CATSCIENCE

PRISM

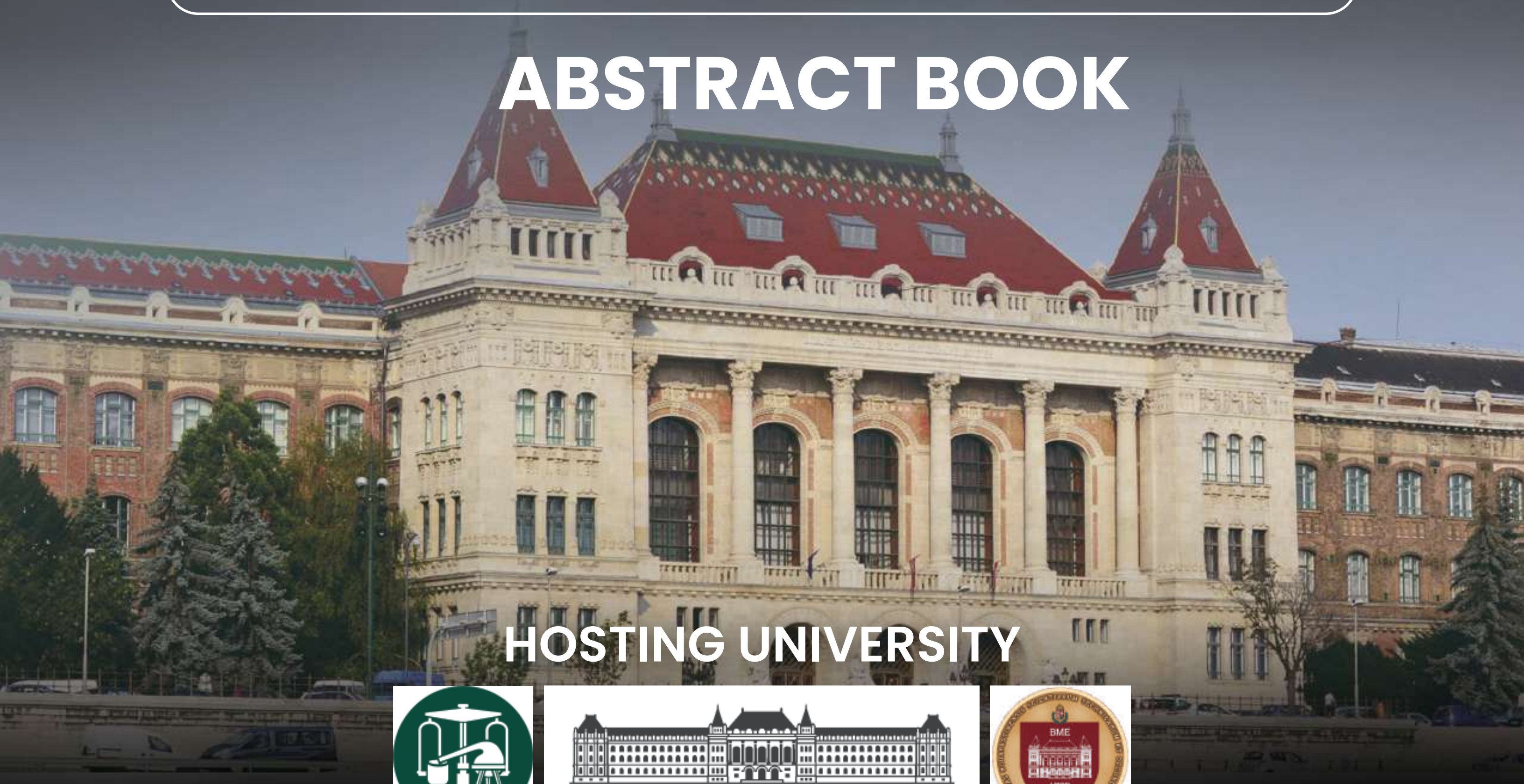
3rd INTERNATIONAL CONFERENCE ON

CATALYSIS SCIENCE AND CHEMICAL ENGINEERING

JULY 21–23, 2025

Budapest University of Technology and Economics, Hungary

ABSTRACT BOOK



HOSTING UNIVERSITY

MŰEGYETEM 1782

www.catalysis-science.com

DAY-1 JULY 21, 2025

Emerging Technologies and AI to Answer to Electronics and Energy Digitalization Demands

