1st CNRS-NTU Chemistry Workshop
September 12th and 13th, 2024
Grenoble, France

Local organizing committee
Dr. Christophe Travelet
Prof. Redouane Borsali

Workshop place :
CTP (Centre technique du papier) – Domaine universitaire
341, rue de la Papeterie – 38610 Gières – France (tram stop : "Bibliothèques universitaires")

Welcoming words

Dear Colleagues, Dear Invited speakers

The CNRS Chemistry and NTU are so thrilled to organize the 1st French Taiwanese workshop on multidisciplinary fields of chemistry, held in Grenoble – France on **September 12thand 13th, 2024** . This 1st edition is gathering well-established scientists from France and Taiwan whose goal is to bring together scientists from both sides to exchange views on the latest developments, uses and applications in Chemistry. Beside the existing IRP (between CNRS and NTU) on "Green Material Science", the idea of this workshop is to provide opportunities to **identify new topics of common interest** and to strengthen the collaboration between the CNRS and NTU. This conference is covering a broad range of topics in the area of Chemistry, namely

- Soft matter : synthesis, elaboration, assemblies, structure, properties, functions
- Molecular architectures : synthesis, mechanisms and properties
- Physical, theoretical and analytical chemistry
- Coordination chemistry, catalysis and processes, interfaces
- Materials chemistry, nanomaterials and processes

The workshop, thanks to the 20 invited speakers (10 from each country), will provide the Taiwanese and French communities with an opportunity to meet and discuss possibilities to bridge the Taiwanese-French collaborations based on the latest developments and new challenges for the 21st century. Mechanisms for more efficient collaborations between Taiwan and French Universities will be pursued as a part of the mission of the conference.

We are looking forward to welcoming you in Grenoble.
With our warmest regards

On behalf of organizing committee

Jacques Maddaluno and **Sophie Guillaume**, Chemistry CNRS, Paris, France
Wen-Chang Chen, President of National Taiwan University and **Cheng-Liang Liu**, NTU, Taiwan
Christophe Travelet and **Redouane Borsali**, UGA-CNRS, CERMAV, Grenoble, France

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Program

30' Time Conference followed by 15'discussion

Thursday September 12th, 2024	
8:45 a.m.	Welcome and registration
9:15 a.m.	*Welcoming words by* • **Prof Wen-Chang Chen**, *President of NTU – Taipei, Taiwan* • **Prof Sophie Guillaume**, *CNRS Chemistry – Paris, France* • **Prof Redouane Borsali**, *UGA-CNRS, CERMAV – Grenoble, France*
9:30	**Feng-Yu Tsai** : *Surface and interface engineering on atomic- and molecular-layer-deposited nano-structured thin films*
10:15	**Delphine Chan-Seng** : *Topology of polymers as a tool to tune properties towards biomedical applications*
11:00	Coffee Break & Picture
11:15	**Cheng-Liang Liu** : *Development of organic thermoelectric materials and devices*
12:00	Lunch On site
1:00 p.m.	**Ken-Tsung Wong** : *Intramolecular or intermolecular charge transfer approach for high efficiency OLED emitters*
1:45	**Géraldine Masson** *: Advances in nitrogen-activated enamide chemistry : asymmetric organocatalysis and photoredox catalysis for the synthesis of chiral amines*
2:30	**Wei-Ssu Liao :** *Interface chemical environment control for sensing technology*
3:15	Coffee Break
3:30	**Laëtitia Chausset-Boissarie** : *Innovative organometallic, photo-, and electrochemical processes through flow technology*
4:15	**Feng-Cheng Chang** : *Technical lignin : Green Bioresources for functional carbon materials applications*
5:00	**Dorothée Laurenti :** *Functionalization of lignocellulosic derivatives towards bio-materials*
5:45	**Jean Raynaud :** *Dynamic inorganic polymers : From boron-containing wonder materials to recycling and circular economy of silicones*
6:30	Conclusion of Day 1 and Departure to downtown – (by Tram)
7:30 p.m.	Dinner at restaurant ***L'Epicurien*** 1, place aux Herbes – 38000 Grenoble - *(downtown)*

Friday September 13th, 2024	
8:45 a.m.	Welcome and registration
9:15 a.m.	*Welcoming words by* **Prof Jacques Maddaluno***, Director of CNRS Chemistry – Paris, France*
9:30	**Ru-Shi Liu** : *Light conversion revolution : Advanced materials technology leading the future*
10:15	**Olivier Joubert** *: A brief overview of the French hydrogen R&D network and a focus on material issues and some solutions*
11:00	Coffee Break & Picture
11:15	**Ru-Jong Jeng** : *A facile strategy to achieve robust polymeric materials from chemical recycling of poly(carbonate)*
12:00	Lunch On site
1:00 p.m.	**Thérèse E. Malliavin :** *Harnessing geometric information for calculating protein structures and exploring conformational space of disordered proteins*
1:45	**Ender Ercan** : *Structural design and self assembly of carbohydrate block copolymers for structure-morphology-property dynamics : A pathway to advanced bio-optoelectronics*
2:30	**Emmanuel Lacôte** *: Low energy-photon radical photopolymerizations in dispersed media*
3:15	Coffee Break
3:30	**Man-kit Leung** *: Recycling and reuse of polyesters and carbon dioxide*
4:15	**Emmanuel Guilmeau** *: From crystal chemistry to thermoelectric properties of ternary and quaternary sulfides*
5:00	**Hao Ming Chen** : *Operando understanding the dynamic structures of electrocatalysts*
5:45	**Carine Michel** : *How to gain atomistic insights on adsorption at the water/solid interface?*
6:30	Conclusion of Day 2 & the Workshop - Departure to downtown – (by Tram)
7:30 p.m.	Diner at restaurant ***Les Jardins de Sainte-Cécile*** 18, rue de l'Alma – 38000 Grenoble - *(downtown)*

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Surface and interface engineering on atomic- and molecular-layer-deposited nano-structured thin films

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Biography

Feng-Yu Tsai is a professor and chairperson of Department of Materials Science and Engineering at National Taiwan University. He received his Ph.D. degree in materials science from University of Rochester in Rochester, New York, U.S.A., following which he worked as a process development engineer with Headway Technologies (San Jose, CA, U.S.A) and as a senior process development engineer with DoPont Displays (Santa Barbara, CA, U.S.A). He joined Dept. Materials Science and Engineering at NTU as a faculty member in 2002. His main research interests lie in the atomic-scale thin film formation mechanisms, their resultant material properties, and their manifestations in a wide variety of coating and surface-functionalization applications spanning from displays, photovoltaics, semiconductor devices, to electrocatalysts for hydrogen production.

Abstract

Atomic layer deposition (ALD) and molecular layer deposition (MLD) offer unique capabilities of precisely tailoring nano-structured thin films to obtain wide-ranging material properties, through facile atomic-scale layer-by-layer combination of different materials. Full realization of such nano-scale constructions as well as the material properties they entail, however, calls for understanding and manipulation of the surface chemistry at the layer-by-layer interfaces, given that ALD and MLD proceed via surface-mediated reactions. This talk will present some of our works on this regard, including studying surface chemistry mechanisms using in-situ and ex-situ analysis techniques, examining relationships between ALD/MLD nanostructures and their resultant properties, and exploring their applications in various types of electronic devices.[1-6]

References

1. H.-N. Hung, C.-Y. Cheng, I.-C. Cheng, J.-J. Shyue, C.-C. Wang, F.-Y. Tsai, Ceram. Int. (2024), 50, 15085–15091, DOI : 10.1016/j.ceramint.2024.01.427
2. H-T Liao, B-W Shih, W-P Hsieh, D-Y Su, F-Y Tsai, Ceram. Int. (2022), 48, 7, 10202-10208, DOI: 10.1016/j.ceramint.2021.12.233
3. M.-H. Tseng, D.-Y. Su, G.-L. Chen, F.-Y. Tsai, ACS Appl. Mater. Interfaces (2021), DOI: 10.1021/acsami.1c03895
4. D.-Y. Su, C.-C. Hsu, W.-H. Lai, F.-Y. Tsai, ACS Appl. Mater. Interfaces (2019), 11, 37, 34212-34221, DOI: 10.1021/acsami.9b09772
5. Y.-Y. Lin, C.-C. Hsu, M.-H. Tseng, J.-J. Shyue, F.-Y. Tsai, ACS Appl. Mater. Interfaces, 7 (2015), 22610–22617, DOI: 10.1021/acsami.5b07278
6. C.-T. Chou, P.-W. Yu, M.-H. Tseng, C.-C. Hsu, J.-J. Shyue, C.-C. Wang, F.-Y. Tsai, Adv. Mater., 2013, 25, 1750-1754, DOI: 10.1002/adma.201204358

