylene glycol at greatly reduced water amount and mild temperature in comparison to conventional industrial process.
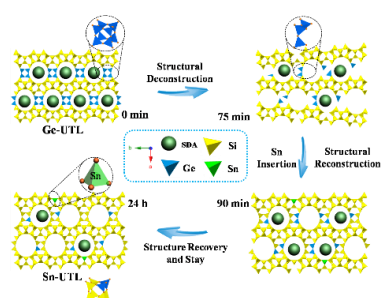

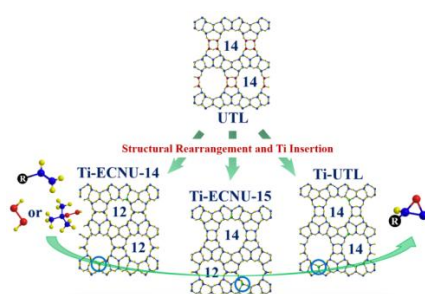**Fig. 1: Post-synthesizing extra-large pore Sn-UTL zeolite through structural rearrangemen**t

Fig. 2: Germanosilicate derived titanosilicates exhibited unique performance in epoxidation
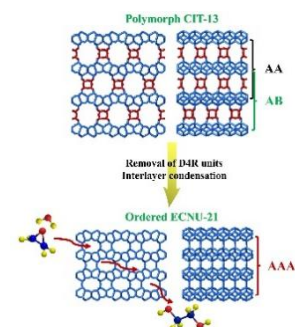

Fig. 3: Purification of polymorph CIT-13 germanosilicate into single crystalline ECNU-21 zeolite

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OC4

Highly active mesoporous catalyst for renewable *1,3*-butadiene from ethanol

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1,3-Butadiene (BD) is a critical unsaturated hydrocarbon used to manufacture various polymers, namely synthetic rubber.[1] However, the common BD production method—steam cracking of heavy hydrocarbons—is unsustainable: fossil fuels are a scarce resource and the process is detrimental to the environment by the emission of greenhouse gases. A time-tested alternative is the catalytic conversion of ethanol to BD, also known as the Lebedev process. Its use of a biomass-derived feedstock makes this technology suitable for a suitable, on-purpose BD production method. Catalytic performance issues are one of the challenges facing the economic viability of the Lebedev process: poor selectivity, low productivity and deactivation are endemic among the many catalysts developed over one hundred years of research on the subject.[2,3] Tackling these problems can be achieved by optimizing the chemical properties of the catalyst; the reaction requires a carefully tuned balance between dehydrogenation, dehydrating and condensing properties. Another strategy is to improve the structural properties of the catalyst.

We report a highly active, yet easily prepared Zn(II) and Ta(V) catalyst supported on mesoporous silica. Ta(V) has long been identified as suitable catalyst for the dehydration and condensation part of the reaction. Zn(II) provides the necessary dehydrogenation activity without a preliminary reduction step often required of other metallic dopants, such as Ag. The simple, one-pot synthesis based on the TUD-1 method combines these two elements, but also provides a morphology suited for the Lebedev process;[4] high specific surface area of 600 m^2/g and mesopores of 12 nm in diameters both facilitate access to the dispersed active sites, but also reduce deactivation by coking. At 400 °C with a $WHSV_{EtOH}$ of 5.3 h^{-1}, the synthesized catalyst is capable of reaching a BD selectivity of 73% at near total ethanol conversion. In terms of BD productivity, this amounts to 2.14 $g_{1,3-BD} \cdot g_{cat}^{-1} \cdot h^{-1}$, which is amongst the highest ever recorded. Furthermore, deactivation by coke formation is significantly reduced compared to other catalysts working under similar conditions and clearly outperform them. These results are ostensibly attributed to the properties listed above.
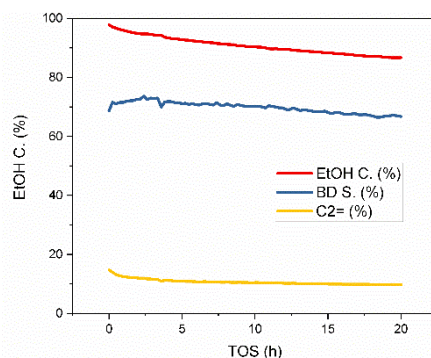

Fig. 1: Ethanol conversion, BD and ethylene ($C_{2=}$) selectivity using ZnTa-TUD-1

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Posters

Bio-inspired manganese mesoporous silica hybrid material as a water compatible antioxidant

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Mn^{III} dinuclear compounds mimicking the active site of the antioxidant Mn-catalase are often instable in water. Fixation of the metal complex inside a functionalized mesoporous silica allows the water compatibility necessary for nanomedicine applications. In this study two functions, pyridine moieties and tetramethylammonium ions, were considered for the matrix functionalization: the former to fix the manganese complex and the second to maintain a suitable pH for an optimal catalase activity [1]. These functions were homogeneously distributed in the pore by sequential surface reactions, using a molecular surface patterning technique [2].

Ultra-fast microwave heating for the synthesis of the silica matrix and minimization of toxic chemicals for its modification were used for a greener preparation. The manganese complex –very active in acetonitrile and inactive in water– becomes very active in water when it is incorporated in the host silica matrix (Fig.1). Moreover, the hybrid material can be advantageously recycled with no significant metal leaching [1].
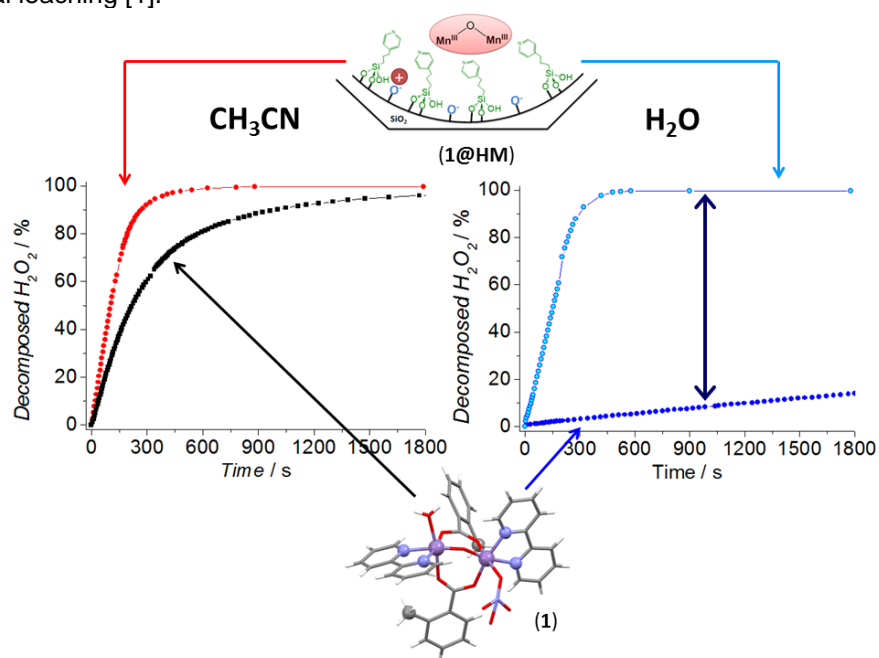

Fig. 1: Comparison of the catalytic activity of the hybrid material (1 @HM) and the molecular analog (1) in acetonitrile and in water.

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P2

HMF in multicomponent reactions: straightforward routes towards novel fine chemicals

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Recently, the production of chemicals, either commodities or specialty / fine chemicals, from renewable biomass has attracted growing interests due to the dwindling reserve of non-renewable fossil resources and the increasing awareness of environmental concerns. 5-Hydroxymethylfurfural (HMF) is an interesting biomass-derived platform chemical.[1] The hydroxyl group in HMF offers more possibilities of derivatization in target molecules compared to furfural. However, the lower stability of HMF weakens its applications in organic synthesis. Thus, developing efficient and mild routes towards existing or novel fine chemicals from HMF is still a challenging task. Multicomponent reaction represents a powerful synthetic tool allowing the straightforward formation of complex molecules directly from simple starting materials.

The Biginelli reaction, involving a condensation of aldehydes, C–H acidic carbonyl compounds and urea-type building blocks, has shown its strong vitality since its discovery more than 120 years ago. However, the direct utilization of HMF in the Biginelli reaction has never been reported. We have investigated the reaction and defined the appropriate conditions for accessing new dihydropyrimidinone libraries.[2]

1,3-Dicarbonyl compounds = 1,3-Diketones, β-keto esters
Urea-type blocks = Urea, thiourea, aminoheterocycles
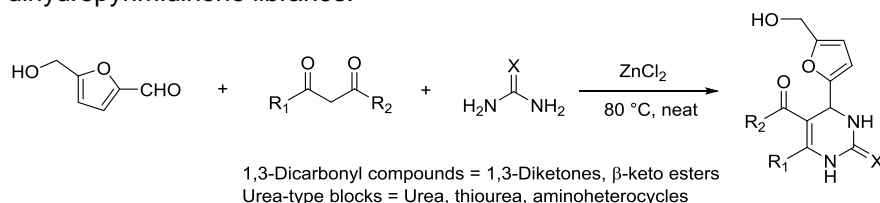
The Kabachnik-Fields reaction, a one-pot condensation of aldehydes, amines and dialkyl phosphites, is the most efficient and convenient strategy to synthesize □-amino phosphonates, which have some significant biological activities. Apart from the sole report involving a two-step synthesis of □-amino phosphonates from HMF, a one-pot strategy has never been reported. We have studied the one-pot conditions to prepare a series of novel HMF-based □-amino phosphonates. The derivatizations on hydroxyl group of the Kabachnik-Fields product and the reaction mechanism were also preliminary investigated.[3]
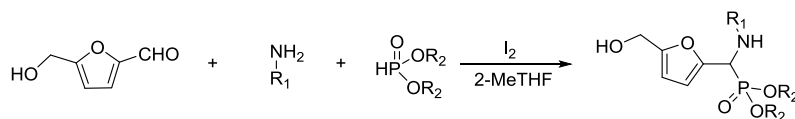
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OMS as catalytic support in NO and NH$_3$ oxidation

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With the economic development, the emission of nitrogen oxides (NO$_x$) has shown a clear upward trend. Nitrogen oxides contribute to the greenhouse effect and take part in photo-chemical reactions, leading to tropospheric ozone and acid rain formation. One of the most efficient technologies for NO$_x$ abatement is the selective catalytic reduction of NO$_x$ by NH$_3$ (NH$_3$-SCR). In this reaction, fast SCR in the presence of equimolar amounts of NO and NO$_2$ exhibits a reaction rate at least 10 times faster than that of reaction which NO$_x$ typically consist of >90% NO under normal combustion conditions. As an attempt to make NH$_3$-SCR technologies processes more efficient, one could think about the partial oxidation of NO upstream of the SCR catalyst to promote fast SCR. Herein we report for the first time the catalytic performance of a series of metal-functionalized manganese octahedral molecular sieves with cryptomelane framework for NO oxidation.

Catalysts were synthesized using a standard method [2] and characterized by ICP-OES, N$_2$ adsorption, XRD, TPR and TEM (Fig. 1A). The catalytic tests for NO oxidation over catalysts were carried out in a fixed-bed quartz reactor at atmospheric pressure. Comprehensive reproducibility and stability tests were performed on all the samples. TPR experiments showed that the addition of noble metals have a clear influence over the redox behavior of the prepared catalysts.
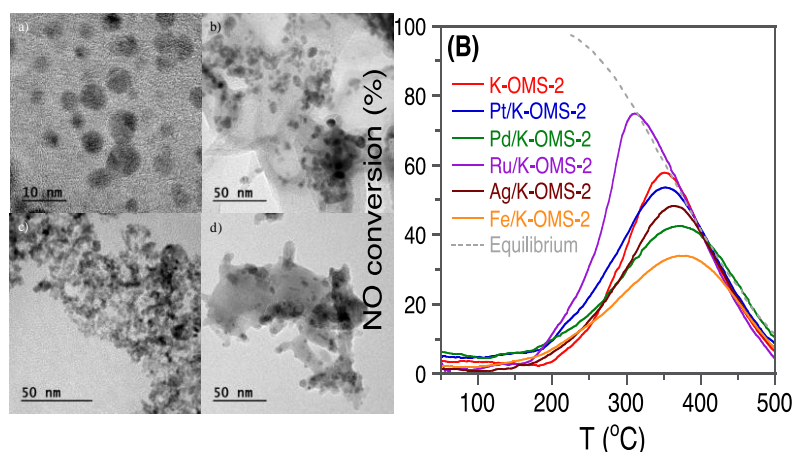

Fig. 1A) TEM micrograph (a) Pt/K-OMS-2. (b) Pd/K-OMS-2. (c) Ru/K-OMS-2. (d) Ag/K-OMS-2 and Fig. 1B) NO conversion as a function of temperature for K-OMS-2 doped with different metals. Experimental conditions: Inlet gas composition = 1000 ppm NO, 8% O$_2$, balance Ar; atmospheric pressure; GSHV = 35,000 h^{-1}; catalyst amount set to provide the same number of Mn equivalents (0.174 mmol Mn).