Rodrigo Martins, P. Barquinha, L. Pereira, E. Carlos, A. Kiazadeh, M. Mendes, D. Nunes, H. Águas E. Fortunato*

CENIMAT/i3N, Department of Materials Science, NOVA School of Science and Technology, NOVA University Lisbon (FCT-NOVA) and CEMOP/UNINOVA, Campus de Caparica, 2829-516 Caparica, Portugal

Keywords: Emerging technologies; Sustainable electronic materials; sustainable energy materials; electronic devices

Abstract

In the current digital era, as the world is growing up with smart technology, at the same time our planet is drowning with materials scarcity, a huge number of unrecycled waste and environmental pollution. The world is facing challenges against rapid climate changes and continuous ecological disturbances, caused by the revolutionary growth in socio-economic developments with the fastest growing trend in smart electronics, plastic-based products, and the continuous dependence on non-recyclable raw materials, besides exhausting our natural resources. On the other hand, a huge significant progress in IoT and wearable smart electronics systems is demanding very high-resolution displays of the communication interface and the use of green technologies, exploiting emerging devices beyond silicon, most of them at a nanoscale basis. Moreover, energy is required to foster and power all these demands.

For festering progress, the use of AI is a demand to which supercomputers are connected and so, energy demands must be considered as a target for developing novel devices with ultra-low power consuming.

The present talk aims to show pathways able to answer to two above identified demands, to which we must add the ones related to minimize the electronic waste (e-waste) caused by the ever-increasing number of disposable electronic devices, where exploitating photocatalysis for energy storage is highlighted.

By doing so, we aim to contribute to future green products, green powered, and make social awareness of green and sustainable technology, which could revolutionize the industry and society both with new business approaches with smart sustainable lifestyles.

Key words: responsible electronics; flexible electronics; transparent electronics; sustainable electronics

Figure 1. Eco-strategies for next generation materials engineering and applications

Reference:

D. Nunes, A. Pimentel, P. Barquinha, M. Mendes, J. Coelho, H. Almeida, E. Fortunato, R. Martins, Flexible devices based on metal oxides: achievements and prospects, in Metal oxide series, editor G. Korotecenkov, 2025, ISBN 04432165689780443216565

G Ferreira, et al in Energy harvesting and movement tracking by polypyrrole functionalized textile for wearable IoT applications, Journal of Energy Chemistry 102, (2024), 230-242

B He, et al in Electrospun Coaxial Nanowire-Based FETs with Annular Heterogeneous Interface Gain for Intelligent Functional Electronics, Advanced Functional Materials 34 (25), (2024), 2316375

G Fagas et al in The INFRACHIP European research infrastructure for emerging and responsible electronics, Nature Reviews Electrical Engineering 1 (6), (2024), 354-355

Molecular Redox Catalysts for the Generation of Solar Fuels

Antoni Llobet

Institute of Chemical Research of Catalonia (ICIQ), Barcelona Institute of Science and Technology (BIST)

Av. Països Catalans 16, E-43007 Tarragona, Spain.