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Topology of polymers as a tool to tune properties towards biomedical applications

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Biography

Delphine Chan-Seng is a CNRS researcher at the Institut Charles Sadron, CNRS research unit associated to the University of Strasbourg. She received a M.Sc. degree in Polymer Sciences from the University of Bordeaux (France) and a Ph.D. degree in Polymer Chemistry from the University of Toronto (Canada). She then conducted postdoctoral research at the University of Massachusetts at Amherst (USA), where she focused on the synthesis of polymers for targeted applications, *e.g*. synthesis of aliphatic polyesters and their post-polymerization functionalization used as coatings for drug-elution cardiovascular stents and synthesis of peptide-based comb polymers used as non-viral vectors for gene therapy. In 2011, she joined the Institut Charles Sadron as a CNRS researcher. Her research activities aim at developing new macromolecules by combining organic chemistry, solid-phase synthesis, and polymer chemistry to modulate the composition, topology, and functionality of macromolecules and thus promote specific intrinsic properties to them. She is currently exploring macromolecular engineering for biomedicine, including comb polymers with pendent peptides for stimuli-triggered drug delivery and materials with antimicrobial properties and hyperbranched polymers grafted on upconversion nanoparticles for bioimaging and theranostics.

Abstract

Advances in the field of polymer chemistry have permitted to prepare polymers of controlled topologies, functionalities and microstructures using various strategies to access complex architectures (*e.g*. star, comb and hyperbranched polymers) with a variety of functional groups positioned at well-defined localizations on the polymer chain.[1] This ability to control the architecture and microstructure of polymers along with their functionalities are an asset to adjust the properties of polymers and tune their performances according to the targeted application.[2-3]
This presentation will illustrate the ability of macromolecular engineering, especially the topology of polymers, to afford polymers of specific and tunable properties. The first example will present the impact of changing the topology of polyarginine from linear into comb polymers onto their thermoresponsiveness in water,[4] while the second one will propose the preparation of hybrid materials based on upconversion nanoparticles (UCNPs) and polymers designed for theranostic applications.[5-6]

References

1. K. Matyjaszewski, Prog. Polym. Sci., 2005, 30, 858-875, doi: 10.1016/j.progpolymsci.2005.06.004
2. C. Zhu, C. Ninh, C. J. Bettinger, Biomacromolecules 2014, 15, 3474-3494, doi: 10.1021/bm500990z
3. N. Gangloff, J. Ulbricht, T. Lorson, H. Schlaad, R. Luxenhofer, Chem. Rev. 2016, 116, 1753-1802, doi: 10.1021/acs.chemrev.5b00201
4. N. Zydziak, M. H. Iqbal, A. Chaumont, A. Combes, E. Wasielewski, M. Legros, L. Jierry, P. Lavalle, F. Boulmedais, D. Chan-Seng, Eur. Polym. J., 2020, 125, 109528, doi: 10.1016/j.eurpolymj.2020.109528
5. A. Kavand, C. Blanck., F. Przybilla, Y. Mély, N. Anton, T. Vandamme, C. A. Serra, D. Chan-Seng, Polym. Chem. 2020, 11, 4313-4325, doi: 10.1039/D0PY00452A
6. A. Kavand, N. Anton, T. Vandamme, C. A. Serra, D. Chan-Seng, Eur. Polym. J. 2020, 137, 109935, doi: 10.1016/j.eurpolymj.2020.109935

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Development of Organic Thermoelectric Materials and Devices

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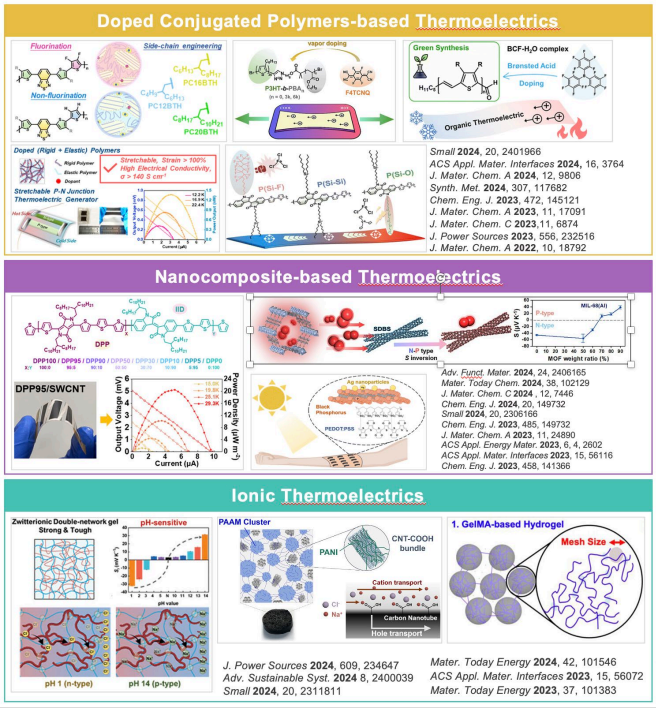
Biography

Prof. Cheng-Liang Liu is a Professor of Materials Science and Engineering at National Taiwan University. He received the B.S. and Ph.D. degrees in Chemical Engineering from National Taiwan University in 2002 and 2007, respectively. He then worked as visiting scientist at the University of Washington (USA) from 2005 to 2006, postdoctoral fellow at National Taiwan University from 2008 to 2010, Assistant Professor at Yamagata University (Japan) from 2010 to 2012, Assistant and Associate Professor at National Central University (Taiwan) from 2012 to 2020, before joining National Taiwan University in 2020. His group focuses on exploring organic polymers and hybrid materials, targeting electronic and energy applications, including transistors, memory devices, solar cells, and thermoelectrics. He currently serves as Associate Editor for Polymer Journal and Journal of Taiwan Institute of Chemical Engineers. For more information, please visit our website: http://homepage.ntu.edu.tw/~liucl/index.html.

Abstract

Organic thermoelectric materials have the potential to directly convert waste heat into electrical power without generating pollution. However, their development is hindered by poor performance, particularly due to low electrical conductivity. This presentation discusses various design strategies aimed at enhancing the performance of organic semiconductors for applications in organic thermoelectrics. We report on a series of solution-processed organic semiconducting molecules, demonstrating that their properties can be effectively modulated through systematic alterations in conjugation length, side chain substituent length, and molecular interactions, based on a combination of molecular design and solution-processing techniques. Additionally, we explore the doping of organic semiconductors and conjugated polymer composites, as well gels with ionic salt or redox couples, to achieve improved thermoelectric performance. The development of flexible and wearable thermoelectric generators based on these advanced materials will also be presented.



References

1. M.-H. Liu, M. G. Mohamed, C.-J. Lin, Y.-J. Sheng, S.-W. Kuo*, **C.-L. Liu**,* *Adv. Funct. Mater.*, **2024**, 24, 2406165.
2. C.-C. Tseng, K.-C. Wang, P.-S. Lin, C. Chang, L.-L. Yeh, S.-H. Tung, **C.-L. Liu**,* Y.-J. Cheng,* *Small*, **2024**, 20, 2401966.
3. L.-C. Lee, K.-T. Huang, Y.-T. Lin, U.-S. Jeng, C.-H. Wang, S.-H. Tung, C.-J. Huang, **C.-L. Liu**,* *Small*, **2024**, 20, 2311811.
4. M.-H. Lin, C.-H. Hsu, D.-Y. Kang,* **C.-L. Liu**,* *Chem. Eng. J.*, **2024**, 485, 149732.
5. P.-S. Lin, J.-M. Lin, S.-H. Tung, T. Higashihara,* **C.-L. Liu**,* *Small*, **2024**, 20, 2306166.
6. S.-H. Hong, C.-C. Hsu, T.-H. Liu, T.-C. Lee, S.-H. Tung, H.-L. Chen, J. Yu,* **C.-L. Liu**,* *Mater. Today Energy*, **2024**, 42, 101546.
7. Y.-T. Lin, C.-C. Hsu, S.-H. Hong, L.-C. Lee, U,-S. Jeng, H.-L. Chen, S.-H. Tung, **C.-L. Liu**,* *J. Power Sources*, **2024**, 609, 234647.