The conversion of NO was clearly affected by the presence of the different metals (Fig. 1B), showing the catalyst containing Ru the highest catalytic activity, and due to the higher reducibility of this catalyst and the contribution of the Ru particles. In the case of NH$_3$ conversion, catalyst containing Ag was the one that showed the best catalytic behavior.

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P4

Au-Cu bimetallic catalysts for the selective oxidation of fatty alcohol ethoxylates to alkyl ether carboxylic acids

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Alcohol ether carboxylic acids (AECAs) are widely used as green nonionic surfactants in the oil and gas, home personal care and industrial formulations [1]. Instead of the using of toxic chloroacetic acid in industrial carboxymethylation process, as a greener alternative, noble metal catalysts can be a good option for the direct oxidation of AEOs using either dioxygen or H_2O_2, affording water as main byproduct. Comparing different possible metals, it is found that Au and its alloys show a superior performance in many alcohol oxidation to acid including AEOs under basic condition [2]. In our work, bimetallic Au-Cu/CeO_2 catalysts were prepared by different methods, then the AEO7 oxidation to AECA6 catalyzed by Au, Cu and their alloy with H_2O_2 as oxidant was performed. The effect of Au/Cu ratio and the catalytic activity, selectivity and stability were studied in detail. A dedicated DFT study was also conducted to assess the role of Cu on the catalytic properties.

Different preparations of the bimetallic catalysts were compared, and the wet impregnation including $NaBH_4$ reduction at room temperature was considered the best one, which both took the high activity and the convenience into account. In the oxidation of AEO7 to AECA6, it was found the best weight ratio of Cu:Au is around 0.10, and the corresponding surface ratio on the alloy should be in the range of 0.2 ~ 1.0 which gives a high yield of AECA6 around 80%. To figure out the role of Cu in the alloy, a DFT study is conducted in the AEO1 oxidation both on the pure metals, and two alloy models as shown in Fig.1. The rate determining transition state on Au and Cu is the HOOH cleavage while changes to the α-C-H cleavage on alloy mainly thanks to the decreasing of the HOOH cleavage barrier caused by the existence of Cu atoms. In experiments, alloys are much more active than the pure metals, and only a little Cu is needed. In DFT results, the catalytic activity is: dimer (63 kJ/mol) > mono (84 kJ/mol) > Au (118 kJ/mol) > Cu (133 kJ/mol)(Energetic span in brackets). The alloy with few Cu atoms shows a much better activity compared to pure metals, the dimer alloy (with the surface ratio of 0.29, which is among the best surface ratio we mentioned above) shows the best activity. The DFT results are well consistent with the experimental results.
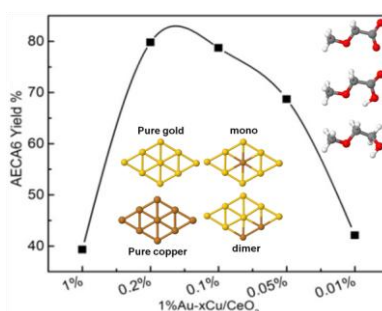

Fig. 1: Effect of Au-Cu formulation on the AEO7 oxidation, 80 °C, 16 h, 20 wt.% AEO7 in water, AEO7/metal = 432 (mol/mol), H_2O_2/AEO7 = 6.4 (mol/mol), H_2O_2 addition during 10 h.

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Non-metallic aerobic oxidation of alcohols over anthraquinone based compounds

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The catalytic performances of substituted anthraquinones were investigated in catalytic oxidation of alcohols like cyclohexanol, benzyl alcohol and 5-hydroxymethylfurfural (HMF) to carbonyl compounds (cyclohexanone, benzyl aldehyde and diformylfuran) (fig.1-a). We have found that reaction proceed at relatively mild conditions (130 °C, 10 bar O_2) with strong effect of oxygen pressure on the activity. The reduction potential of anthraquinone plays the key role in the oxidation reaction. TOF numbers and selectivities to carbonyl compounds pass through the maximum with increase of the reduction potential (fig.1-b). The maximum activity and selectivity (>80 %) is observed for sulfonated and carboxylated anthraquinones with intermediate reduction potential ($\approx$ 0.3 V) [1]. Grafted 2-carboxyanthraquinone catalyst has demonstrated comparable catalytic performance to the parent molecule and might be used as heterogeneous catalyst. The oxidation reaction was found to have radical character with transfer of hydrogen from alcohol to anthraquinone and subsequent oxidation of hydrogenated anthraquinone by oxygen.
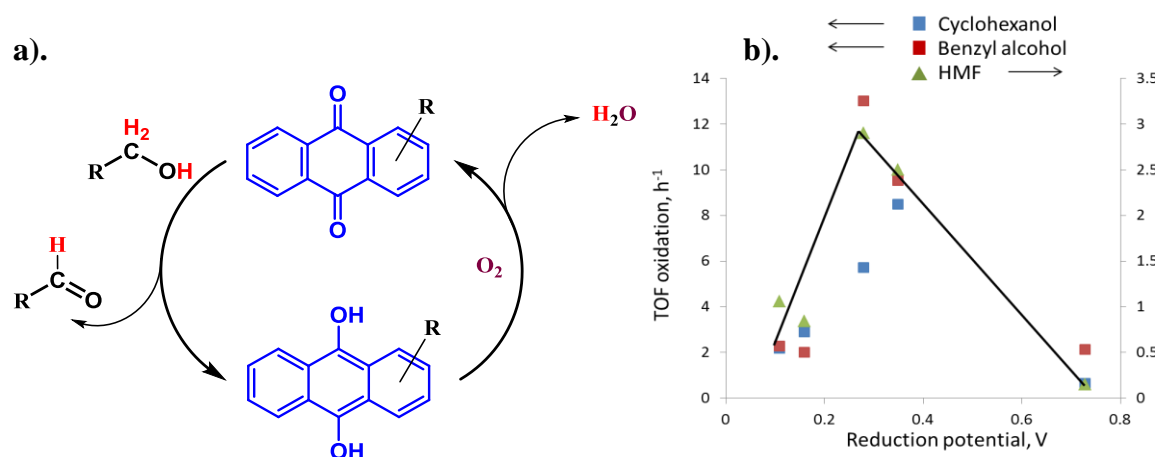

Fig. 1: (a) Schematic representation of the metal-free aerobic oxidation of alcohols in presence of Anthraquinone-based compounds; (b) TOF numbers of alcohols oxidation to carbonyl compounds at comparable conversion 60 %.
Conditions: cyclohexanol (T=130 °C, 1 mol/mol %, p(O_2)=10 bar, 2h), benzyl alcohol (T=150 °C, 1 mol/mol %, p(O_2)=10 bar, 2h) and HMF (T=130 °C, 1 mol/mol %, p(O_2)=10 bar, 2h)

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[1] DFT-calculated aqueous reduction potentials vs SHE / Method: B3LYP/6-311+G(d,p), PBF/6-31G(d).

P6

Unveiling the role of choline chloride
on furfural synthesis from a highly concentrated xylose

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Furfural has recently been emphasized as a versatile platform chemical for the production of top value-added chemicals such as fuel additives [1-2], being identified as one of the key chemicals produced from biomass [3]. The conversion of xylose to furfural occurs in an acidic media trough a dehydration reaction. Many research are devoted to this reaction, but starting from a low concentrated solution of xylose (up to 20 wt%). Indeed, the conversion of highly concentrated solution of xylose to furfural is scarcely reported in the literature due to polymerization reactions leading to a low selectivity to furfural. The main challenge of this reaction is to control the selectivity of this reaction by preventing the formation of humins.

We have studied the conversion of a highly concentrated solution of xylose (up to 50 wt%) to furfural in the presence of choline chloride, a cheap ammonium salt in the presence of HCl. We were pleased to see that 70% yield of furfural was obtained and that the initial production rate was enhanced due to the formation of choline-xyloside intermediate exhibiting higher reactivity than xylose(Scheme 1). A mechanism describing the action of choline chloride during xylose hydrolysis is proposed based on the kinetic and computational studies and will be presented. [4]
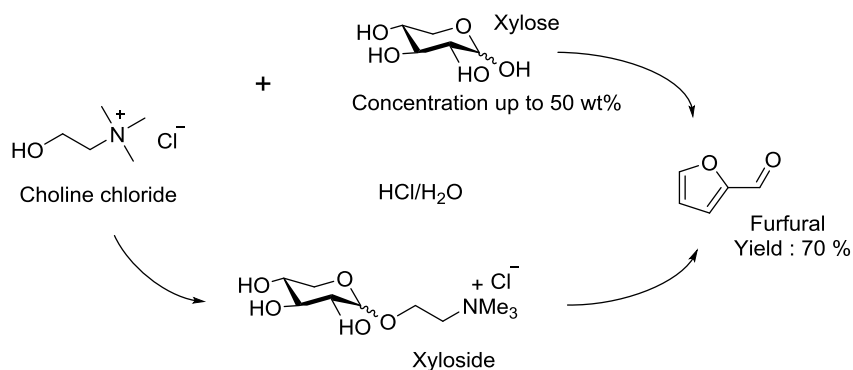
**Scheme 1 : Synthesis of furfural from a high concentrated feed of xylose
in the presence of choline chloride and HCl : formation of a high reactive choline-xyloside.**

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Single-site carbon-based cun₄ material as a selective electrocatalyst for CO_2 reduction to ethanol

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The direct electroreduction of CO_2 into gaseous and liquid fuels is currently considered as a promising strategy to store sustainable sources of energy while transforming a greenhouse gas into high value-added chemicals. It is generally believed that CO_2 electroreduction to multi-carbon products such as ethanol or ethylene may be catalyzed with significant yield only on metallic copper surfaces, implying large ensembles of copper atoms. We have been investigating an inexpensive Cu-N-C material prepared *via* a simple pyrolytic route that exclusively feature single copper atoms with a CuN_4 coordination environment, atomically dispersed in a nitrogen-doped conductive carbon matrix [1]. This material achieves aqueous CO_2 electroreduction to ethanol at a Faradaic yield of 55%, as well as CO electroreduction to C_2 products (ethanol and ethylene) with a Faradaic yield of 80%. This paves the way for the industrial application of inexpensive single-atom catalysts for the selective synthesis of multi-carbon products from anthropogenic CO_2 emissions.
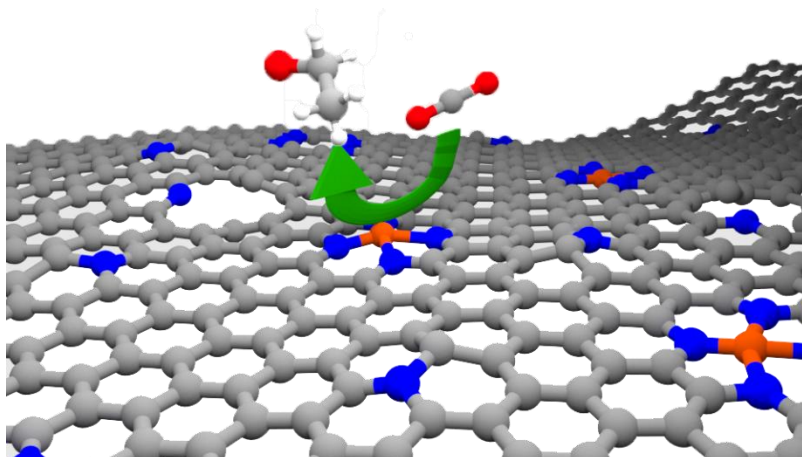

Fig. 1: Schematic representation of Cu-N-C material

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P8

Reductive amination of biomass-based aldehydes in aqueous solution over versatile Ni_yAlO_x catalysts

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Amines are key intermediates in the chemical industry with extensive applications in the manufacture of agrochemicals, pharmaceuticals, detergents, fabric softeners, lubricants, polymers and food additives. Biomass-based furanic aldehydes such as furfural and hydroxymethylfurfural (HMF), with various functional groups and associated reaction sites, opens the door to a wide range of chemical modifications making them versatile renewable building blocks. The reductive amination of aldehydes with ammonia in aqueous solution offers compelling advantages such as mild reaction conditions, the use of relatively cheap reagents and a wide availability of substrates over the other classical amine synthesis methods [1].