Abstract

The replacement of fossil fuels by a clean and renewable energy source is one of the most urgent and challenging issues our society is facing today, which is why intense research is devoted to this topic.[1] Nature has been using sunlight as the primary energy input to oxidize water and reduce CO2 to generate carbohydrates (a solar fuel) for over a billion years. Inspired but not constrained by nature, artificial systems can be designed to capture light and oxidize water and reduce protons or other useful substrates such as CO2 to generate chemical fuels. One of the key aspects for the efficient design of devices for the making solar fuels is the understanding and mastering of the catalysts involved in both the anodic and cathodic reactions. The talk will describe the initial developments up to the state of the art, of molecular catalysts and their anchoring on conductive and semiconductive surfaces. The latter is crucial for the generation of powerful hybrid molecular anodes and cathodes for the production of solar fuels.[2] [1] (a) Llobet, A. et al. Nat. Rev. Chem. 2019, 3, 331–341. (b) Llobet, A. et al. Chem. Soc. Rev. 2023, 52, 196-211. [2] (a) Llobet, A. et al. Nat. Chem. 2020, 12, 1060–1066. (b) Llobet, A. et al. Adv. Energy Mat. 2020, 2002329. (c) Llobet, A. et al. J. Am. Chem. Soc. 2021, 143, 11651–11661. (d) Llobet, A. Nat. Catal. 2022, 5, 79-82, (e) Llobet, A. et al. ACS Energy Lett. 2023, 8, 1, 172–178. (f) Llobet, A. et al., Adv. Energy Mat. 2024, 14, 2402070. (g) Llobet, A. et al., J. Am. Chem. Soc. 2025, 147, 12686–12695.

Biography

PhD, Univ. Autònoma de Barcelona (UAB) July 1985. Post-doc at the Univ. of North Carolina at Chapel Hill and Texas A&M Univ. in the USA. In 1993 joined the Univ. de Girona and in 2004 the UAB as a Full Professor. In September 2006, he was appointed as Group Leader at the Institute of Chemical Research of Catalonia (ICIQ) in Tarragona. In 2018 he was awarded with the "Animesh Chakravorty" Endowment Lecture by the Chemical Research Society of India (CRSI) and the "Alexander von Humboldt Research Award" for a career achievement by the Humboldt Foundation from Germany.

Carbon-based Metal-free Electrocatalysts for Energy and Chemical Conversions

Liming Dai

Australian Carbon Materials Centre

The ARC Centre of Excellence for Carbon Science and Innovation

University of New South Wales, Sydney, NSW 2052, Australia

Presentation mode (Plenary Speaker)

Abstract

Since our discovery of the first carbon-based metal-free electrocatalyst (C-MFEC, *i.e.*, N-doped carbon nanotubes) for oxygen reduction in fuel cells in 2009, the field of C-MFEC has grown enormously. C-MFECs, as alternatives to noble metal-based electrocatalysts, have been widely demonstrated for efficient oxygen reduction, oxygen evolution, hydrogen evolution, carbon dioxide reduction, nitrogen reduction, and many other electrocatalytic reactions. Recent worldwide research effort has shown great potential for applications of C-MFECs in fuel cells for clean energy conversion, metal-air batteries for energy storage, water splitting for hydrogen fuel generation, and other electrochemical processes for value-added chemical production to reduce or even eliminate greenhouse emissions. Further research and development of C-MFECs could revolutionize clean energy and green chemical technologies. In this talk, I will summarize some of our work on the development of C-MFECs for clean energy and chemical conversions, along with an overview of recent advances, current challenges, and future perspectives in this exciting field.

Biography

Liming Dai joined University of New South Wales in 2019 as an Australian Laureate Fellow and a UNSW Scientia Professor. He is also Director of the ARC Centre of Excellence for Carbon Science and Innovation. Before joining UNSW, he worked in Cavendish Laboratory and CSIRO. He was then an associate professor of polymer engineering at University of Akron, the Wright Brothers Institute Endowed Chair Professor at University of Dayton, and the Kent Hale Smith Professor at Case Western Reserve University. His expertise covers the synthesis and device fabrication of conjugated polymers and carbon nanomaterials for energy, environmental and biomedical applications.