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Intramolecular or Intermolecular Charge Transfer Approach for High Efficiency OLED Emitters

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Biography

Ken-Tsung Wong is working as Professor at Department of Chemistry, National Taiwan University, and a Joint Research Fellow of Institute of Atomic and Molecular Science (from 2012), Academia Sinica, Taiwan. Ken obtained his B.S. degree from Catholic Fu-Jen University in 1989, Ph.D. degree from National Taiwan University (supervisor: T.-Y. Luh) in 1993. He conducted his postdoctoral researches at University of Illinois at Urbana-Champaign (supervisor: S. E. Denmark) in 1995-1996 and Université Louis Pasteur, Strasbourg (supervisor: J.-M. Lehn) in 1996-1998. He joined the Department of Chemistry at National Taiwan University as Assistant Professor in 1998, then promoted to Associate Professor in 2002 and Professor in 2006. Ken has published more than 350 SCI papers with a H-index of 83 (Google scholar). Currently, he serves as the associate editor of *Synthetic Metals* and the editorial advisory broad member of *ACS Applied Materials & Interfaces*.

Ken established a strong interdisciplinary research program engaging domestic and international collaborations. His research mainly focuses on the molecular design and organic synthesis of novel pi-conjugated materials for optoelectronic applications such as organic light-emitting device (OLED), electrogenerated chemiluminescence (ECL), solid-state light-emitting electrochemical cells (LEC), transistors, organic photovoltaics (OPVs), organic photodetectors (OPDs), and memory devices. Ken also worked on hydrogen-bonding directed self-assembly for making organic nano structures and studying their light-emitting applications. In addition to optoelectronics, his small-organic-molecule materials have been explored to show promising nanomedicine applications recently.

Abstract

Organic materials that display thermally activated delayed fluorescence (TADF) are striking functional materials that have led to booming progress in OLED material developments. Organic TADF emitters can be achieved by the subtle manipulations of the intramolecular charge transfer process and the HOMO-LUMO overlap with tailor-made molecular structures. [1] In addition, efficient TADF character can also be realized by blending electron-donating (D) and -accepting (A) molecules for giving “exciplex” by intermolecular charge transfer.[2] Creating high-efficiency TADF emitters requires sophisticated molecular design strategies to bring the structural features both for realizing high photoluminescence quantum yield (PLQY) and high horizontal emission dipole ratio (Θ//) together. In this conference, our recent progress in organic TADF emitters achieved by the intermolecular charge transfer approach, particularly for the exciplex-forming systems with detailed donor-acceptor interactions, will be presented. Our new progress shall stimulate the evolution of innovative ideas for molecular design, leading to the development of new exciplex-forming materials for achieving high-efficiency OLED devices.

References

[1] (a) Lin, T.-A.; Chatterjee, T.; Tsai, W.-L.; Lee, W.-K.; Wu, M.-J.; Jiao, M.; Pan, K.-C.; Yi, C.-L.; Chung, C.-L.; Wong, K.-T.; Wu, C.-C. *Adv. Mater.* **2016**, *28*, 6976. (b) Yi, C.-L.; Lin, C.-Y.; Tang, Y.; Wang, C.-Y.; Huang, C.-W.; Gong, X.; Gong, S.; Wu, C.-C.; Wong, K.-T. *Adv. Optical Mater.* **2022**, 2101791. (c) Lin, C.-Y., Lu, C.-H., Kuo, K.-H., Wu, C.-C., Wong, K.-T. *Adv. Optical Mater.* **2023**, 2202292.

[2] (a) Wang, M.; Huang, Y. H.; Lin, K. S.; Yeh, T. H.; Duan, J.; Ko, T. Y.; Liu, S. W.; Wong, K.-T.; Hu, B. *Adv. Mater.* **2019,** *31*, 1904114. (b) Al Amin, N. R.; Kesavan, K. K.; Biring, S.; Lee, C.-C.; Yeh, T.-H.; Ko, T.-Y.; Liu, S.-W.; Wong, K.-T. *ACS Appl. Electron. Mater.* **2020,** *2*, 1011. (c) Lin, C.-Y.; Hsu, C.-H.; Hung, C.-M.; Wu, C.-C.; Liu, Y.-H.; Shi, E. H.-C.; Lin, T.-H.; Hu, Y.-C.; Hung, W.-Y.; Wong, K.-T. *Nature Chem.* **2024**, 16, 98-106.

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Advances in Nitrogen-Activated Enamide Chemistry: Asymmetric Organocatalysis and Photoredox Catalysis for the Synthesis of Chiral Amines

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Biography

Géraldine Masson is a CNRS Research Director at the Institute of Chemistry of Natural Substances (ICSN), part of Paris-Saclay University. She also leads a joint lab (Laboratoire commun) HitCat with SEQENS and CNRS.
She received her Ph.D. in 2003 from Grenoble University in France under Dr. Sandrine Py and Prof. Yannick Vallée. Afterward, she conducted postdoctoral research as a Marie Curie fellow from 2003 to 2005 at the University of Amsterdam in the Netherlands with Profs. Jan van Maarseveen and Henk Hiemstra. She joined ICSN as a CNRS researcher in late 2005 and was promoted to CNRS Research Director DR2 in 2014 and DR1 in 2020.
Her research focuses on catalytic methods to create biologically active molecules, especially in asymmetric organocatalysis, photoredox catalysis, and electrochemistry. Géraldine Masson has received awards, including the CNRS Bronze Medal, the J.-M. Lehn Prize from the Organic Chemistry Division of the French Chemical Society (2019), and the Cannizzaro-Arnaudon Lectureship from the Italian Chemical Society (2022).
She currently serves as an Associate Editor of The Journal of Organic Chemistry and Deputy Editor of ACS Organic & Inorganic Au.

Abstract

Nitrogen-activated carbon-carbon double bonds present significant potential for constructing a diverse array of nitrogen-containing products. To broaden the utility of these substrates, our research focused on exploring the reactivity of promising enamide derivatives.

We developed innovative methods for the α,β-difunctionalization of enamides using a synergistic two-step strategy that combined asymmetric organocatalysis and photoredox catalysis. A pivotal aspect of our approach was employing thiol as a transient reaction partner which played a crucial in ensuring the success of these processes and enabling the synthesis of a diverse range of enantioenriched α,β-substituted amines.[1]

Additionally, we successfully implemented stereoselective enantioselective photocatalytic processes for synthesizing both α- and β-chiral amines. In these approaches, sulfoxide and sulfonyl groups proved to be ideal linchpins, facilitating selective transformations and ensuring high enantioselectivity.[2,3]

This lecture will present our contributions, emphasizing their application in synthesizing biologically active natural and synthetic compounds.

References

1. Y D. Bouchet, T. Varlet, G. Masson, *Acc. Chem. Res*. **2022**, 55, 3265.
2. M. Leone, J. Milton, D. Gryko, L. Neuville, G. Masson, *Chem. Eur. J.* **2024**, *30*, e202400363
3. W.-Y. Ma, M. Leone, E. Derat, P. Retailleau, C. R. Reddy, L. Neuville, G. Masson, *Angew. Chem. Int. Ed.* **2024**, e202408154

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Interface Chemical Environment Control for Sensing Technology

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Biography

Wei-Ssu Liao is a Professor at National Taiwan University, Chemistry Department, with joint appointments at Center for Emerging Material and Advanced Devices, and Graduate School of Advanced Technology.
He obtained his BS from National Cheng Kung University in 2000 and his MS from National Taiwan University in 2002. He received his PhD from Texas A&M University in 2009, working under the direction of Prof. Paul Cremer. Thereafter, he worked as a postdoctoral scholar with Prof. Paul Weiss and Prof. Anne Andrews at UCLA between 2009-2013. In 2013, he joined Department of Chemistry, National Taiwan University as a faculty member.
Prof. Liao's research experience and interests lie in bioanalytical chemistry, surface science, functional nanomaterials, and analytical devices.

Abstract

Appropriate interface chemical environment control plays an important role in nanofabrication and corelated sensor designs. I will discuss how interface chemical controls affect nanomaterial properties and sensing capabilities in this talk. Both substrate and colloid based approaches will be included, and the significance of interface environment managements from nanofabrication, sensor designs, toward innovative device developments will be highlighted. For next-generation sensor integration and functional device design, delicate controls over the interface environment should be considered. This can open avenues for the capability improvement of sensors and the functionality breakthrough of devices. Future challenges and potential solutions, with prospective opportunities in this research field will also be included.

References

1. Kar, Guerra, Liao, *Advanced Sensor Research* 2024, 2400031.
2. Chen, Wang, Chiang, Chang, Lo, Liao, *JACS Au* 2024, 4, 2151.
3. Chang, Chen, Wang, Chang, Liao, *Cell Reports Physical Science* 2024, 5, 101887.
4. Kar, Wang, Liao, Chang, Liao, *JACS Au* 2023, 3, 1118-1130.
5. Chen, Tan, Hsieh, Wang, Shibata, Maejima, Wang, Hiruta, Citterio, Liao, *ACS Sensors* 2020, 5, 1314-1324.
6. Liao, Cheunkar, Cao, Bednar, Weiss, Andrews, *Science* 2012, 337, 1517-1521.