In this work, $NiAlO_x$ catalysts were developed for the reductive amination of various aldehydes and ketones in aqueous ammonia under mild reaction conditions. The influence of the Ni/Al molar ratio was demonstrated and the optimal $NiAlO_x$ catalyst was determined. This catalyst offers high selectivity and yield to the primary amine FAA, which can be further hydrogenated to THFAA by reacting the carbonyl compounds with aqueous ammonia solution (Fig. 1). Furthermore, HMF could also react with various primary and secondary amines to afford the corresponding amine products employing our catalytic route. The catalyst can also be recycled without loss of activity.
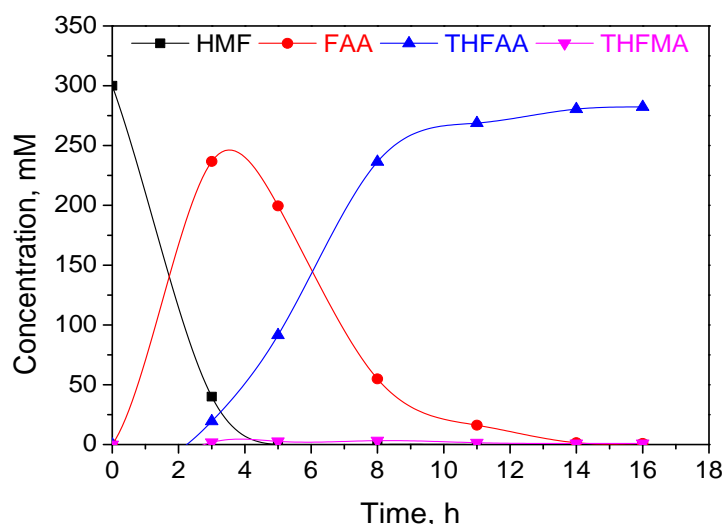

Fig. 1: Concentration profile as a function of time for the reductive amination of HMF over $NiAlO_x$ catalyst.

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Exploring the advances and challenges for innovation in green chemistry for the pharmaceutical world of tomorrow
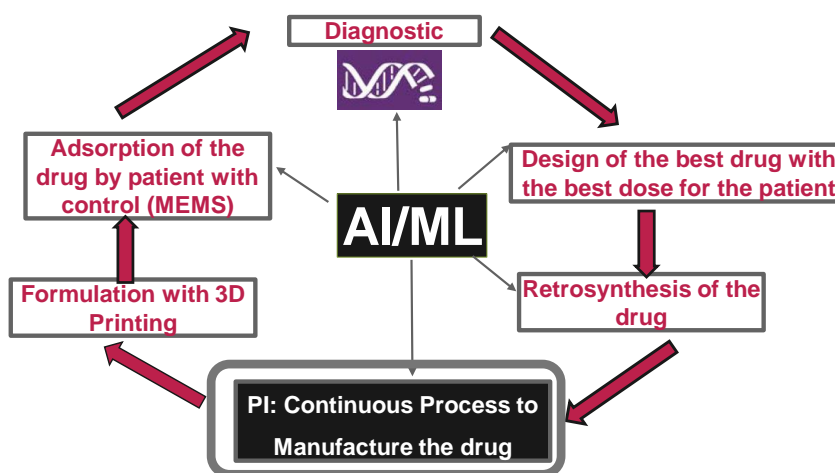
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Due to the different constraints, the pharmaceutical world must change his way of working and must integrate the new technologies to survive for developing a personalized medication. Innovation is the key of success to develop new drugs for a personalized medication. By taking the last disruptive innovations, AI/ML – 3Dprinting/3DBioprinting – IoT - Robots- MEMS- Process Intensification (Continuous chemical and biological process)-…, which are going to change the world, it can be developed new drug with a new process to get a personalized medication with the best drug for the patient by developing new green chemical and biological processes. An example concerning an antiepileptic drug will be shown. By transforming the batch process to a continuous process intensification (PI) with a multidisciplinary team, private and public researchers, it has been drastically reduced time production, (from several weeks to some hours), solvent consumption, energy consumption while increasing the global yield by 2.5. It has been developed a green chemistry by reducing CAPEX and OPEX. Furthermore, the full process can be done everywhere on a mobile unit on a skid. It is the pharmaceutical world of tomorrow.…

Fig. 1: the future: a personalized medication

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Patent: WO2017/076737 A1: "Continuous process for preparing Brivaracetam"
* Edith Lecomte Norrant is the future CEO of Legomedic

P10

One-pot synthesis of d-phenylalanine-functionalized multi-walled carbon nanotubes: a metal-free chiral catalyst for the asymmetric electroreduction of aromatic ketones

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Asymmetric synthesis is attracting considerable research attention given the increasing demand for chiral pharmaceuticals [1]. Many synthesis methods of chiral drugs have been established. However, such methods are generally catalyzed by precious metal catalysts, such as Ir, Ru, and Rh complexes [2]. In this study, we explored a chiral-functionalized multi-walled carbon nanotubes (MWCNTs) catalyst for asymmetric electroreduction. The catalyst can immobilize the chiral inducer onto the cathode material, thereby enabling the reuse of chiral inducer, reducing the use of metals.

p-MWCNTs functionalized by different dosages of D-4-amino-phenylalanine were obtained by an analogical method, and the corresponding samples were designated as D-PHE-MWCNTs-1, D-PHE-MWCNTs-2, D-PHE-MWCNTs-3, and D-PHE-MWCNTs-4.

Apart from the preparation and characterization of D-PHE-MWCNTs, we further explored the catalytic capability in asymmetric electroreduction. D-PHE-MWCNTs were fabricated as a chiral electrode to catalyze the asymmetric electroreduction of ketones. 2,2,2-Trifluoroacetophenone was selected as a model substrate. The cyclic voltammograms (Fig. 1) showed that the peak currents of functionalized MWCNTs were higher than those of p-MWCNTs, indicating that the MWCNTs enhanced catalytic activity for reducing the carbonyl group of the model substrate after functionalization.

The asymmetric electroreduction of the model substrate 2,2,2-trifluoroacetophenone was performed by galvanostatic method. The yields obtained on the functionalized MWCNTs (Table 1, entries 3-6) were higher than those on the p-MWCNTs (Table 1, entry 2). The ee values obtained from the D-PHE-MWCNTs (Table 1, entries 3-6) were markedly higher than those of p-MWCNTs (Table 1, entry 1), indicating that the functionalized MWCNTs cathodes were more beneficial as heterogeneous catalyst.
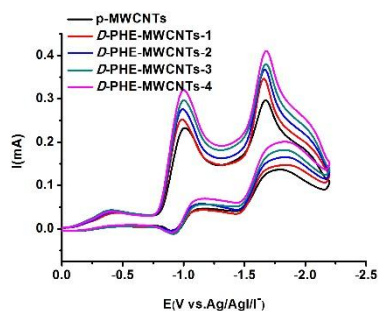

Fig. 1 Cyclic voltammograms of 50 mM 2,2,2-trifluoroacetophenon in MeCN/n-amyl alcohol (1/1)-0.1 M TEAI with the scan rate of 0.1 V s^{-1} on different electrodes: p-MWCNTs, *D*-PHE-MWCNTs-1, *D*-PHE-MWCNTs-2, *D*-PHE-MWCNTs-3, *D*-PHE-MWCNTs-4.

Table 1 Effect of cathode on the enantioselective electroreduction of 2,2,2-trifluoroacetophenon[a]

Entry	Cathode	Yield[b] (%)	ee[b] (%)
1[c]	p-MWCNTs	22	1
2[d]	p-MWCNTs	21	0
3	*D*-PHE-MWCNTs-1	23	20
4	*D*-PHE-MWCNTs-2	24	27
5	*D*-PHE-MWCNTs-3	25	32
6	*D*-PHE-MWCNTs-4	25	39

[a] Anode: Mg, 20 mL co-solvent (MeCN/n-amyl alcohol=1/1), 0.1 M substrate: 2,2,2-trifluoroacetophenone, supporting electrolyte: 0.1 M TEAI, current density: 3 mA cm^{-2}, charge: 2 F mol^{-1}, temperature: 25 $^{\circ}$C. [b] Determined by GC with a chiral column. [c] *D*-PHE added into reaction solution, the ratio of the *D*-PHE and p-MWCNTs is consistent with the *D*-PHE-MWCNTs-4. [d] No *D*-PHE added.

In summary, D-PHE-MWCNTs were prepared through one-step method and performed as a heterogeneous chiral catalyst in the asymmetric electroreduction of aromatic ketones. Chiral inducer-functionalized MWCNTs could be ideal chiral-modified electrodes available in asymmetric electroreduction of aromatic ketones.

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Metal – polyamine combined approach towards CO$_2$ capture and conversion

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In the quest for the ideal CO$_2$ sorbent, able to capture the gas in a diluted stream and then to release it with the minimal amount of heat possible, this work focuses on Diethylentriamine: this easily accessible amine shows a cooperative CO$_2$ absorption system reminding that of Hemoglobin towards oxygen. The shift from a low to a high loaded form on the amine depends on a supramolecular self-assembling process between two of the many members of the rich carbamated library resulting in a DETA methanolic solution upon CO$_2$ loading (Fig.1).
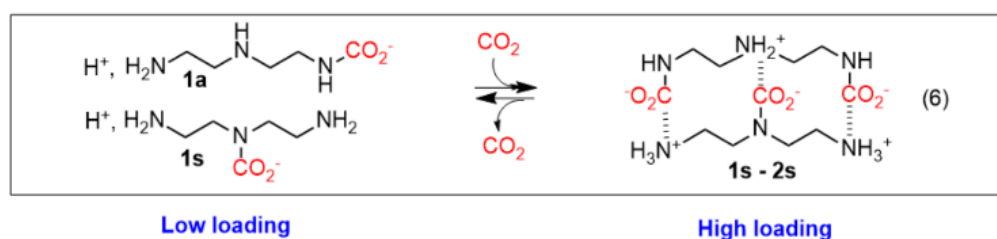

Low loading   **High loading**

Fig. 1. DETA carbamates shift from low to high loaded form in a CO$_2$ poor/rich environment

The affinity between high density charged metals and carbamated DETA can push cooperativity in strongly dissociative mediums such as water: Cobalt induces a disproportionation equilibria from two DETA monocarbamates to a bicarbamate which has been characterized by NMR, IR, UV-Vis and DFT calculations [2].

DETA is also versatile organic building block: a green, one step macrocyclisation forming polyazamacrcycles or nitrogen-rich cryptates and sepulchrates containing catalytic centres with which could be applied in integrative CCUS processes.