A New Generation of Modified TiO2 Based Photocatalytic Hybrid Structures

G. Kiriakidis 1,2 and V. Binas 1,2,3

1. PCN Materials pc, Anopolis, Heraklion,7008, Crete, Greece

2. TCMD/ IESL, FORTH, Voutes, Heraklion,70013, Crete, Greece

3. Chemistry Dpt, Aristotle University of Thessaloniki, 57001, Greece

Living in a healthy indoor environment has recently become of paramount importance all over the globe. Materials with depolluting and disinfecting properties for more efficient control of the indoor environment can have a beneficial impact on the improvement of Indoor Air Quality (IAQ), energy consumption, and human health

Among the existing various techniques to mitigate the problem of contamination and restrictions on the proliferation of airborne pathogens, particularly in the indoor environment, photocatalysis has been demonstrated as the most effective, durable, economical, and promising solution2-4. Bringing together the accumulated scientific and technological knowledge on visible-light activated TiO2 powders, a new generation of photocatalytic coatings incorporating structural and transition-metal modified TiO2 was optimized for developing a new generation of effective air cleaning products and devices. These range from the development of indoor wet-paints and coatings on metallic, cementitious, fabric, glass, and ceramic substrates, to hybrid microfibrillated cellulose / photocatalytic compounds, applied to packaging and high-traffic objects.

1. “Smart Surfaces: Heterogeneous Photo-Catalysis on TiO2 Based Coatings for De-pollution Purposes in Indoor and Outdoor Environments”. https://doi.org/10.1007/s11244-020-01351-7

2. “Modified TiO2-based photocatalysts for improved air and health quality” https://doi.org/10.1016/j.jmat.2016.11.002

3. “Metal oxide semiconductors as visible light photocatalysts” https//DOI: 10.3938/jkps.65.297

4. “Studies on photo-induced NO removal by Mn-doped TiO2 under indoor-like illumination conditions” https://doi.org/10.1016/j.jphotochem.2011.04.037

Application of Ionic Liquids in Organic Catalysis

Rita Skoda-Földes*, Dávid Ispán, Attila Máriás, Enikő Nagy, Lilla Maksó

University of Pannonia, Hungary

Presentation mode (Plenary)

Abstract

Ionic liquids (ILs) have attracted increasing interest in the last decades with a diversified range of applications. In organic synthesis, ILs can be used not only as just alternative reaction media. They can act as catalysts, as multifunctional compounds like solvents and ligands, solvents and catalysts, or stabilizing agents for the catalysts or intermediates.

In the past few years, our research has focused on the development of methodologies for catalyst recycling, exploiting the unique features of ILs. Palladium nanoparticles stabilized on supported ionic liquid phases served as catalysts in carbonylation and coupling reactions of heterocycles, such as benzofurans and imidazole [1,2-a] pyridines. [1] The catalytic effect of the ILs themselves has been utilized in hetero-Michael additions, and the formation of reversible ILs made it possible to recycle organic base catalysts in aza-Michael and Claisen-Schmidt reactions. [3,4] The latter methodologies were applied to produce steroidal derivatives with pharmaceutical importance.

In this presentation, some examples of the application of ILs in the catalytic reactions mentioned above will be discussed.

Biography

[1] (a) E. Nagy, Z. Nagymihály, L. Kollar, M. Fonyó, R. Skoda-Földes, Synthesis 2023, 55, 131-140. (b) E. Nagy, A. Máriás, M. Kovács, R. Skoda-Földes, Molecules 2024, 29, 5048

[2] D. Ispán, Á. Küzdő, M. Fonyó, Á. Gömöry, N.Tumanov, J. Wouters, S. Mahó, Gy. Lendvay, R. Skoda-Földes, Eur. J. Org. Chem. 2023, 26, e202300560

[3] L. Maksó, B. Szele, D. Ispán, Á. Gömöry, S. Mahó, R. Skoda-Földes, Org. Biomol. Chem., 2024, 22, 2465–2473

Effect of strong metal-support interaction on the improvement of Mo-doped titania-carbon composite supported Pt Electrocatalysts Performance

András Tompos[1]*, Cristina Silva[1], Irina Borbáth[1], Gábor P. Szijjártó[1], Erzsébet Dodony[2], Dániel Olasz[2], György Sáfrán[2], Kristóf Zelenka[1], Ágnes Szegedi[1], Zoltán Pászti[1]

[1]Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Magyar Tudósok körútja 2, H-1117 Budapest, Hungary

[2]Institute for Technical Physics and Materials Science, HUN-REN Centre for Energy Research, Konkoly-Thege M. út 29-33, H-1121 Budapest, Hungary

Presentation Mode Keynote

Abstract

Recent studies demonstrated that the strong metal-support interaction (SMSI) phenomenon offers possibilities for enhancing stability and functionality of catalysts. SMSI can occur in reducible oxide supported catalysts, usually resulting in electron transfer between the metal and the oxide, accompanied by the decoration of the metal particles with ultra-thin layers of the support material upon annealing under reductive conditions.