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Innovative Organometallic, Photo-, and Electrochemical Processes Through Flow Technology

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Biography

After graduating from CPE Lyon with an engineering degree, Laëtitia Chausset-Boissarie obtained her PhD in organic chemistry in 2011, from the University of Geneva, under the supervision of Prof. E. P. Kündig. Her graduate research focused on the total synthesis of Lythraceae alkaloids. She was then awarded a Swiss National Science Foundation fellowship to carried out postdoctoral research in the group of Pr. V. K. Aggarwal at the University of Bristol working on novel applications of chiral boronic esters in asymmetric synthesis. This was followed in 2012 by postdoctoral stint in the group of Prof. I. Gillaizeau at Orléans University to develop novel strategies for the functionalization of heterocycles and ATER (temporary assistant professorship) position at Paris Descartes University in bio-chemistry. In 2015, she was appointed CNRS research associate at Lille University before moving to Rouen Normandie University in late 2022. Laëtitia Chausset-Boissarie expertise is focused on developing new synthetic methods mostly relying on microflow microreactors and High-Pressure activation. She is an active member of the steering committee for the French research network Synth_Flux and was recently awarded the CNRS Emergence@International 2023 grant.

Abstract

To date, numerous examples demonstrated the advantages of microfluidic systems in terms of reaction efficiency and selectivity, showcasing their value in modern chemical synthesis and manufacturing. Continuous flow technology, thanks to their high surface-to-volume ratio, enhances heat and mass transfer and offers significant advantages for reactions involving very short-lived or highly reactive intermediates[1] as well for photo- and electrochemical processes, which use “traceless” reagents like photons or electrons.[2] We will present recent results on chloromethyllithium of esters, photoinduced generation of *o*-benzyne and functionalization of nitrogen heterocycles such as sulfonylation of imidazopyridines,[3] trifluoromethylation of 2-pyridones,[4] and oxy- and trifluoromethylation of endocyclic enamides.[5]

References

1. J.-I Yoshida, Y. Takahaashi & A. Nagaki *Chem. Commun.* **2013**, *49*, 9896
2. M. B. Plutschack, B. Pieber, K. Gilmore & P. H. Seeberger *Chem. Rev.* **2017**, *117*, 11796Y.
3. E. Leclercq, M. Boddaert, M. Beaucamp, M. Penhoat & L. Chausset-Boissarie *Org. Biomol. Chem.* **2021**, *19*, 9379.
4. E. Leclercq, A. Moncomble, C. Debavelaere, M. Beaucamp, M. Penhoat, & L. Chausset-Boissarie *Green Chem.* **2022**, *24*, 7388
5. E. Leclercq, W. Barakat, R. Maazaoui, M. Penhoat, I. Gillaizeau, & L. Chausset-Boissarie *Adv. Synth. Catal.* **2024**, *366*, 2919

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Technical lignin: Green Bioresources for Functional Carbon Materials Applications

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Biography

Dr. Feng-Cheng Chang holds a Ph.D. in Wood Science from the University of British Columbia. He has served as a postdoctoral researcher at UBC, an Assistant and Associate Professor at the School of Forestry and Resource Conservation, National Taiwan University, and an adjunct lecturer at the University of Tsukuba, Japan. His research focuses on developing lignocellulosic fibers and composites, reusing industrial waste for value-added applications, enhancing biomaterial properties, and studying material viscoelasticity and long-term behavior.

Abstract

Lignin, an abundant and cost-effective biomass resource, possesses an intricate structure that renders it an excellent precursor for the production of carbon fiber. Despite lignin-based carbon fibers exhibiting relatively low mechanical strength, their unique properties make them ideal candidates for functional applications, particularly as adsorbents and in electrochemical devices. The potential for utilizing technical lignin in carbon production faces challenges, primarily due to its limited commercial viability and the need for a deeper understanding of its structural composition and thermal characteristics. By enhancing our knowledge of technical lignin's properties and optimizing processing techniques, we can unlock its full potential as a sustainable alternative to petrochemical-derived carbon materials. This research highlights the promise of lignin-based functional carbon materials, particularly in energy storage applications, positioning lignin as a key player in the development of eco-friendly and economically viable materials that can meet the growing demands of modern technology. As we explore these avenues, lignin may emerge as a pivotal resource in the transition towards more sustainable energy solutions.

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Functionalization of lignocellulosic derivatives towards bio-materials

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Biography

Dorothée Laurenti is a CNRS Director of research at Lyon 1 University in the Institute of Research on Catalysis and Environment (IRCELYON). She is responsible of the team CATREN (Heterogeneous Catalysis for the Energy Transition) at IRCELYON, and director of the GDR THERMOBIO on "Biomass and wastes thermochemical conversion" which gathers 30 academic teams in France and some private companies. After a PhD at Marseille University in organic chemistry/homogeneous catalysis (1999), she had a postdoc position in Green Chemistry group at York University (UK) and then in the laboratory of organometallic surface chemistry at Lyon, France. She has co-directed 20 PhD, 8 Postdoctoral researchers with various academic or industrial collaborations and published 80 papers.

Dr Laurenti's expertise is focused on heterogeneous catalysis in various fields:

- Biomass valorization, functionalization
- Hydroconversion/upgrading of (bio-)oils
- Characterization of complex mixtures (Fossil fuels, Bio-oils)
- Catalytic processes, kinetics

Abstract

Faced with depleting fossil fuel reserves, and ever-increasing demand for energy, chemicals and materials, the valorization of renewable resources such as lignocellulosic biomass has become essential. The main components of lignocellulose, lignin and cellulose, can be valorized in various ways into different platform chemicals by depolymerization. However, we are often confronted with very complex product charges containing mixtures of monomers and oligomers, whose separation and characterization must be optimized [1-3]. The use of these bio-polymers directly as material precursors for polymer or other type of industry is attracting the attention of researchers. In this presentation, we will present and compare several approaches to the valorization of lignin or cellulose into materials applications, preferably using heterogeneous catalysis.

The first targeted application is the production of polyols for the synthesis of non-polyurethane (NIPU) polymers by the incorporation of lignin oligomers having high OH density [4]; the second one is the production of bio-binder for bitumen in combination with maleinized used cooking oils (UCO). It consists in the functionalization of lignin or cellulose in order to increase hydrophilicity and reach interesting rheological properties by mixing with UCO [5].

References

1. B. Joffres, M. T. Nguyen, D. Laurenti*, C. Lorentz, V. Souchon, N. Charon, A. Daudin, A. Quignard, C. Geantet, Appl. Catal. B: Environmental 184 (2016) 153-162.
2. A. Margeriat, A. Bouzeggane, C. Lorentz, D. Laurenti, N. Guilhaume, C. Mirodatos, C. Geantet, Y. Schuurman, J. Appl. Anal. Pyrol. 130 (2018) 149-168.
3. J. Pu, T.-S. Nguyen, E. Leclerc, C. Lorentz, D. Laurenti, I. Pitault, M. Tayakout-Fayolle, C. Geantet, Appl. Catal. B: Env. 256 (2019) 117769-117781.
4. H. Lilti Thesis Lyon1 – BIOPOLIOL Project – ANR-21-CE43-0026
5. N. Daridon Thesis Lyon1 – POP Project – ANR-22- CE43-0010

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Dynamic Inorganic Polymers:
From boron-containing wonder materials to recycling and circular economy of silicones

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Biography

Dr. Jean Raynaud was appointed as a CNRS researcher in 2013. His research focuses on sustainable catalysis for polymerization with an emphasis on Fe, and on dynamic polymers with energy-storage capabilities as well as on depolymerization chemistries. His expertise ranges from polymer chemistries to organic and organometallic strategies for catalysis. After graduating from Bordeaux University in 2010 from the LCPO (PhD thesis: "N-heterocyclic carbenes (NHCs) as multitask organic activators for group-transfer and ring-opening polymerizations), he got a 2&1/2 year post-doctoral position in the Ritter group at Harvard University on a Marie-Curie IOF grant, working on organometallic Palladium(III) polymer and copolymer assemblies for Superconductivity. He is currently involved in multiple collaborative projects harnessing the use of homogeneous and heterogeneous Iron catalysis for olefin and diene (co)polymerization, silicone and polycondensates/polyadducts crosslinking and recycling, but also Boron-based dynamic polymers for energy-storage (in particular H_2) applications as well as energetic Nitrogen-containing polymers. His recent research efforts deal with chemical recycling of polymers, either via depolymerization to produce monomers/functional oligomers or through repurposing of waste polymers via reactive extrusion. Circular Economy and Energy/Matter efficiency are thus at the center of his research towards sustainable polymers. **Catalysis to construct, de-construct and re-construct polymers.**
He has partnerships with several industrial companies and several international collaborations (notably with ETH Zürich, Kyoto University & National Taiwan University). He has his HDR ("habilitation à diriger des recherches") and has co-authored 42 research papers, 25 patents, and 30 oral communications at conferences (9 invited).