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P12

Structure-sensitive and insensitive reactions in alcohol amination over non-supported Ru nanoparticles

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The reaction rates and selectivity of many metal-catalyzed reactions depend on the size of metal particles in the nanoscale range. Primary amines are important platform molecules in chemical industry. In the present work [1], the catalytic performance of non-supported Ru nanoparticles with the sizes from 2 to 9 nm was investigated in direct amination of octanol and other alcohols into primary amines in the presence of ammonia. The 90 % selectivity to octylamine was obtained over small Ru nanoparticles (d=2 nm) even at 92 % conversion, whereas for larger Ru non-supported and supported nanoparticles, the octylamine selectivity dropped as the octanol conversion approaches 70-80 %. Primary reaction of alcohol amination into octylamine was found to be nearly a structure insensitive reaction. The selectivity to primary amine drops over large Ru particles at higher conversion, because of the secondary highly structure sensitive reaction of amine self-coupling (Figure 1). Over small negatively charged metal nanoparticles, the amine self-coupling is hindered, because of suppression of secondary imine hydrogenation. Similar structure sensitivity of the reactions involved in alcohol amination was observed for different substrates.
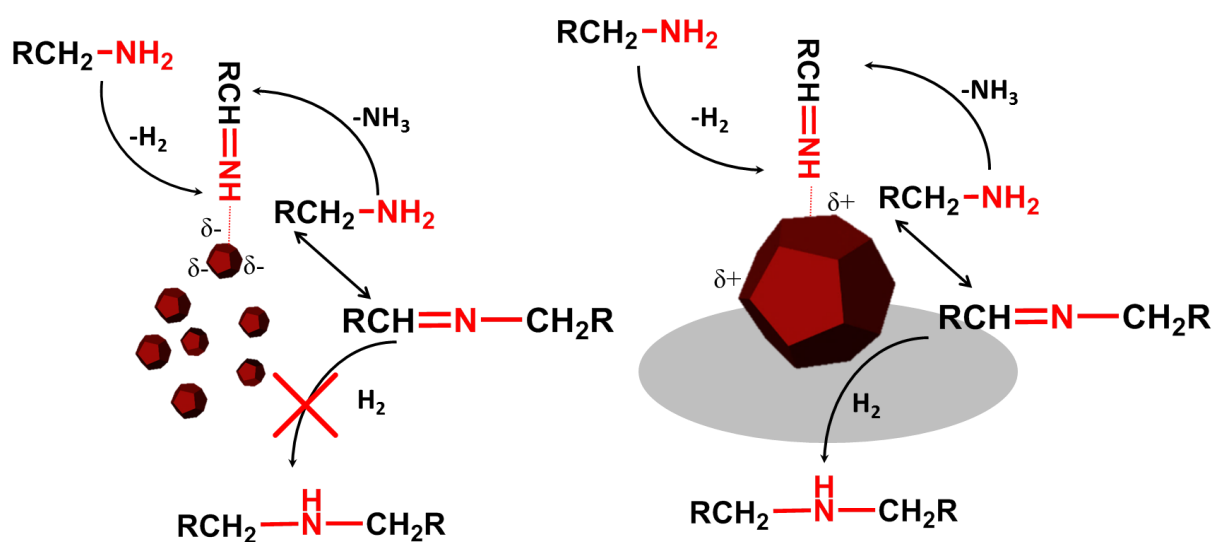

Fig. 1: Ru NP size and effect of support on self-coupling of primary amines

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Colloidal tectonics for tandem synergistic pickering interfacial catalysis: oxidative cleavage of cyclohexene oxide into adipic acid

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Organic syntheses using biomass-derived reagents usually encompass the reaction of immiscible reagents showing low catalytic activity due to resilient mass transfer limitations. *Pickering Interfacial Catalysis* (PIC) has recently emerged as a potential solution for overcoming such limitations. In this concept, the reagents are emulsified by solid amphiphilic catalysts, generating a large interfacial surface area that accelerates mass transfer.

Supramolecular preorganization and interfacial recognition can provide useful architectures for colloidal building. To this aim, a novel approach, based on colloidal tectonics involving two surface-active particles containing both recognition and catalytic sites, has been developed for controlling the formation and the properties of Pickering emulsions (Fig. 1). This was illustrated through the combination of dodecyltrimethylammonium phosphotungstate particles, $[C_{12}]_3[PW_{12}O_{40}]$, and silica particles functionalized with alkyl and sulfonic acid groups, $[C_n/SO_3H]@SiO_2$. The interfacial self-assembly occurs by the penetration of the alkyl chains of $[C_n/SO_3H]@SiO_2$ into the $[C_{12}]_3[PW_{12}O_{40}]$ supramolecular porous structure constituted of polar and apolar regions. These emulsions were used as a non-nitric acid route for adipic acid synthesis from the one-pot oxidative cleavage of cyclohexene oxide with aqueous H_2O_2. The catalytic performance was boosted due to the synergistic interactions between the particles.
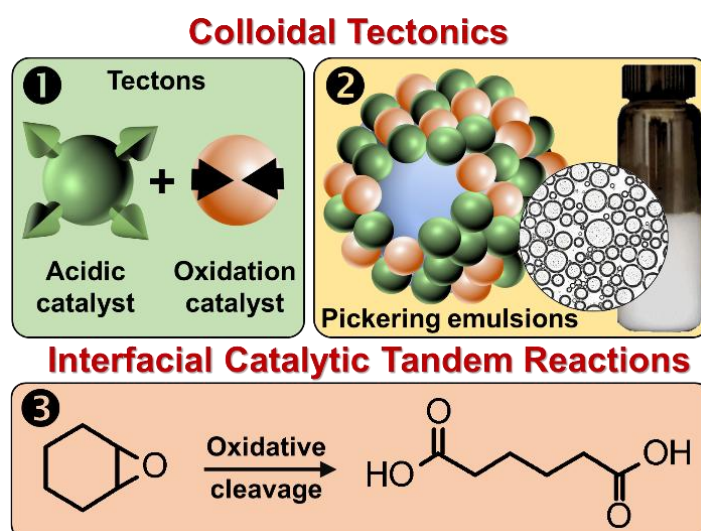

Fig. 1: Concept of colloidal tectonics for catalytic tandem reactions at the liquid/liquid interface

P14

Merging metathesis and photochemistry: a sustainable access to heterocyclic structures

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Since the discovery of powerful ruthenium based catalysts which are not sensitive to oxygen and can be easily handled, metathesis of alkenes can be considered nowadays as one of the most suitable method to directly functionalize alkenes. In parallel, olefins play a central role in synthetic organic photochemistry. Merging these two topics is therefore of great interest to reach efficiently unusual complex structures in a real sustainable manner. By using this concept, we already reported the access to various structures as lactones [1], macrolides [2] including some natural products.as amphiasterin B4 [3]. More recently, we have combined a metathesis reaction and a photochemical C-H activation reaction involving either an organocatalyst, either an organic photosensitizer, to deliver furofuranones or functionalized hexenolides [Fig 1] [4,5].
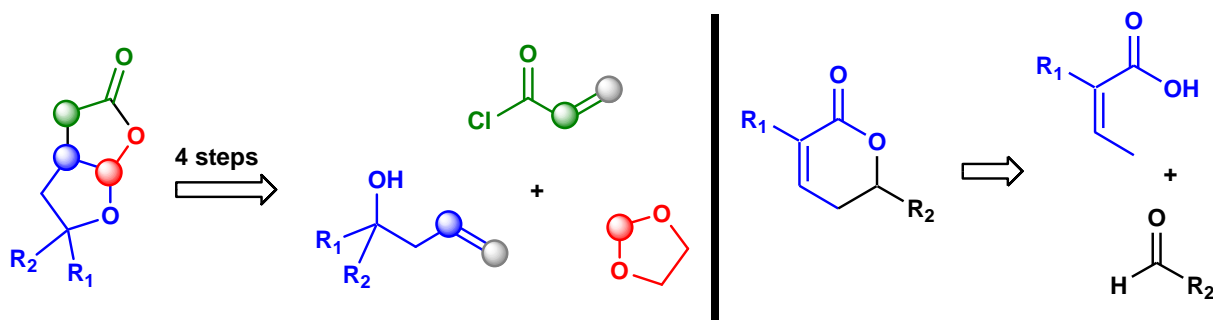

Fig. 1: Access to furofuranones and functionalized hexenolides

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P15

Carbohydrate amphiphiles: resource for biobased surfactants

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Surfactants are commodity chemicals used by all human beings in everyday life, with applications ranging from household and cleaning detergents, home and personal care products, cosmetics, foods, paints, inks, pesticides, polymers, textiles, lubricants, pharmaceutics, mining, to oil and gas recovery. Considering their very large tonnages and their end-of-life in the waste water or environment, they require novel design and processes for preventing undesired pollution or toxic effects. Among greener approaches, renewable resources, better than fossil ones, should be preferred. The natural hydrophilicity and hydrophobicity of carbohydrates and lipids, respectively, provides the necessary duality for designing surfactants. The strategy offers environmental benefit and opportunities for better added value to agricultural crops and co-products.

Based on the recent chapter that we have produced for the volume on *Green Chemistry and Engineering* edited by Prof. Buxing Han and Tianbin Wu, part of the new edition of the Spinger *Encyclopedia of Sustainability Science and Technology* [1], the poster gives an overview of the field of glycoamphiphilicity and biobased surfactants. Based on historical and more recent original amphiphilic compound families [2-6], it exemplifies the strategies either from native polyhydroxylated sugars or from furanic platform molecules obtained by dehydration (HMF and analogues). It highlights the wide range of properties possibly reached by subtle shape and functional modifications which arise from the variability of carbohydrate structures and the multiple ways to connect the hydrophobic moiety.
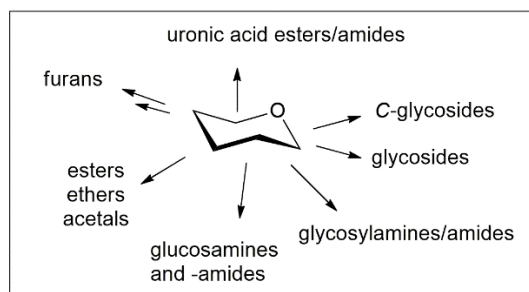

Fig. 1: connective strategies for derivation of carbohydrates to surfactants

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P16

Electrochemical CO_2 valorization to dicarboxylic acids and propiolactones

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Electrochemical synthesis could provide an elegant and efficient means to exploit the largely available C1 building block CO_2. Electrochemical synthesis allows very often a selective and single step synthesis where other methods fail to succeed. However, the activation of the stable CO_2 requires reactive co-reactants, high potential (around 2.1 V vs SHE) and more efficient electro-catalysts. In our laboratory study we could selectively synthesize dicarboxylic acids or propiolactones from olefines with CO_2 in a single step at room temperature. The change of the selectivity from the preferred diacid to the lactone was achieved by adding a catalyst into the reaction solution. Remarkable to mention is the fact that four member ring lactones are difficult to synthesize with common organic methods. Normally, the classical synthesis requires at least a 3-step reaction with expensive and toxic homogeneous catalysts. Synthesis routs that are described in the literature result in a low yield and six member ring lactones as main side product.[1] In our approach we achieve in a single step in moderate conditions 2-methyl-2-(propen-2-yl)-propiolactone with 20% yield and over 95% selectivity.

Lactones have a possible wide range of applications: they could be used as building block for fine chemicals, fungicide/herbicide in agro sector, and pharmaceuticals; they could find applications as fragrant or solvents and as monomer for polymers such as polyesters or surfactants. Ring opening of the lactone furthermore gives access to beta-hydroxy carbonic acids with tailor-made functional groups.
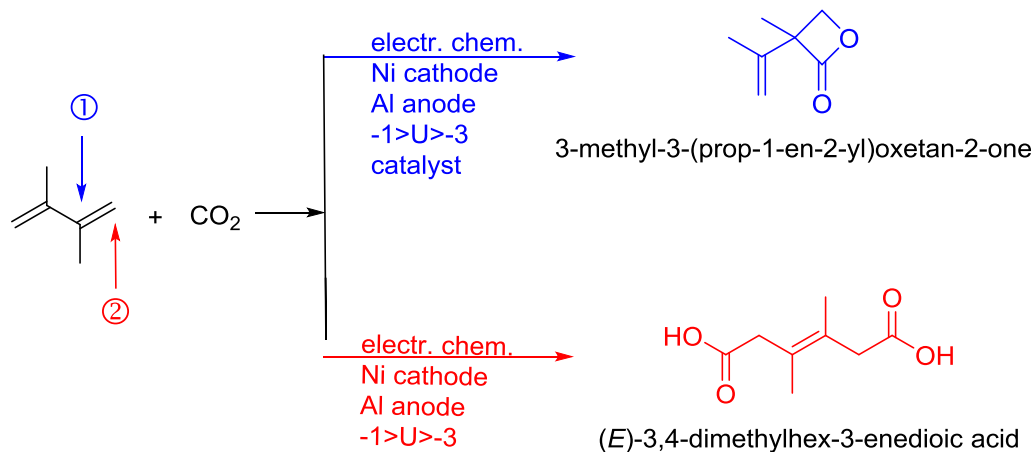

Fig. 1: The addition of catalyst changes the selectivity of the CO_2 attack resulting in propiolactone formation

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Carbon-based catalytic frameworks for green chemistry

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Confining catalytic sites can cause fundamental changes, affecting the system's entropy and creating cage-wall effects. To study these changes, we combine two-dimensional materials into 3D porous frameworks that host catalytic sites. Here we report the results for studies on graphene oxide.