This work focuses on the development of SMSI and its influence on the catalytic performance of the $Pt/Ti_{0.8}Mo_{0.2}O_2$-C system, a representative of the mixed oxide-carbon composite supported Pt electrocatalyst family. XPS combined with in situ H_2 exposition clearly demonstrated appearance of very easily reducible Mo species after the reductive pretreatment, which evidences migration of Mo species to the surface of the Pt particles. Beneficial metal-support interactions developing at the Pt-oxide-carbon junctions contribute to higher activity and better stability of the catalysts, which may allow design of effective electrodes with decreased Pt content. Based on the experiment in a single cell test device using 100 ppm CO/H_2 fuel, the $Pt/Ti_{0.8}Mo_{0.2}O_2$-C catalyst demonstrates a clear advantage over the conventional Pt/C catalyst in terms of CO tolerance. Better CO tolerance of $Pt/Ti_{0.8}Mo_{0.2}O_2$-C can be attributed to SMSI effect, which reduce CO adsorption on the active catalytic sites due to the electronic ligand effect and improve surface cleaning, presumably due to the bifunctionality of adjacent, Mo^{n+} and Pt containing, surface sites.

Biography

András Tompos, director of Institute of Materials and Environmental Chemistry in HUN-REN Research Centre for Natural Sciences, graduated as chemical engineer at Budapest University of Technology in 1994. As a PhD student at the Central Research Institute for Chemistry, he designed catalysts for the selective hydrogenation of unsaturated carbonyl compounds. He defended his PhD thesis in 1999. Until 2001 he was post doc at RWTH Aachen studying enantioselective ring opening of mezzo epoxides by means of salen complexes. After his return to Hungary, his attention was drawn to combinatorial tools. He designs electrocatalysts for fuel cells.

Synthetic Fuel Production based on CCU technologies

András Sápi[1]

University of Szeged, Hungary

Presentation mode: Oral

Abstract

We are focusing on direct hydrogenation of carbon-dioxide with high activity and controlled selectivity of C_1 as well as C_{5+} products using of designed nanoparticles and supports as well as interfaces followed by molecular level understanding of the reactions. In this talk, I will discuss our research on the field from the last 5 years evidenced by >20 scientific publications show plenty of results on the field of nanocatalysis and CO_2 activation reactions towards a new sight into green catalysis, we are scaling up Fe-catalyst based C_{5+} production to 5-10 kg liquid product/day based on solar power-motored H_2 generation.

Biography

Andras Sapi is an associate professor of The Institute of Chemistry, University of Szeged with a PhD and habilitation in Chemistry. Having > 100 papers in the field of heterogeneous catalysis, material science and solving environmental problems focusing on the atomic level understanding as well as the industrialization. Holder of the Prize for the Environment 2025 and the Best Young Scientist 2022 prize as well as the innovation price of Szeged 2020 & 2024.

From Ionic Liquids to Functional Poly (Ionic Liquid) Aerogels: Green and Catalytic Platforms for CO_2 Capture and Conversion

Raquel V. Barrulas1,2, Henrique Bule1 , Maria Morais1 , Marcileia Zanatta, Ricardo Chagas4, and Marta C. Corvo 1* 1 i3N|Cenimat, Materials Science Dep., NOVA School of Sciences and Technology, Caparica, Portugal; 2 MESA+ Institute & Fac. Science and Technology, Univ. of Twente, The Netherlands; 3 Institute of Advanced Materials (INAM),