Abstract

Boron-containing polymers possess extremely valuable chemical and mechanical properties, owing to the sp2-sp3 modularity at the boron center. This tunable hybridization can be advantageous in either hydrogen-storage hybrid materials or dynamic glasses [1]. Architecture tuning can help adjust H_2 release temperature, transfer-hydrogenation from dihydrogen bonding, radical generation from B-H bonds but also glass-transition of these wonder boron-based materials.
Silicones are another example of high-performance inorganic polymers. Harnessing catalysis can help establish a structure/properties/recyclability relationship allowing for the eco-design and circular economy of silicones [2].

References

1. a) Raynaud, J. & Lacôte, E. et al. *Angew. Chem. Int. Ed.* **2015**, *54*, 15744; b) Raynaud, J. & Lacôte, E. et al. *Angew. Chem. Int. Ed.* **2019**, *58*, 15239; c) Montarnal, D. & Raynaud, J. et al. *Angew. Chem. Int. Ed.* **2019**, *58*, 12216; d) Raynaud, J. & Lacôte, E. et al. *Chem. Eur. J.* **2024**, *30(1)*, e202300145; e) Lacôte, E., Chui, C.-W. & Raynaud, J. et al. *manuscript in preparation*; f) D'Agosto, F., Ouchi, M. & Raynaud J. et al. *manuscript in preparation*
2. a) Raynaud, J. & Monteil, V. et al. *Green Chem.* **2023**, *25*, 3869-3877 Front Cover of issue; b) Monteil, V. & Raynaud, J. et al. *submitted manuscript & ChemRXiv* DOI : 10.26434/chemrxiv-2024-vfkz0 ; c) Raynaud, J. & Monteil, V. et al. *Catal. Sci. Technol.* **2021**, *11*, 4849-4856; d) Raynaud, J. & Monteil, V. et al. & Elkem Silicones© Patents: 3 pending and WO2023031525A1, WO2023031524A1, WO2019008279A1 & WO2018115601A1

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Light Conversion Revolution: Advanced Materials Technology Leading the Future

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Biography

Professor Ru-Shi Liu received his Bachelor's degree in Chemistry from Soochow University (Taiwan) in 1981. He got his Master's Degree in nuclear science from the National Tsing Hua University (Taiwan) in 1983. He obtained two Ph.D. degrees in Chemistry from National Tsing Hua University in 1990 and the University of Cambridge in 1992. He joined Materials Research Laboratories at the Industrial Technology Research Institute as an Associate Researcher, Research Scientist, Senior Research Scientist, and Research Manager from 1983 to 1995. Then, he became an Associate Professor at the Department of Chemistry of the National Taiwan University from 1995 to 1999. Then, he was promoted to Professor in 1999. In July 2016, he became the Distinguished Professor.

He got the Excellent Young Person Prize in 1989, the Excellent Inventor Award (Argentine Medal) in 1995, and the Excellent Young Chemist Award in 1998. He got the 9th Y. Z. Hsu Scientific Paper Award due to his excellent energy-saving research in 2011. He received the Ministry of Science and Technology awards for distinguished research in 2013 and 2018. In 2015, he received the distinguished award for Novel and Synthesis by IUPAC and NMS. In 2017, he received the Chung-Shang Academic Paper Award. He got "Highly Cited Researchers" by Clarivate Analytics in 2018, 2019, 2020, 2021, and 2023. He got the Hou Chin-Tui Award in 2018 due to his excellent research on basic science. He received the 17th Y. Z. Hsu Chair Professor Award for contributing to excellent research on "Green Science & Technology" in 2019. He then got the 26th TECO award for his contribution to combining materials chemistry's academic and practical application in 2019. He received the Academic Award of the Ministry of Education and the Academic Achievement Award from the Chemical Society Located in Taipei in 2020. He obtained the FutureTech Award from the Ministry of Science and Technology and the Journal of the Chinese Chemical Society Best Paper Award in 2021.

His research is concerned with Materials Chemistry. He is the author and co-author of more than 600 publications in international scientific journals with total citations >32,073, h-index: 91. He has also been granted more than 200 patents.

Abstract

Prepare to be illuminated by cutting-edge research that's lighting up the future! This groundbreaking study explores the fascinating world of light transformation, unlocking its potential in ways you never imagined. This research covers everything from revolutionary solid-state lighting that could change how we illuminate our world to game-changing energy solutions that might power our tomorrow and even to life-saving medical breakthroughs.

Discover how:

- Phosphors and quantum dots are revolutionizing LED technology[1,2]
- Light could be the key to solving our energy crisis through water splitting and next-gen batteries[3,4]
- Nanomaterials are opening new frontiers in cancer therapy[5]

Join us on this enlightening journey as we shed light on the possibilities that await us!

References

1. V. Rajendran, K. C. Chen, W. T. Huang, M. Kamiński, M. Grzegorczyk, S. Mahlik, G. Leniec, K. M. Lu, D. H. Wei, H. Chang & R. S. Liu, ACS Energy Lett. 8, 2023, 2395–2400.
2. V. Rajendran, M. H. Fang, W. T. Huang, N. Majewska, T. Lesniewski, S. Mahlik, G. Leniec, S. M. Kaczmarek, W. K. Pang, V. K. Peterson, K. M. Lu, H. Chang & R. S. Liu, J. Am. Chem. Soc. 143, 2021, 19058–19066.
3. K. Iputera, J. Y. Huang, S. C. Haw, J. M. Chen, S. F. Hu & R. S. Liu, J. Mater. Chem. A. 10, 2022, 3460–3468.
4. Z. Tong, S. B. Wang, M. H. Fang, Y. T. Lin, K. T. Tsai, S. Y. Tsai, L. C. Yin, S. F. Hu & R. S. Liu, Nano Energy, 85, 2021, 105972.
5. W. T. Huang, T. Y. Su, M. H. Chan, J. Y. Tsai, Y. Y. Do, P. L. Huang, M. Hsiao & R. S. Liu, Angew. Chem. Int. Ed., 60, 2021, 6955–6959.

1st CNRS-NTU Chemistry Workshop
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A brief overview of the French hydrogen R&D network and a focus on material issues and some solutions

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Biography

Olivier Joubert (1965) is the director of the French Research Network on Hydrogen Energy which assembles the major French academic research groups in the field of electrolysis production and storage of hydrogen and also its conversion to electricity using fuel cell. He is presently full professor in Chemistry of Materials at University of Nantes and is Chair of electrochemical storage and conversion of energy group (ST2E) of "Institut des Matériaux Jean Rouxel (CNRS-IMN)". The major research interests of professor JOUBERT revolve around development of new materials for technological applications such as high and intermediate temperature ceramic Solid Oxide (SO) fuel or electrolyser cells (SOFC and SOEC). He is co-author of 120 publications, 25 invited talks and 5 patents.

Abstract

In France, the Research network on Hydrogen energy (FRH2) brings together about 300 experts working in the field of hydrogen. FRH2 aims to promote and structure an interdisciplinary field of research with competences in solid oxide or proton exchange polymer membrane fuel cells/ electrolysers, hydrogen storage and systems. The first part of the presentation will give a brief overview of this CNRS network including some highligts.

The second part of the talk will be dedicated to scientific results focusing on the development of materials for the next generation of electrolysers or fuel cells. Among the different technologies, I will focus on solid oxide (SO) electrolysis which shows high efficiency but suffers from short life time due to the high operating temperature, and also on strategy for recycling and recovery of Solid Oxide Cell components.