We succeeded in synthesizing porous graphene frameworks (PGFs) that remain stable at temperatures up to 200°C. The graphene oxide sheets are first linked together by amine linkers that bind covalently to the sheets (see figure 1a). Then, the material is reduced, using the thermal instability of graphene oxide (figure 1b).

The linker can be modified with catalytically active groups. We modified the ethylene diamine linker arms of one such PFG with iodomethane into amine hydrohalides (figure 1c), a known catalyst for the insertion of CO_2 into epoxides [1]. Using styrene oxide as model system we reached 90% conversion and 96% selectivity while suppressing polymerization (figure 1d). We are now studying confinement effects for this reaction.

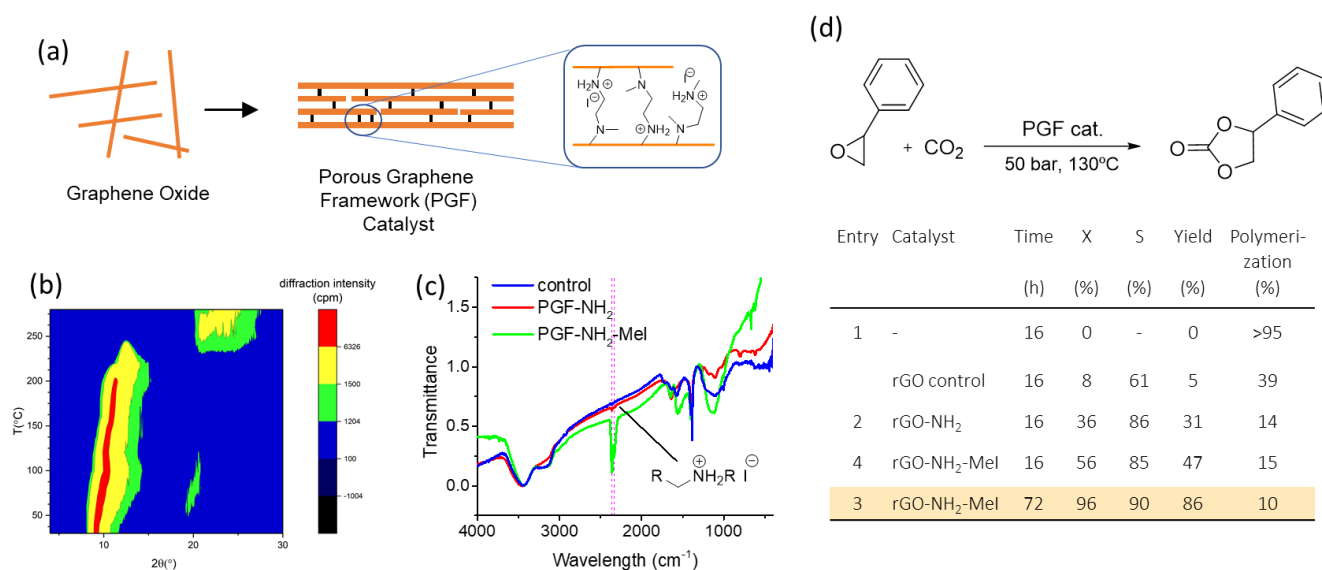| Entry	Catalyst	Time	X	S	Yield	Polymeri-zation
		(h)	(%)	(%)	(%)	(%)
1	-	16	0	-	0	>95
	rGO control	16	8	61	5	39
2	rGO-NH$_2$	16	36	86	31	14
4	rGO-NH$_2$-MeI	16	56	85	47	15
3	rGO-NH$_2$-MeI	72	96	90	86	10

Fig. 1: (a) synthesis of novel PGF-based catalyst, (b) XRD data showing thermal reduction of graphene oxide exploited in its synthesis (c) FTIR spectra showing presence of amine-hydrohalide groups and (d) catalytic results of the PGF catalyst for CO_2 cycloaddition.

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P18

Regulation of framework titanium siting in Ti-MWW by boron and aluminum incorporation and its effect on the catalytic performance in cyclohexene oxidation

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As a typical representative of the green chemistry, titanosilicates/H_2O_2 system has attracted great interests as applied in environmentally friendly chemical process for liquid-phase catalytic oxidation of various organic compounds. And the improvement of accessibility of Ti active centers is considered to be the main means to the effective utilization of titanosilicates. There are eight crystallographic T positions in the MWW skeleton and to control the distribution of Ti by introducing heteroatom Al is one of the possible ways.

The proper amount of aluminium source was added into the synthesis process of Ti-MWW, and the result showed the MWW structure was well preserved with the content of the framework "Ti" almost unchanged while an inversely proportional relationship between the heteroatom B and Al was found, which indicated an competition occupancy of the T position. Furthermore, the ^{27}Al MAS NMR analysis confirmed the introduction of the framework Al atoms which mainly located in the sinusoidal channel of MWW[1]. Combined with the experimental data that the cyclohexene conversion increased progressively but almost the same TON of "Ti" in 1-hexene oxidation, it is concluded that the heteroatom "Ti" tied to the the B atoms[2] were pushed into the outer surface of the zeolite through the insertion of Al atoms, therefore increasing the contact probability between the substrates and "Ti" active centers.
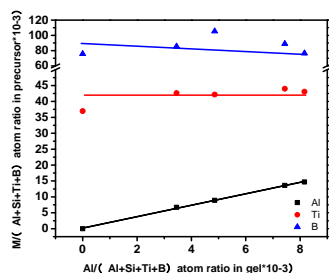

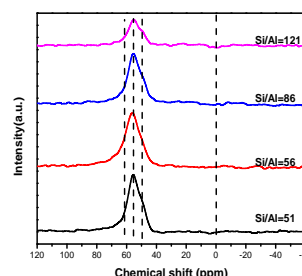**Figure 1. The dependence of the Al/(Si + Ti + B+Al) ratio in the as-synthesized samples**

Figure 2. The ^{27}Al MAS NMR in the as- synthesized samples

Table 1. The catalytic activity in the oxidation of cyclohexene

No	Si/Al[a]	distribution of Al species(%)[b]			Conv.(cyclohexene) (mol%)	Conv.(H_2O_2) (mol%)	Eff.(H_2O_2) (mol%)	Sel[c].(Epo) (mol%)
		Al$_{(49)}$	Al$_{(55)}$	Al$_{(60)}$				
1	∞	-	-	-	4.5	17.0	19.5	73.0
2	123	25.6	60.3	14.1	8.3	24.7	20.9	62.6
3	135	23.7	63.3	13.0	7.3	23.2	21.5	68.0
4	203	20.7	64.8	14.5	6.9	25.7	19.4	72.1
5	280	18.2	73.2	8.6	4.7	16.3	20.0	69.6
6[d]	∞	-	-	-	2.6	21.5	9.5	79.5
7[d]	123	25.6	60.3	14.1	1.3	32.9	3.3	82.1
8[d]	203	20.7	64.8	14.5	1.1	35.1	2.6	80.4

Reaction conditions: catalyst Ti-MWW(Si/Ti=45) 0.1 g; cyclohexene: 5 mmol; H_2O_2 (30 wt %): 5 mmol;CH_3CN: 10 ml; T = 333 K; t = 2 h. a:measured by ICP b:Al(50), Al(56) and Al(61) are the fractions of three Al species in the total Al species resolved at 49, 55, and 60 ppm, respectively. c:cyclohexene oxide, cyclohexene-1,2-diol d:The poisoning of samples was conducted by adding 1 mmol of 2,4-dimethylquinoline into the reaction mixture.

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Solventless conditions for the Baylis-Hillman reaction of HMF and GMF

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Carbohydrates and their derived furanic platform molecules are interesting substrates for fine chemistry and useful resources for making biobased chemicals, especially in the fields of surfactants and monomers [1-3]. We have recently developed a new approach to carbohydrate-containing derivatives based on the Baylis-Hillman reaction of hydroxymethylfurfural (HMF) or other furanic systems with acrylic reagents, leading to new biobased α-hydroxymethyl-alkenes [4-6].

We report here our investigations on the no-solvent conditions for the reaction of HMF and analogs with methyl acrylate. For HMF or its simpler analog furfural, the reaction can proceed even with very low excess methyl acrylate or even using a 1:1 stoichiometry, with yields up to ca. 80 % although in slower reactions. The study included the much more polar GMF (glucosyloxymethylfurfural), an interesting HMF analog derived from the disaccharide isomaltulose. However, GMF being a solid, the no-solvent conditions are less appropriate and then low-solvent conditions (syrups made with minimal amounts of MeOH: 1ml/20mmol) are required for the reaction to proceed with acceptable yields.
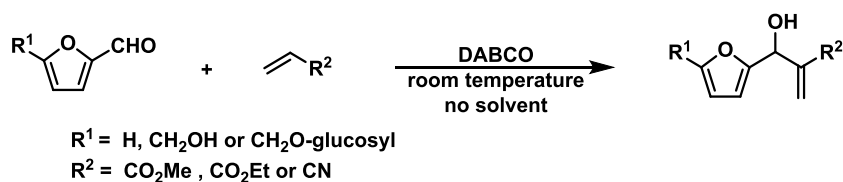

R^1 = H, CH_2OH or CH_2O-glucosyl
R^2 = CO_2Me, CO_2Et or CN

Fig. 1: Baylis-Hillman reaction of HMF and GMF

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P20

Iodization of palladium-supported catalyst for ethers production from bio-derived feedstocks

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Surface modification of metal catalysts is an important strategy for fine-tuning chemoselective reactions. Recent works have focused on the fabrication of organic monolayers like thiols and amines on noble metals surface by tuning the steric effect [1, 2]. However, the modification of metal surfaces with inorganic atoms, such as iodine, remains challenging due to the strong interaction between iodine and metals which normally causes total catalyst deactivation. Herein, we report an efficient palladium-iodide catalyst for direct production of ethers from aldehydes and alcohols. As shown in fig. 1, the adsorbed iodine atoms located on the surface of Pd with high electronic density favors the stabilization of H^+ species (hydrogen spillover-type mechanism) during the hydrogenation reaction. The protons grafted on iodine are able to activate the aldehydes and then, to produce acetal-like intermediates in the presence of alcohols. Hydrogen atoms from bare-Pd sites disassociate the C-O bond to form the target ethers. The proposed formation of protons on Pd-I catalyst was determined by in-situ pyridine-FTIR analysis. An obvious peak located on 1540 cm^{-1}, assigned to Brønsted acid sites, was observed when pyridine and hydrogen were present at the same time on the catalyst surface. Interestingly, after removing hydrogen, this peak disappeared, and appeared again after re-charging hydrogen. These results confirmed the hydrogen spillover-type mechanism from bare-Pd to Ads-I on the iodine-modified Pd surface, which is a key step for the etherification reaction.
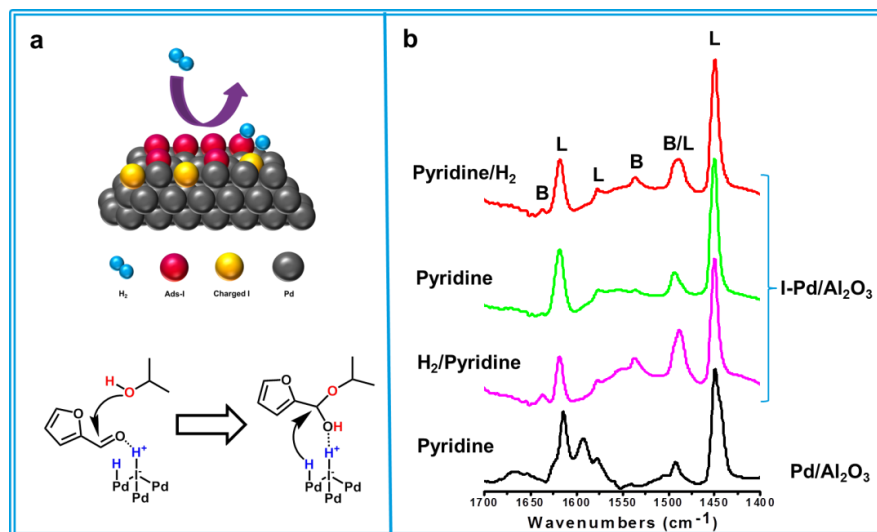

Fig. 1: (a) Illustration of the hydrogen spillover over I-Pd/Al$_2$O$_3$ catalyst and the activation of furfural; (b) In-situ pyridine-FTIR for I-Pd/Al$_2$O$_3$ catalyst and Pd/Al$_2$O$_3$ catalyst.