Universitat Jaume I, Castelló de la Plana, Spain; 4 LAQV-REQUIMTE, Chemistry Dep., NOVA School of Science and Technology, Caparica, Portugal

Presentation mode: Oral

Abstract

The escalating levels of atmospheric CO_2, now surpassing 400 ppm, underscore the urgent need for materials that not only efficiently capture CO_2 but also facilitate its transformation through sustainable processes. While ionic liquids (ILs) have emerged as highly selective solvents, their fluid nature and regeneration costs have prompted interest in more robust and multifunctional alternatives. Our work traces the evolution from ILs to poly(ionic liquids) (PILs), culminating in the development of porous PIL-based aerogels (AEROPILs) [1]. These materials combine the ionic tunability of ILs with the structural integrity and catalytic flexibility of solid supports. Importantly, AEROPILs offer enhanced surface area, morphology control, and thermal stability—features that enable superior catalytic CO_2 transformation, particularly in cycloaddition and related reactions [2]. To align with green chemistry principles, recent studies have focused on incorporating biodegradable polyhydroxyalkanoates (PHA) into the aerogel matrix. This addition imparts hydrophobicity and promotes environmental. Parallel efforts include the embedding of ZnO nanoparticles, introducing Lewis acidity to expand the material's catalytic scope. Together, these modifications support the design of recyclable, low-impact materials tailored for integrated CO_2 capture and utilization (CCU). This presentation will explore the synthesis, characterization, and catalytic behavior of these next-generation AEROPILs, emphasizing how molecular and structural design choices drive sustainability, multifunctionality, and catalytic efficiency in the quest for greener carbon management technologies [3]. 3rd International Conference on Catalysis Science and Chemical Engineering (CatScience 2025) July 21 - 23, 2025| Budapest University of Technology, Hungary [1] R.V. Barrulas et al., Int. J. Mol. Sci. 23, 200, 2022. [2] R.V. Barrulas et al., J. CO2 Util. 83, 102771, 2024. [3] R.V. Barrulas et al., Carbon Capture Science & Technology, 15, 100390, 2025. Acknowledgements: National Funds via FCT – Portuguese Foundation for Science and Technology (LA/P/0037/2020, UIDP/50025/2020, UIDB/50025/2020), PIDDAC (POCI-01–0145-FEDER007688) for i3N, AERO2cycle; Pacto Bioeconomia Azul (C644915664-00000026) co-financed by the PRR - Recovery and Resilience Plan of the European Union (Next Generation EU). RC and MCC thank FCT for the researcher contracts (CEECIND/09397/2023 and CEECIND/08064/2023, respectively).

Biography

Marta C. Corvo has a PhD in Chemistry from NOVA University in Lisbon, Portugal. She currently leads the Ion Gels team at the Institute of Nanostructures, Nanomodelling and Nanofabrication (i3N) at CENIMAT, as an Associate Researcher. Her research interests include ionic liquids and ion gel materials, as well as NMR studies in both solid-state and solution. Marta focuses on various applications, including CO2 capture and conversion, art conservation, energy, and tissue engineering.

Synthesis of Multi-metallic Sub-nanocatalysts Using a Dendrimer Reactor

Kimihisa Yamamoto

Tokyo Institute of Technology, 4259 Nagatsuta, Yokohama 226-8503, Japan

Presentation mode (Oral)

Abstract

Dendrimers are highly branched organic macromolecules with successive layers or "generations" of branch units surrounding a central core. Organic inorganic hybrid versions have also been produced, by trapping metal ions or metal clusters within the voids of the dendrimers. Their unusual, tree-like topology endows these nanometer-sized macromolecules with a gradient in branch density from the interior to the exterior, which can be exploited to direct the transfer of charge and energy from the dendrimer periphery to its core.