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A Facile Strategy to Achieve Robust Polymeric Materials from Chemical Recycling of Poly(carbonate)

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Biography

Ru-Jong Jeng is a Professor at National Taiwan University (NTU). He currently serves as the Director of Institute of Polymer Science & Engineering, NTU, Taiwan.
R. J. Jeng earned his Master and Ph. D. in Polymer Science & Engineering Program at University of Massachusetts Lowell, US. After doing his post-doctoral work at National Tsing Hua University, Taiwan, he joined the Department of Chemical Engineering, National Chung Hsing University, Taiwan in 1994. Subsequently he moved to NTU in 2011. He has approximately 240 publications, and more than 50 patents (Taiwan, Japan and US).
For the past decade, Prof R. J. Jeng has been mainly focusing on polymer recycling and green processes, including chemical recycling of polycarbonates, and syntheses and applications of water-borne polyurethanes and epoxy polymers

Abstract

This study demonstrates a simple and convenient two-step one-pot, highly efficient process of recycling poly-(bisphenol A carbonate), i.e., PC, into versatile intermediates for polymers such as polyurethanes (PUs) and epoxy polymers.[1-5] Via a highly efficient and selective amine carbonylation reaction, PC is depolymerized by aliphatic diamines forming hydroxyl-N,N'-diphenylene-isopropylidenyl biscarbamates (hydroxyl DP-biscarbamates) as major interim prepolymers. Both short- and long-chained prepolymers are prepared with their respective diamines, and the prepolymers are chain-extended or functionalized with commercially available reagents o produce a variety of PUs or epoxy polymers. Hence, PC is cleaved into pieces of soluble hydroxyl DP-biscarbamates first and then reassembled into new polymeric materials without resorting to a separation process. Different from PC-recycling processes reported in the literature, each carbonate group of PC in this new process is fully utilized for making one carbamate group and one hydroxyl terminated intermediate in the absence of catalyst under mild conditions. Most significantly, this process attains 100% atom-economy efficiency and the feasibility of converting one functional polymer into another.

References

1. C. H. Wu, L. Y. Chen, R. J. Jeng, and S. A. Dai, ACS Sustain. Chem. Eng., 6 (2018) 8964−8975.
2. Y. C. Huang, Y. H. Huang, L. Y. Chen, C. A. Dai, S. A. Dai, Y. H. Chen, C. H. Wu, and R. J. Jeng, Polymer, 212 (2021) 123296 (9 pp).
3. S. W. Chen, J. H. Yang, Y. C. Huang, F. C. Chiu, C. H. Wu, and R. J. Jeng, Chemical Engineering Journal Advances, 11 (2022) 100316 (8 pp).
4. Y. C. Huang, L. F. Chen, Y. H. Huang, C. C. Hu, C. H. Wu, and R. J. Jeng, Chemical Engineering Journal, 452 (2023) 139262 (13 pp).
5. S. W. Hsu, Y. C. Huang, C. H. Wu, and R. J. Jeng, ACS Sustainable Chemistry & Engineering, 11 (2023) 17907−17919.

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Harnessing geometric information for calculating protein structures and exploring conformational space of disordered proteins

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Biography

Thérèse E. Malliavin is a CNRS research Director at University of Lorraine. She is actually animating a team at the Laboratoire de Physique et Chimie Théoriques (LPCT) and is the french leader of an International Research Project (IRP) with Prof Jung-Hsin Lin (Academia Sinica, Taipei).
Before her actual position, she was group leader at the Structural Bioinformatics Unit (Institut Pasteur) and she served as appointed member of CNRS National Committee.
TE. Malliavin was a visiting scientist at Academia Sinica. She spent her Post-doc at Shemyakin-Ovchinnikov Institute, Moscow, Russia. She has more than 95 publications.
Prof. T. E. Malliavin's expertise focused during the last decade on the development of bioinformatics methods for analyzing the conformational space of intrinsically disordered proteins, leading to:

- the TAiBP algorithm to overcome the exponential complexity present in the enumeration of protein conformations
- a mixture model RamaMix for quantifying the relative populations of protein conformations from the distribution of backbone angles
- applications to cases of intrinsically disordered proteins playing a significant role in biology

Abstract

Structural bioinformatics plays an increasingly important role in the prediction and calculation of biopolymer structures, leading to a better definition of their function. In addition, intrinsically disordered proteins (IDP) and intrinsically disordered regions (IDR) are at the center of numerous regulation and control pathways in the cell, and attract consequently extreme interest nowadays in structural biology.[1] The optimization problem that arises for protein structure determination is more complex for such objects as the convergence criterion is more difficult to set up and the size of the conformational space is a obstacle to exhaustive exploration. The threading-augmented interval Branch-and-Prune (TAiBP), based on a reformulating of the Distance Geometry Problem (DGP), provides a theoretical frame for the fast generation of protein conformations, avoiding the combinatorial explosion of the Branch-and-Prune approach due to exponential complexity.[2,3] An original finite mixture approach RamaMix has been developed for the quantification of IDP conformations from the global distributions of backbone torsion angles.[4] The TAiBP pipeline was applied to a whirlin tandem domain, a protein involved in hearing and vision in which two PDZ domains are connected by a disordered linker (IDR) and provided a quantitative description of the conformational space.[5] It is also currently used to investigate the conformational space of the Small EDRK-Rich Factor 1A (SERF1A), a protein fostering the oligomerisation and fibrils appearance of α-synuclein.

References

1. Huang, SY., Chang, CF., Lin, JH., **Malliavin* TE** (2023) In: Nielsen, F., Barbaresco, F. (eds) *Geometric Science of Information.* GSI 2023. Lecture Notes in Computer Science, vol 14072, pp 532-540. Springer, Cham. Doi: 10.1007/978-3-031-38299-4_55
2. Worley B, Delhommel F, Cordier F, **Malliavin T**, Bardiaux B, Wolff N, Nilges M, Lavor C, Liberti L. *Journal of Global Optimization*, (2018) https://doi.org/10.1007/s10898-018-0635-0
3. **Malliavin TE**, Mucherino A, Lavor C, Liberti L. J Chem Inf Model. 2019 Oct 28;59(10):4486-4503. doi: 10.1021/acs.jcim.9b00215. Epub 2019 Sep 6. PMID: 31442036.
4. Förster D, Idier J, Liberti L, Mucherino A, Lin JH, **Malliavin* TE**. Sci Rep. 2022 Nov 9;12(1):19057. doi: 10.1038/s41598-022-21648-9. PMID: 36352011; PMCID: PMC9646904
5. **Malliavin TE**. Sci Rep. 2021 Aug 19;11(1):16925. doi: 10.1038/s41598-021-96370-z. PMID: 34413388; PMCID: PMC8376923.

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Structural Design and Self Assembly of Carbohydrate Block Copolymers for Structure-Morphology-Property Dynamics: A Pathway to Advanced Bio-optoelectronics

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Biography

Dr. Ender Ercan is an Assistant Professor in the International Bachelor Program in Engineering, with a joint appointment in the Department of Chemical Engineering and Materials Science at Yuan Ze University, Taiwan. Dr. Ercan is a dedicated materials scientist specializing in advancing semiconducting materials and their applications in optoelectronics. His research focuses on soft optoelectronic polymers and inorganic/organic composite materials, covering a wide array of areas including field-effect transistors, memory devices, and light-emitting diodes. Dr. Ercan delves into the complex relationships among structure, property, and performance, exploring materials such as polymers, block copolymers, perovskites, quantum dots, and organic chromophores. He holds degrees in Chemical Engineering from Turkey (B.Sc. and M.Sc.) and a Ph.D. from National Taiwan University. He has also served as a member of the Advanced Research Center for Green Materials Science and Technology at National Taiwan University. Dr. Ercan has contributed 29 outstanding scientific papers published in reputable international journals, with 12 as the first author and 7 as co-corresponding author, reflecting his commitment to impactful scientific research. Over the past decade, Dr. Ercan's expertise has increasingly focused on material nanostructures, leading to significant advancements in the following fields;

- Composite Materials: Perovskite/Polymer, Chromophore/Polymer & Biocomposite Systems
- Polymer Science and Engineering
- Self-Assembly of Nanostructures (0D, 1D & 2D Geometries) & Electrospun Fibers
- Stimuli Responsive Glycoconjugates
- Soft Optoelectronic: Field-effect Transistor, Synapse, Memory, Photomemory, Light-emitting Diode

Abstract

Owing to the ever-increasing environmental impacts of electronic waste and the cost-inefficiency of physical miniaturization through current engineering approaches, there has been significant attention on the development of biobased and nanomaterials. Among biomaterials, carbohydrate-based block copolymers (BCPs), as "high χ - low N" BCPs, offer recyclability, biocompatibility, and the ability to form self-assembled nanostructures with sub-10 nm domain features. This report presents a comprehensive study of sugar BCPs, focusing on their self-assembly through: **a)** structural design of conjugated/insulating, linear/cyclic, and pendent blocks; **b)** the introduction of oligosaccharides with functional groups and varying lengths; and **c)** various formation methodologies including thermal annealing,[1] solvent vapor annealing,[2] and solvo-microwave annealing.[3] This presentation provides a thorough guide for the development of sugar BCPs and their structure-morphology-performance relationships for next-generation advanced bio-optoelectronics.