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Addressing some fundamental questions in alcohol amination

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Synthetic amines, which are widely used as solvents, agrochemicals, pharmaceuticals, and detergents, are historically produced from feedstocks such as nitriles, carboxylic acids, and alkyl halides. With the development of many biomass-based technologies, alcohols become a potential and promising source for the production of amines, and the direct amination of alcohols is an ideal route for the synthesis of amines with water being the only byproduct [1].

Our group has been working on the direct amination of alcohols with ammonia for the synthesis of primary amines in the last few years. Recently we tried to address some fundamental questions in alcohol amination that have not been covered in the literature, such as the effect of metal particle size on the activity and selectivity, and the stability of different catalysts under amination conditions. Some preliminary results will be presented. In the amination of 1-octanol, we found that Ru-based catalysts were stable under reaction conditions, whereas a cobalt catalyst deactivated quickly. The cause of the deactivation will be discussed relying on a combination of characterization techniques (*e.g.*, H_2-TPR, Fig. 1). By studying the same reaction over Ru catalysts with varying particle sizes, we will show that the reaction is structure insensitive on Ru surfaces.
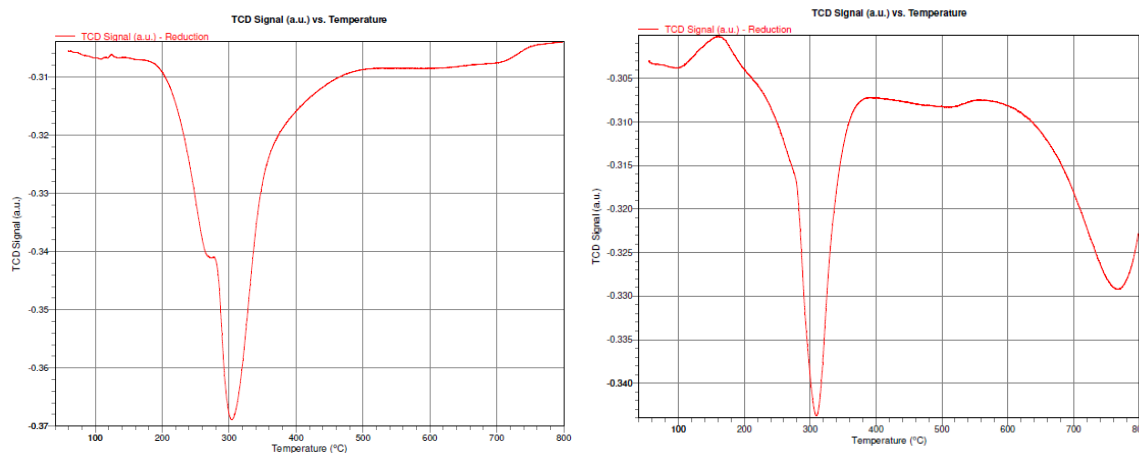

Fig. 1: TPR profiles of fresh (left) and deactivated (right) cobalt catalysts.

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P22

Fluorescent metallosupramolecular functional materials

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Over the past three decades, the preparation of fluorescent discrete metallosupramolecular architectures through coordination-driven self-assembly has garnered great attention due to their promising applications such as chemical sensors, optical devices, supramolecular biomedicines, and so on.[1] However, many problems are still far from being fully resolved in this area. For example, it is quite challenging to investigate the processes and dynamics of coordination-driven self-assembly due to the existence of multiple intermediates and many possible processes.[2] Moreover, the dynamic nature of coordination bonds sometimes lead to the instability of the obtained metallosupramolecular architectures, which might be decomposed under the relatively harsh conditions.[3] Therefore, the development of new method for the exploration of the processes and dynamics of coordination-driven self-assembly and the construction of functional metallosupramolecular architectures with the improved stability are particularly necessary.

Recently, we have presented the first successful example on real-time monitoring the process and dynamics of coordination-driven self-assembly by employing fluorescence-resonance energy transfer (FRET) (Fig. 1a).[4] The high sensitivity and efficiency of FRET allowed for monitoring the self-assembly process and dynamics of the metallosupramolecular architectures in real time. This work undoubtedly deepens the understanding of the coordination-driven self-assembly process, thus allowing for the design of new functional metallosupramolecular materials in the future.

Moreover, we have provided the successful fabrication of porphyrin-containing fluorescent metallacycles in the confined cavities of mesoporous carbon FDU-16 (Fig. 1b).[5] Employment of the ordered cavities as a platform to anchor and isolate porphyrin-containing metallacycles prohibited their self-dimerization and oxidative degradation, which allowed for the enhancement of photosensitization efficiencies and catalytic activities.
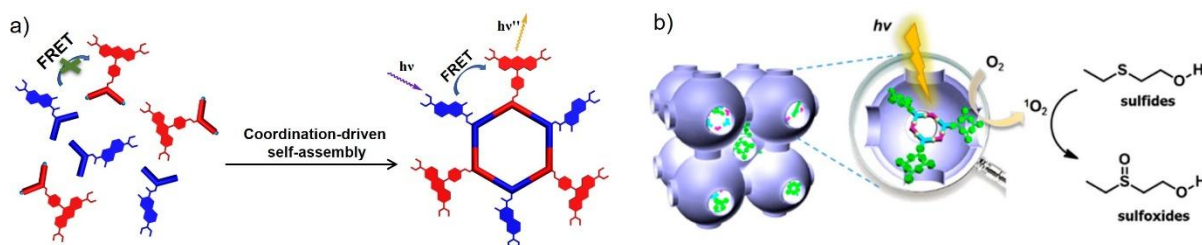

Fig. 1. a) Real-time monitoring the dynamics of coordination-driven self-assembly by employing FRET. b) Schematic presentation of self-assembly of trisporphyrin metallocycle in cavities of mesoporous carbon FDU-16 and the application of photooxidation of sulfides.

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The p band intermediate state (PBIS) tailors photo-luminescence emission at the nanoscale interface

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The availability of a range of excited states has enriched low dimensional quantum nanostructures with interesting luminescence properties. However, few breakthroughs concerning their photoluminescence (PL) emission origin limited the practical applications. Using metal nanoclusters (NCs) as a model system, by judiciously manipulating the delicate surface ligand interactions on single metal nanocluster or in superlattice, the resulting interplay of various noncovalent interactions leads to the precise modulation of emission colours and quantum yield (QY). A new p band state, resulting from the strong overlapping of p orbitals of the paired or more adjacent heteroatoms (O, N and S) bearing on the protecting ligands, was identified as a dark state to activate triplet state of the surface aggregated chromophores, allowing for the development of bright and practical metal NCs luminophores and rational engineering of closely relevant light emitting and harvesting quantum structures.
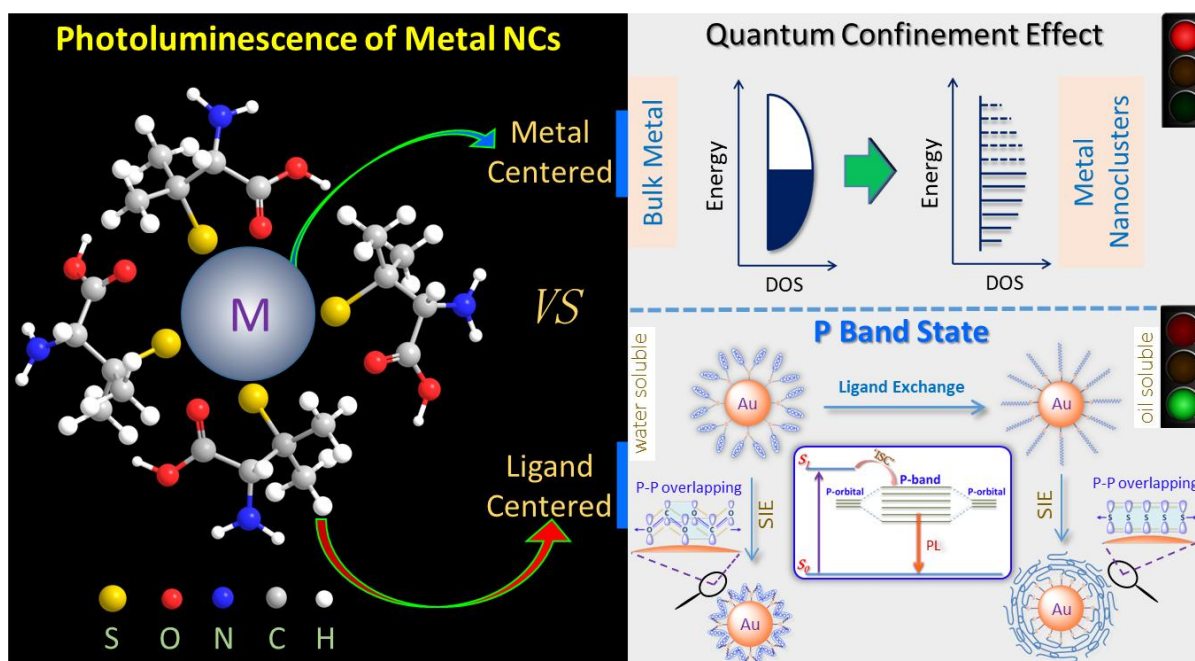

Fig. 1. P band intermediate state (PBIS) plays the relaxation of excited state at the nanoscale interface.