References

1. Ender Ercan,* Yan-Cheng Lin, Yoko Sakai-Otsuka, Redouane Borsali, Wen-Chang Chen,* "Harnessing Biobased Materials in Photosynaptic Transistors with Multibit Data Storage and Panchromatic Photoresponses Extended to Near-Infrared Band" Advanced Optical Materials, doi: 10.1002/adom.202201240, 2023, 10, 21, 2201240.
2. Tiffany Mulia, Ender Ercan, Muhammad Mumtaz, Yan-Cheng Lin, * Redouane Borsali, * Wen-Chang Chen, * "Carbohydrate-based block copolymers with sub-10 nm face-centered cubic nanostructures for low-power-consuming and ultraviolet light-triggered synaptic phototransistors", Carbohydrate Polymers, doi: 10.1016/j.carbpol.2024.122476, 2024.
3. Tiffany Mulia, Muhammad Mumtaz, Ender Ercan, Wei-Chen Yang, Chen-Fu Lin, Yan-Cheng Lin*, Redouane Borsali*, Wen-Chang Chen* "Exploring the Charge-Trapping Behavior of Self-Assembled Sugar-based Block Copolymers with a Pendent Design in Photoassisted Memory" ACS Applied Polymer Materials, doi: 10.1021/acsapm.2c02214, 2023, 5, 3898−3911.

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Low energy-photon radical photopolymerizations in dispersed media

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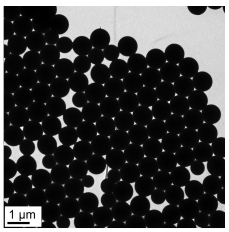
Biography

Emmanuel Lacôte is a CNRS Research Director at Université Claude Bernard Lyon 1. He is the director of LHCEP, a joint research institute for spacecraft propulsion.
After his undergraduate studies at the École Normale Supérieure in Paris he prepared a French/Swiss Ph. D. at Sorbonne University and the University of Fribourg under the supervision of Max Malacria and Philippe Renaud. He then moved to Stanford (CA) for a postdoc with Paul Wender devoted to total synthesis. He joined CNRS in 2000 as a junior researcher, where he moved up-rank to his current position.
Emmanuel is a trained radical chemist. His current research is at the interface between organic & main group/inorganic chemistry (NHC-Boranes, Highly Nitrogenated energetic molecules) and polymers (main group polymers of B and N and photopolymerizations in dispersed media). He has been invited professor at several Universities in Japan (Tokyo, Osaka Prefecture University), Germany (Münster), Canada (Queen's), etc. He received a Bessel Award from the Humboldt Foundation for his work on Boron Chemistry. He and Prof. Ching-Wen Chiu (NTU) shared an ORCHID grant on Boron cations and radicals.

Abstract

In this talk we will first present how NHC-Boryl or sulfur-based radicals can be formed via visible (blue) light irradiation, and how this can be used to initiate efficient photopolymerizations in emulsion[1] and dispersion,[2] overcoming the scattering of the photons by the particles formed. The latexes generated are made of monodisperse particles with sizes up to the micrometer-scale.



We will then examine how one can transition toward the red[3] and how the organic surfactant can be replaced by inorganic CeO_2 nanoparticles toward the photochemical formation of latexes of Pickering-stabilized filmogenic CeO_2-armed polymer particles.

References

1. "Visible-light Emulsion Photopolymerization of Styrene" Le Quéméner, F.; Subervie, D.; Morlet-Savary, F.; Lalevée, J.; Lansalot, M.; Bourgeat-Lami, E.; Lacôte, E. *Angew. Chem. Int. Ed.* **2018**, *57*, 957-961; DOI: 10.1002/anie.20171048.
2. "Visible-Light Initiated Dispersion Photopolymerization of Styrene" Canterel, R.; Lalevée, J.; Bourgeat-Lami, E.; Lacôte, E.; Lansalot, M. *Angew. Chem. Int. Ed.*, **2023**, e202309674; doi.org/10.1002/anie.202309674.
3. "A Methylene Blue/Sodium sulfinate Photo-Initiating System for the Red-Light Emulsion Photopolymerization of Methyl Methacrylate" Kalout, H.; Lansalot, M.; Bourgeat-Lami, E.; Morlet-Savary, F.; Lacôte, E.; Lalevée, J. *Adv. Funct. Mater*. **2024**, accepted for publication.

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Recycling and Reuse of Polyesters and Carbon Dioxide

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Biography

Man-kit Leung received his BSc. and MSc. degrees from The Chinese University of Hong Kong. During 1986-1991, under the supervision of Professor Walter S. Trahanovsky at the Department of Chemistry, Iowa State University, he earned his Ph.D. on the work of reactive conjugated alkenes. During 1991-1993, he spent his Post-doc at the Department of Chemistry, Cornell University with Professor Jean. M. J. Fréchet on photoresist and photosensitive polymers. During 1993-1994, he started his career as an assistant professor at The Chinese University of Hong Kong. Later, he moved to the Department of Chemistry at National Taiwan University and was promoted to full professor in 1999.

Honors and Awards

2003 NTU Excellent Teaching Award; Outstanding Teaching Award: 2000, 2001, 2007, 2008, 2017; National Taiwan University.
2024 NTU Distinguished Academic Advisors
1999 Excellent Young Chemist Award, The Chinese Chemical Society Located in Taipei.
2019 Yeefong Lectureship

Career

Prof Man-kit Leung's expertise is in supermolecules, electro-polymerization and electro-chromism, organic light emitting materials, polyester recycling, and CO_2 recycling chemistry.

Abstract

During the past few decades, sustainability has become a major concern in chemistry. Using electrical energy efficiently for lighting and reusing recycled plastics are two major fields to explore. Our research team tried to combine these two concepts and has recently demonstrated the potential of recycling polylactic acid for vitrimer synthesis. Furthermore, we can use the vitrimer as a host for quantum dots that show superb dispersion properties and high photoluminescence efficiency. We have also developed polymer-based catalysts for CO_2 recycling. [1-4]

References

1. Yong-Yun Zhang, Kuan-Ting Liu, Mu-Huai Fang, Man-kit Leung, “Quantum Dot-Vitrimer Composites: An Approach for Reprocessable, Self-Healable, and Sustainable Luminescent Materials,” *ChemSusChem* **2023**, 16(13), e202300227
2. Jia-Yu Chuang, Kuan-Ting Liu, Monica Mengdie Lin, Wen-Yueh Yu, Ru-Jong Jeng, Man-kit Leung, "Two novel types of heterogeneous catalysts apply to synthesize cyclic carbonates through CO_2 fixation on epoxides under mild condition" *J. CO_2 Util.*, **2023**, 76, 102592.
3. Z. Syeda, H.-y. Chen, M.-k.Leung, Amino alcohols as recycling-catalysts for degradation of PET to oligoethylene terephthalates *Polym. Degrad. Stabil.* **2023**, *214,* 110387.
4. K.-T. Liu, J.-Y. Chuang, R.-J. Jeng, M.-k. Leung, Sustainable Synthesis of Cyclic Carbonates from Terminal Epoxides by a Highly Efficient CaI_2/ 1,3-Bis[tris(hydroxymethyl)methylamino]propane Catalyst, *ACS Omega,* **2021**, 6(41), 27279-27287.

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From crystal chemistry to thermoelectric properties of ternary and quaternary sulfides

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Biography

Emmanuel Guilmeau is a CNRS Director of Research at the CRISMAT Laboratory (France). He received a Ph.D. in Materials Chemistry in 2003 from the University of Caen (France). He was a postdoctoral fellow at AIST (Ikeda, Japan) in 2004 and at LCIS (Liège, Belgium) in 2005. He is a board member of the Solid State Chemistry Division of the French Chemical Society (SCF), European Thermoelectric Society (ITS) and president of the scientific board of the French Thermoelectric Society (GIS-TE).
His research interests are in the area of synthesis, material chemistry and physics, and compositional design of thermoelectric materials, with different processing and characterisation methods.
He has authored more than 200 journal publications, 4 book chapters and 2 patents. He has given 60 invited talks at national and international conferences.

Abstract

Thermoelectricity offers a promising solution to address energy scarcity by enabling the efficient conversion of waste heat into useful electricity. Continued research and development in this field can lead to the development of more efficient and cost-effective thermoelectric materials, which can play a significant role in addressing the global energy challenge. The scientific challenge is here to synthesize a material in which the electrical and thermal properties are decoupled. In short, how can we develop an electrical conductor that conducts very little heat?
In this context, numerous studies have demonstrated the potential of sulfide materials for thermoelectric applications over the temperature range 300 – 700 K. Although most materials have high thermal conductivities, recent works demonstrated that extremely low thermal conductivities could be achieved in sulfides through order/disorder phenomena, rattling dynamics, and structure low dimensionality.
During my presentation, recent advances in synthetic minerals and sulphide compounds will be shown. Some peculiar structural features in connection with materials processing, chemical bonds, and atomic and nanoscale order/disorder phenomena were carefully examined to establish rules and correlations between the crystal structures, nano-microstructures, electronic structures, vibrational and thermoelectric properties. [1-7]

References

[1] P. Acharyya, K. Pal, B. Zhang, T. Barbier, C. Prestipino, P. Boullay, B. Raveau, P. Lemoine, B. Malaman, X. Shen, A. Renaud, B. Uberuaga, C. Candolfi, X. Zhou, E. Guilmeau, *J. Amer. Chem. Soc.* 146 (2024) 13477
[2] K. Maji, B. Raveau, P. Lemoine, P. Boullay, P. Acharyya, X. Shen, A. Renaud, V. Pelletier, R. Gautier, V. Carnevali, M. Fornari, B. Zhang, X. Zhou, B. Lenoir, C. Candolfi, E. Guilmeau, *J. Amer. Chem. Soc*. 146 (2024) 9741
[3] Z. Zeng, X. Shen, R. Cheng, O. Perez, N. Ouyang, Z. Fan, P. Lemoine, B. Raveau, E. Guilmeau, Y. Chen, *Nature Comm*. 15 (2024) 3007
[4] K. Maji, P. Lemoine, A. Renaud, B. Zhang, X. Zhou, V. Carnevali, C. Candolfi, B. Raveau, R. Al Rahal Al Orabi, M. Fornari, P. Vaqueiro, M. Pasturel, C. Prestipino, E. Guilmeau, *J. Amer. Chem. Soc*. 144 (2022) 1846
[5] V. Pavan Kumar, A. R. Supka, P. Lemoine, O. I. Lebedev, B. Raveau, K. Suekuni, V. Nassif, R. Al Rahal Al Orabi, M. Fornari, E. Guilmeau, *Adv. Energy Mater*. 9 (2019) 1803249
[6] P. Lemoine, G. Guélou, B. Raveau, E. Guilmeau, *Angew. Chemie Int. Ed*. 61 (2022) e202108686
[7] C. Bourgès, Y. Bouyrie, A. Supka, R. Al Rahal Al Orabi, P. Lemoine, O. I. Lebedev, M. Ohta, K. Suekuni, V. Nassif, V. Hardy, R. Daou, M. Fornari, Y. Miyazaki, and E. Guilmeau. *J. Am. Chem. Soc*. 140 (2018) 2186–2195

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Operando understanding the dynamic structures of electrocatalysts

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Biography

Hao Ming Chen is a full Professor at National Taiwan University, Taiwan.
He is the recipient of Bau Family Award in Inorganic Chemistry, Chinese Organic Chemists (ISCOC) and Chinese Inorganic Chemists (2023), Outstanding Researcher Award, Asia-Pacific Association of Catalysis Societies (2023), Lectureship Award for the Asian and Oceanian Photochemists Sponsored by Eikohsha (The Japanese Photochemistry Association 2019) and has been featured in the 2018 *JACS* Young Investigator Issue. He is also the recipient of numerous awards, including Outstanding Research Award and the Dr. Ta-You Wu Memorial Award (the Ministry of Science and Technology), Outstanding Young Chemist Award (Chinese Chemical Society Located in Taipei), Young Scholar Innovation Award (the Foundation of the Advancement of Outstanding Scholarship), the Academia Sinica Research Award for Junior Research Investigators, and the Outstanding Researcher Award (Asia-Pacific Association of Catalysis Societies).
H. M. Chen spent his Post-doc at UC Berkeley, US –He earned his BS and PhD in chemistry at National Taiwan University, Taiwan. He has more 150 publications.
Prof R. Chen's expertise is focused during the last decade on the Liquid/solid interfacial study, leading to:

- Operando methodology
- Catalytic chemistry
- In situ X-ray spectroscopy (XAS, RIXS, XRD)

Abstract

Electrochemical reduction of CO2 is heavily pursued as a potential solution of CO2 recycling and realizes the high-density renewable energy storage. Among numerous types of catalysts, copper-based catalysts have been shown to perform interesting nature toward hydrocarbon products. Nevertheless, achieving practical CO2RR selectivity toward desired products on the state-of-the-art copper-based catalysts is still facing great challenges. The great challenge for promoting the CO2RR selectivity may arise to a fact that this electrochemical process is a multiple proton-electron-transfer step and highly surface-sensitive, implying that the surface state of electrocatalyst may be dynamic and unpredictable under practical situations. By employing the comprehensive in-situ techniques we developed during past few years, we have demonstrated the first empirical demonstration to track the dynamic structural reconstruction/transformation in a model bimetallic system, which establishes a good understanding of the correlation between catalyst surface structure and catalytic selectivity. Furthermore, we also realized a very important achievement to develop an operando seconds-resolved X-ray absorption spectroscopy to uncover the chemical state evolution of working catalysts. We aim to establish an indispensable in situ research model for future studies and offers exciting research prospects for catalytic scientists.

References

1. Wang, J.; Hsu, C.-S.; Wu, T.-S.; Chan, T.-S.; Suen, N.-T.; Lee, J.-F.; Chen, H. M. *Nature Commun.* **2023**, 14, 6576.
2. Hsu, C.-S.; Wang, J.; Chu, Y.-C.; Chen, J.-H.; Chien, C.-Y.; Lin, K.-H.; Tsai, L.-D.; Chen, H.-C.; Liao, Y.-F.; Hiraoka, N.; Cheng, Y.-C.; Chen, H. M. *Nature Commun.* **2023**, 14, 5245.
3. Chang, C.J.; Lai, Y.-A.; Chu, Y.-C.; Peng, C.-K.; Tan, H.-Y.; Pao, C.-W.; Lin, Y.-G.; Hung, S.-F.; Chen, H. M. *J. Am. Chem. Soc.* **2023**, 145, 6953-6965.
4. Wang, J.; Tan, H.-Y.; Qi, M.-Y.; Li, J.-Y.; Tang, Z.-R.; Suen, N.-T.; Xu, Y.-J.; Chen, H. M. *Chem. Soc. Rev.* **2023**, 52, 5013.
5. Tan, H.-Y.; Lin, S.-C.; Wang, J.; Chen, J.-H.; Chang, C.-J.; Hou, C.-H.; Shyue, J.-J.; Kuo, T.-R.; Chen, H. M. *J. Am. Chem. Soc.* **2023**, 145, 27054.

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How to gain atomistic insights on adsorption at the water/solid interface?

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Biography

Carine Michel received her PhD in 2007 in Theoretical Chemistry at the Université Joseph Fourier, Grenoble, France, under the supervision of Pr. A. Milet. She focused mainly on modelling the chemical reactivity of various homogeneous systems. Then, she spent one year as a post-doctoral fellow under the supervision of Pr. E.J. Baerends at the VU University, Amsterdam in the field of C-H oxidation.
In 2009, she was appointed at the Laboratoire de Chimie as a CNRS researcher to focus on the catalytic valorisation of biomass into chemicals. She extended her research themes to the study of reactive solid/liquid interfaces with a focus on the life cycle of catalysts, from preparation to deactivation.
She received the Bronze medal of the CNRS (2015) and defended her Habilitation à Diriger des Recherches in 2016 ('Computational Studies across Catalysis'). She was the head of the LIA Funcat (with uOttawa- and is now the head of the IRP ELINE (with UCLA). She was appointed vice-director of the Laboratoire de Chimie in 2021 and then director of this research lab in 2024.

Abstract

Reactions at the water/solid interface are central to develop more sustainable processes, from biomass upgrading to the use of unconventional activation as in photocatalysis and electrocatalysis. To gain atomistic insight on those reactions, modelling approaches were constantly improved in the past decade. Several approaches are available nowadays from continuum models to a full explicit description of the liquid water. We will discuss the pros and cons of those methods using several examples.

References

[1] Steinmann, S. N. & Michel, C. How to Gain Atomistic Insights on Reactions at the Water/Solid Interface? ACS Catalysis, 2022, 12, 6294-6301

The CNRS even present at Grenoble main train station in June and July 2024 !

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