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P24

Reaction-induced CoO@Cu$_2$O nanocomposites in-situ onto SiC-foam for gas-phase oxidation of bioethanol to acetaldehyde

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Acetaldehyde (AC) is one of the most widely used commodity chemicals, and the gas-phase oxidation of bioethanol (EtOH) to acetaldehyde (AC) is thus greatly important to the green and sustainable goals for the chemical industry. The Ag catalysts, such as electrolytic Ag and oxides supported nano-Ag, have been commercialized for the titled reaction by air, but suffer from either low activity for electrolytic Ag or sintering for nano-Ag. Recently, a promising Au/MgCuCr$_2$O$_4$-spinel was tailored, offering full conversion and 95% AC selectivity with a single-run lifetime of 500 h at 250 $^\circ$C[1]. However, the limited availability of noble metals spurs intense efforts to develop the cheap catalysts based on oxides. In addition, this process is strongly exothermic, which requires the catalyst with high heat-transfer ability to dissipate the reaction heat. Herein, we discover a silicon carbide (SiC) foam supported CoO@Cu$_2$O nanocomposites (i.e., large CoO particle partially covered with small Cu$_2$O particles)[2], which is active, selective and stable for the titled reaction. Interestingly, the catalyst CoO@Cu$_2$O/SiC-foam is obtainable exclusively via in situ transforming the cobalt and copper nitrates supported onto the SiC-foam in the real reaction stream. Details of catalyst preparation, catalyst characterization, and catalyst evaluation are available in the Ref. [2]. For comparison, we also prepared other catalysts by precipitation (CuCo-PPT/SiC-foam), surface impregnation combustion (CuCo-SIC/SiC-foam), and colloidal nanosynthesis (CuCo-NANO/SiC-foam) methods. Unfortunately, CuCo-PPT/SiC-foam and CuCo-SIC/SiC-foam deliver the EtOH conversion of below 18%; CuCo-NANO/SiC-foam gives a slightly increased conversion of 40.3%. Interestingly, the CoO@Cu$_2$O/SiC-foam catalyst gives very high performance: 95% conversion with 97.8% selectivity at 280 $^\circ$C, more active than the Ag catalysts and comparable to the Au-based catalysts such as Au/CuMgCr$_2$O$_4$-spinel[2]. The CoO@Cu$_2$O/SiC-foam was characterized by TEM, and an interesting CoO@Cu$_2$O ensemble was imaged, thus offering abundant CoO-Cu$_2$O interface (Fig. 1A). To confirm such "CoO@Cu$_2$O"-governed EtOH oxidation, a similar "CoO@Cu$_2$O" nanostructure was tailored by nanosynthesis technology (Fig. 1B) and supported on SiC-foam, delivering a comparable EtOH conversion of 89%. Moreover, another inverse nanostructure of Cu$_2$O@CoO was tailored (Fig. 1C), but delivers a very low conversion of only 20%. One more mixed-oxide nanostructure of CoO&Cu$_2$O with both size of 50-100 nm was also synthesized (Fig. 1D); as expected, only 21% conversion is obtainable due to the insufficient interface and the reduction of Cu$_2$O to Cu^0. Moreover, steady conversion of 91-95% is achieved at 280 $^\circ$C with 95-97% selectivity for at least 200 h without any signs of deactivation, indicating a high stability of such Cu$_2$O@CoO nanostructure for the titled reaction.
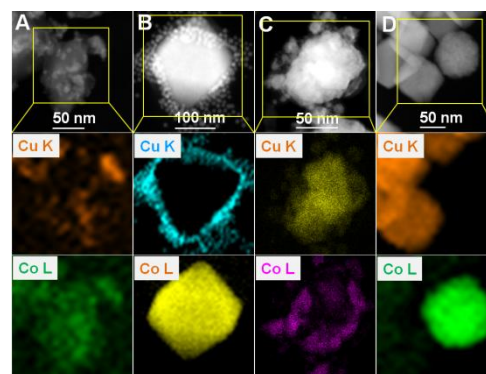

Fig. 1: High-angle annular dark field STEM image and elemental maps: (A) Reaction-induced CoO@Cu$_2$O for the CoO@Cu$_2$O /SiC-foam, as-synthesized nanostructures of (B) CoO@Cu$_2$O, (C) Cu$_2$O@CoO, and (D) CoO&Cu$_2$O through nanosynthesis technology[2].

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Mild reduction of phosphine oxides by phosphites

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Organophosphorus compounds are an important class of organic compounds, with a widespread application in various fields such as agriculture, medicine, biology and industry. Currently, the reduction of phosphine oxides to produce phosphines is a particularly interesting approach to industry, as a number of large-scale processes generate phosphine oxides as byproducts[1]. At present, three main systems are used to reduce phosphine oxides to phosphines: (1) metal hydrides; (2) silanes, especially $HSiCl_3$; (3) Lewis acids or Brønsted acids with silanes as reducing agents[2]. However, for these systems, reagents are usually difficult to be handled with under air and moisture, and harsh reaction conditions are often required, *e.g.* high reaction temperature and long reaction time.
.

Therefore, it is necessary to develop a new process which overcomes the above described disadvantages. A mild protocol for the reduction of phosphine oxides to phosphines was developed in our group by using inexpensive diphenyl phosphite (DPPhite) as reducing agent and iodide (I_2) as oxidant at room temperature[3]. Eight different phosphines were obtained with moderate to good isolated yields.
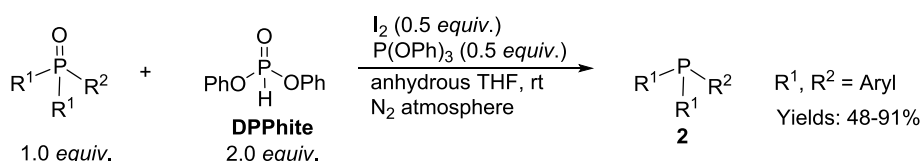

Fig. 1: The reduction of phosphine oxides to phosphines with DPPhite and I_2

Based on experiments and DFT calculations, we proposed a mechanism involving oxygen transfer between the starting phosphine oxide reagent and DPPhite *via* an iododiphenylphosphate $(PhO)_2P(O)I$. This highly reactive species easily undergoes nucleophilic attack by the oxygen atom of phosphine oxide. The dissociation of the formed intermediate results in the transfer of the oxygen atom of phosphine oxide to yield diphenyl phosphate $(PhO)_2P(O)OH$ and the [phosphine–I_2] adduct. Finally, another molecule of DPPhite reacts with [phosphine–I_2] adduct to release phosphine and to regenerate $(PhO)_2P(O)I$.

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P26

Utilization of CO$_2$ as a C1 building block for the synthesis of cyclic carbonates and carbamates

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The development of green carbon science is a very important task for the sustainable chemistry. [1] In this context, the efficient synthesis of fuels and value-added chemicals by using CO$_2$ as an inexpensive, nontoxic and renewable C1 synthon has attracted ever-increasing attention. Among the known more than 20 reactions, the synthesis of cyclic carbonates and carbamates using CO$_2$ as starting material is of current research interest. Despite significant achievements in this area, the development of new catalyst systems and new reactions is still important.

We have reported a bifunctional phosphorane-(salen)CoI complex as a new type of efficient catalysts for the coupling reaction of CO$_2$ with epoxides or aziridines under ambient conditions with a catalyst loading of 0.1-2.5 mol%.[2] The key to the efficiency is the activation of (salen)CoI by a phosphorane, which could not only enhance the Lewis acidity of the Co center for electrophilic activation, but also simultaneously generate an iodide to facilitate the ring-opening process.

We also developed a novel tandem asymmetric A^3-coupling-carboxylative cyclization sequence for the facile synthesis of chiral *N*-aryl 2-oxazolidinones from simple starting materials with CO$_2$ as C1 synthon under mild conditions, which constitutes a rare example of asymmetric tandem reactions capable of CO$_2$ fixation.[3] Notably, the combination of 1,3-diphenylguanidine (DPG) with silver salts was essential for the carboxylative cyclization of *N*-aryl propargylamines and CO$_2$. Take advantage of this catalyst system, an unprecedented highly efficient carboxylative cyclization of homopropargyl amine with CO$_2$ for the construction of six-membered 2-oxazinones was realized recently.[4]
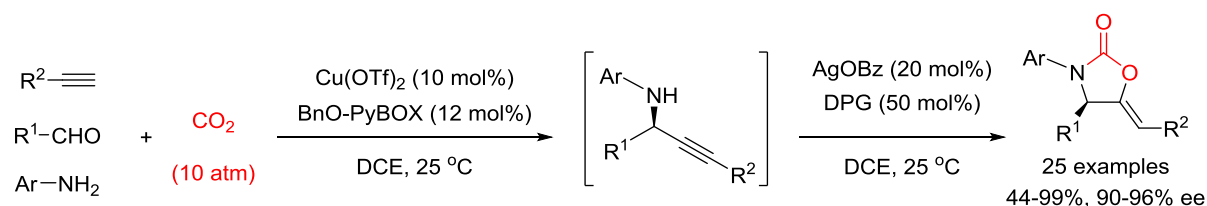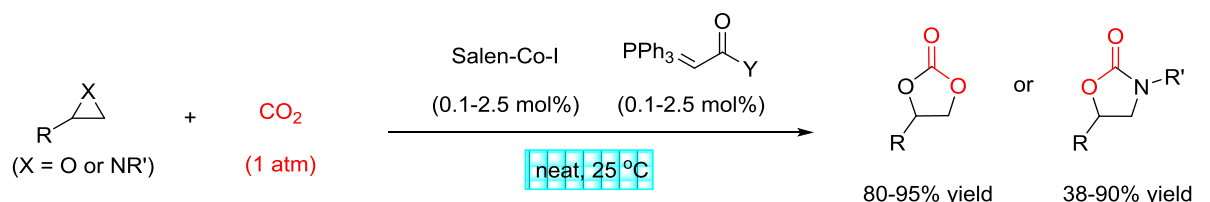
Chemical fixation of CO$_2$ to cyclic carbonates and carbamates

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Pickering-assisted catalysis for efficient solvent-free oxidative desulfurization using H_2O_2 and polyoxometalates

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Carbon functionalized silica was used as an emulsifier for the biphasic oxidative desulfurization of benzothiophene (BT) dissolved in catalyzed by $H_3PW_{12}O_{40}$ (HPW) using H_2O_2 as an oxidant. In this concept that we have termed here as Pickering-Assisted Catalysis (PAC), the silica favors the formation of a water/decalin emulsion, enhancing mass transfer between the immiscible phases without using a cosolvent, whereas the HPW catalyst is hosted is the water phase (Fig.1).[1,2] The effect of the operation variables such as the type of silica, the amount of HPW, the H_2O_2/BT molar ratio and the reaction time, was studied in detail. The results show that the PAC concept could significantly enhance the BT conversion up to a value of 79% compared to a non-emulsified biphasic reaction system due to the formation of Pickering emulsions stabilized by the silica nanoparticles. Furthermore, the addition of less than 1 vol% of methanol or ethanol to the emulsified system could further enhance the BT conversion to 95% at a much lower H_2O_2/BT molar ratio (from 4 to 2.5) due to both a more favorable extraction of the sulfone product from the oil to the water phase, and a facilitated formation of Pickering emulsions. Last but not least, the BT conversion kept almost unchanged during four consecutive runs. This result demonstrates the high level of recycling and the integrity of the silica nanoparticles and the HPW catalyst during operation.
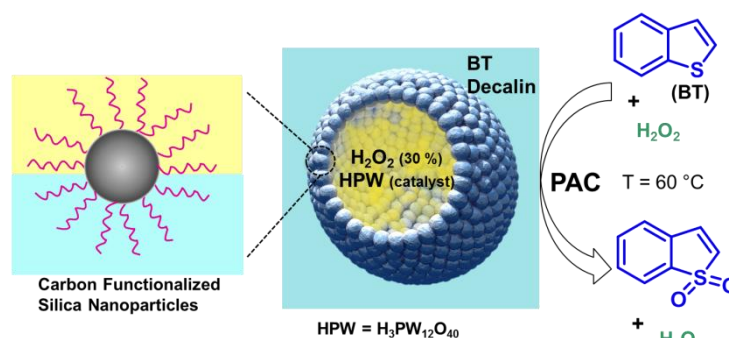

Fig1. Biphasic Oxidative Desulfurization catalyzed polyoxometallate using amphiphilic silica nanoparticles as emulsifier under PAC.

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P28

Valorization of biomass ketoses to surfactants through aldolisation

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From several decades, the surfactant industry has developed quite fast since surfactants are widely applied in our daily life. For example, surfactants can be used as pesticides auxiliaries in agriculture, as ingredients for detergency and cosmetics, as additives in pharmaceutical industry, also in paint, lubricant, food and fuel industry [1]. Most of the commercially available surfactants are ester-linked, so they are not stable in acidic and basic conditions. In this context, we have previously developed new C-C bond-linked surfactants (Scheme **1**). The aldolisation of dihydroxyacetone (DHA, the simplest ketose) has been realized with various aldehydes, followed by a hydrogenation step, to give tetraol surfactants.
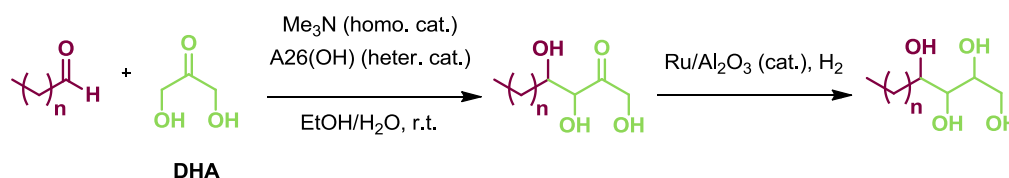
Scheme 1: Surfactants from biomass DHA through aldolisation

The substrate scope of the aldolisation-hydrogenation process has been extended under the selected conditions by using some biosourced aldehydes (such as citronellal, furfural). After obtaining a series of alkyltetraols, their physico-chemical properties have been studied by measuring the critical micelle concentration (CMC) for evaluating their performance as surfactants. The results are quite interesting and are compared with commercially available surfactants [2].

Furthermore, fructose has been taken into account as biomass substrates since they are abundant in Nature and are relatively inexpensive. The aldolisation of fructose has been carried out using the previously optimized conditions with DHA, unfortunately, very limited yield has been achieved. As a consequence, the conditions were re-optimized and with the help of Phase Transfer Catalyst (PTC) [3], to give fructose derived alkyl surfactants. To the best of our knowledge, this is the first example to make the direct aldolisation on unprotected fructose.
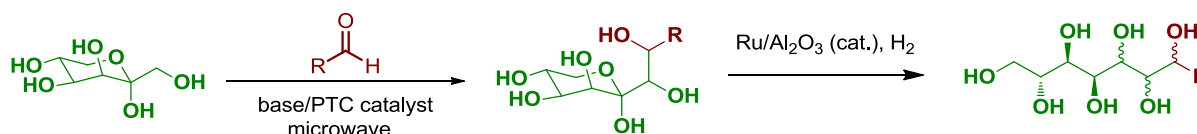
**Scheme 2: Surfactants from fructose through aldolisation**

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Natural products total synthesis and medicinal studies

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The chemical synthesis of structurally interesting and biologically relevant natural products has served as a driving force for developing new methodologies, testing the scope of existing synthetic methods. It also provides the platform for the further identification of their specific biological targets and mechanistic mode of action. Our research interests are devoted to develop synthetic useful methodologies to address natural target molecules that have novel molecular structure, potent biological activity, and the potential for mechanistic studies. In this poster, we will introduce our synthetic studies towards polycylic natural products uisng different strategies including photo-Nazarov and photoenolization/Diels–Alder (PEDA) reactions.
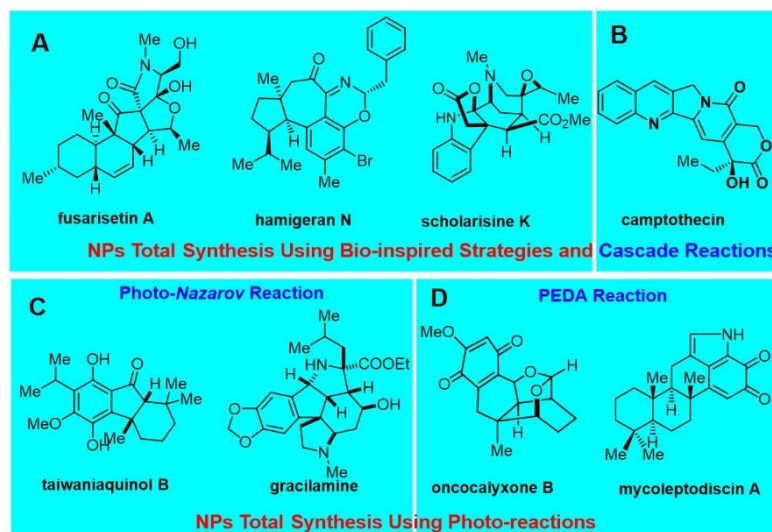
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P30

Interfacial interaction regulated CO oxidation over transition metal atoms on hexagonal boron nitride

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We investigated the electronic structure and CO oxidation mechanisms over transition metal (TM) atoms, namely Au and Pt, immobilized by vacancy defects on gas-exfoliated hexagonal boron nitride (h-BN). We showed that chemical bonds at TM/h-BN interface not only alter the thermodynamics and kinetics for the aggregation and effectively immobilize TM atoms, but also significantly change the composition and energetic distribution of the electronic states of the composites. First-principles based thermodynamics analysis show that coadsorption of CO and O_2 is favored over other surface phase at conventional reaction conditions. This further regulates the CO oxidation over TM/h-BN to proceed only through a Langmuir-Hinshelwood mechanism, involving the formation and dissociation of a peroxo intermediate and the reduction of the composites. The calculated reaction barriers for CO oxidation over TM/h-BN are all lower than 0.50 eV. The microkinetics simulations over Au/h-BN also show a maximum TOF of 1.28 s^{-1} for CO oxidation at 298.15 K with P_{O_2}= 20 Pco = 0.2 bar and is already comparable to that of reported single atom catalysts over transition metal oxides. The findings highlight the in-situ CO oxidation mechanisms and finely explain the potential superior performance of transition metal atoms deposited over non-redox-active support.

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95

Informations and Indexes

General Information and Internet Connection

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You may show this address to the taxi drivers: 中山北路 **3663** 号华东师范大学
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Public Transportation from / to the conference location (Zhongshanbei Campus of ECNU)

1. Metro Line 3 & 4: get off at Jinshajiang Rd. Station, ten minutes' walk to ECNU.

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3. Railway Station

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Wireless internet access is available in the Conference building.
Free wifi is available at the Coffee bar of Yifu hotel, close to the Lobby

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It is located in the Entrance Hall of the Building. You will collect your delegate badge and conference documentation at the registration desk and then check in. Please note that lecture halls, restaurant, and social events are accessible only with your name badge.

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

Poster Area
The poster session will take place on the corridor on the two and third floors of Shanghai Key Lab of Green Chemistry and Chemical Processes (see map on next page Building No. 28)

Certificate of attendance
All registered participants will be delivered a certificate of attendance.

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The organizers do not accept responsibility for individual medical, revel or personal insurance.
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Midday buffet lunches will be served in the Western Cafeteria (西餐厅) (see map building No. 33 on next page).

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Location:
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Public Transport Map

List of Participants

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GAO	Shuanhu	East China Normal University, Shanghai
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LIU	**Xiaoyan**	East China Normal University, Shanghai
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LIU	**Xue**	East China Normal University, Shanghai
LIU	**Ye**	East China Normal University, Shanghai
LIU	**Yueming**	East China Normal University, Shanghai
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LU	**Yong**	East China Normal University(ECNU) , Shanghai
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Author Index

GERARD	Jean-François	IL21
GIL	Sonia	P3
GIMBERNAT	Alexandra	IL18
GIRARDON	Jean-Sébastien	IL18
GIROIR-FENDLER	Anne	P3
GLENADEL	Quentin	P14
GU	Qingyi	P4
GUEHL	Marie	IL18
GUN'KO	Yurii	OC1
GUO	Yanglong	P3
GUO	Yanna	IL15
HASAN	Tawfique	IL17
HE	Mingyuan	P18
HU	Zhi-Yi	IL17
HERNANDEZ ENCISO	Willington Y.	P5, P20
HUANG	Yongji	P8
JACQUEL	Nicolas	IL22
JACQUIN	Marc	IL29
JAOUEN	Frederic	P7
JEROME	François	IL33, P6
JIANG	Jingang	OC3
JIANG	Shi	P6
KARAPINAR	Dilan	P7
KHODAKOV	Andrei Y.	P12, P20
KONG	Lingzhao	IL11
KUSEMA	Bright T.	P8, P21
LAI	Jonathan	IL33
LECLAIRE	Julien	IL20, P11
LECLERCQ	Loic	P13
LECOMTE-NORRANT	Edith	P9
LEINEKUGEL LE COQ	Damien	IL29
LEMAIRE	Marc	P28
LI	Jerry Peng	P8
LI	Li	P18
LI	Li-Yuan	IL17
LI	Peng	P25
LI	Qingyuan	P27
LI	Xiaomin	IL2
LIANG	Guanfeng	P12
LINGERRI	Roberto	P30
LIU	Haichao	IL27
LIU	Xin	P30
LIU	Xue	OC3
LIU	Ye	P24
LIU	Yueming	P18
LOPES FERREIRA	Nicolas	IL18

LU	Jia-Xing	P10
LU	Yong	IL19, P24
MA	Changru	P6
MAESTRO	Patrick	IL5
MAROCCO-STUARDI	Francesca	P11
MEHAULT	Camille	IL25
MENG	Changgong	P30
MENG	Xiangju	IL31
MÉTIVIER	Pascal	P25
MICHEL	Carine	IL7, P4
MONSAN	Pierre	IL12
MOUGEL	Victor	P7
NARDELLO-RATAJ	Véronique	P13
NASSAR	Youssef	P14
ORDOMSKY	Vitaly V.	IL 32, P5, P12, P20
PACHECO	Nuno	IL29
PAN	Xiaxia	P24
PANNAKAL	Steve	IL28
PASCAULT	Jean-Pierre,	IL22
PELOTIER	Béatrice	P14
PERA-TITUS	Marc	P3, P4, P6, P8, P13, P21, P27
PERRET	Noémie	IL24
PHILIPPE	Régis	IL25
PINEL	Catherine	IL24
PIVA	Olivier	P14
POMALAZA	Guillaume	OC4
POPOWYCZ	Florence	IL26, P2
QUENEAU	Yves	P2, P6, P15, P19
RAFFIER	Ludovic	P14
RANJBAR	Nastaran	P7
RANNOUX	Claire	IL29
RICHARD	Dominique	IL25
RICHARD	Romain	IL29
ROTHENBERG	Gadi	IL9, P17
ROUSSEAU	Alain	IL22
ROY	Nita	IL28
SAID	Achraf	IL24
SAINT-LOUP	René	IL22
SCHMITT	Véronique	P13
SCHWIEDERNOCH	Renate	P16
SCODELLER	Ivan	IL33
SEPTAVAUX	Jean	IL20
SHI	Feng	P8
SHIJU	N. Raveendran	IL9,P17
SHU	Haosheng	P16

SLOT	Thierry	P17
STREIFF	Stéphane	IL32, IL33, P8, P16
SU	Baolian	IL17
SU	Fangzheng	P8, P27
SUN	Ming-Hui	IL17
SUN	Shigang	IL13
SUN	Yuhan	IL11
TAN	Haibo	IL15
TANG	Jing	IL15
TANG	Yong	IL4
TANG	Zhimou	P18
TARASCON	Jean-Marie	IL14
TAVERNA	Dario	P7
TOUATI	Nadia	P7
TRAN	Huan Ngoc	P7
TURNER	Stuart	IL17
VANOYE	Laurent	IL25
Van TENDELOO	Gustaaf	IL17
VERRIER	Charlie	P6
VIOLET	Leo	IL25
WAKERLEY	David W.	P7
WAN	Lijia	IL4
WANG	Huan	P10
WANG	Hui	P10
WANG	Jia	P18
WANG	Liang	IL31
WANG	Lianjie	P15, P19
WANG	Shuo	P10
WANG	Xu-Qing	OC2
WANG	Yang-Dong	IL17
WANG	Ye	IL10
WISCHERT	Raphael	IL33, P4, P25
WU	Dan	P5, P20
WU	Mengjia	P16
WU	Peng	OC3
WU	Qinming	IL31
XIAO	Fengshou	IL31
XIE	Shi-Liang	P26
XIE	Zai-Ku	IL17
XU	Lin	P22
XU	Hao	OC3
XU	Meng	P30
YAMAUCHI	Yusuke	IL15
YAN	Zhen	P8, P21
YANG	Bingyu	P13
YANG	Hai-Bo	OC2, P22

YANG	Tai-qun	P23
YANG	Weimin	IL30
YU	Jihong	IL34
YU	Yunkai	P18
YUAN	Hangkong	P8
YUE	Ying-Na	P10
ZANNA	Sandrine	P7
ZENG	Sheng	P10
ZHANG	Wei	IL9
ZHANG	Kun	P23
ZHAO	Dongyuan	IL2
ZHAO	Guofeng	IL19, P24
ZHAO	Jingpeng	P5, P12
ZHAO	Yang	P4
ZHENG	Jianxia	P25
ZHOU	Feng	P26
ZHOU	Jian	IL17
ZHOU	Wenjuan	P4, P5, P27
ZHOU	Yage	P12
ZHU	Biwen	P28
ZHU	Hongdan	P30
ZITOLO	Andrea	P7