We show that $AuCl_3$, $SnCl_2$, $FeCl_3$, and so on complexes to the imines groups of a spherical polyphenyl-azomethine dendrimer in a stepwise fashion according to an electron gradient, with complexation in a more peripheral generation proceeding only after complexation in generations closer to the core has been completed. By attaching an electron-withdrawing group to the dendrimer core, we are able to change the complexation pattern, so that the core imines are complexed last. By further extending this strategy, it should be possible to control the number and location of metal ions incorporated into dendrimer structures, which might and uses as tailored catalysts, building blocks, or fine-controlled clusters for advanced materials. The metal-assembly in a discrete dendrimer molecule can be converted to a size-regulated metal particle with a size smaller than 1 nm as a molecular reactor. Due to the well-defined number of metal clusters in the subnanometer region, its property is much different from that of bulk or general metal nanoparticles. The chemistry of nanocatalysts on the sub-nanometer scale is not yet well understood because precise multi-metallic nanoparticles are difficult to synthesize with control over size and composition. The template synthesis of multi-metallic sub-nanocalaysts is achieved using a phenylazomethine dendrimer as a macromolecular template.

References

K. Yamamoto et al. *Nature Rev. Chem.*, 5, 5, 338, 2021, *Chem. Rev.*, 120, 2, 1397, 2020, *Nature. Commun.* 2018, *9*, 3758, *Nature. Commun.* 2018, *9*, 3873, *Science Adv.* 2017, *3*, e1700101, *Nature. Commun.* 2017, *8*, 688. *Nature Chem*, 2009, 1, 397, *Nature Nanotech.*, 2008, 2, 106., *Nature*, 2002, 415(6871), 509

Biography

Kimihisa Yamamoto received PhD degrees from Waseda University in Polymer Chemistry in 1990. He joined the Department of Chemistry at Keio University from 1997 as professor. Currently, he is a professor in Tokyo Institute of Technology since 2010. His present research interests are in developing supra-metallomolecules for nanosynthesizers involving nanoparticles, subnanoparticles, and superatoms.

Design Strategy of Carbon Catalysts for Oxygen Reduction and Mixed-Potential-Driven Catalysis

Kotaro Takeyasu

Institute for Catalysis, Hokkaido University, Japan

Presentation mode (Oral)

Abstract

Nitrogen-doped carbon (N–C) catalysts have emerged as promising alternatives to platinum for the oxygen reduction reaction (ORR) in polymer electrolyte fuel cells, owing to their high durability and activity in alkaline media. However, their performance deteriorates significantly in acidic electrolytes due to reduced catalytic activity. We identified that the protonation of pyridinic nitrogen (pyri-N), which forms the active site, lowers the redox potential for oxygen adsorption, thereby hindering ORR activity in acidic conditions. To counter this, we designed hydrophobic cavities around pyri-NH^+ sites to suppress hydration and maintain high redox potential. Additionally, ionomer-coated SiO_2 particles were embedded to enhance local proton conductivity, allowing the catalyst to retain high onset potentials and current densities under acidic conditions.

Beyond conventional electrocatalysis, we developed a theoretical framework for mixed-potential-driven catalysis, where anodic and cathodic reactions occur simultaneously on a single catalyst surface without external bias. This concept was experimentally validated using room-temperature CO oxidation and enzyme-like glucose oxidation as model systems. Short-circuit current measurements confirmed mixed-potential behavior, and kinetic modeling based on the Butler–Volmer equation elucidated how overpotential partitioning governs reaction rates and selectivity.

Our work offers a unified design approach that bridges molecular-level understanding and system-level performance, not only enhancing the applicability of N–C catalysts in acidic media but also expanding the design space for hybrid electrochemical systems. These findings pave the way for advanced electrocatalysts for both fuel cell and selective chemical conversion applications.

Biography:

Kotaro Takeyasu received his Ph.D. degree under the supervision of Prof. Katsuyuki Fukutani at the University of Tokyo. After postdoctoral work with Prof. Michio Okada at Osaka University, and Prof. Yoshiyasu Matsumoto at Kyoto University, he started working as an Assistant Professor at University of Tsukuba with Professor Nakamura in 2018. He started a career in Institute for Catalysis, Hokkaido University as an Associate Professor from 2024 focusing on surface science and mixed-potential-driven catalysis on carbon catalysts.

Day 2, 22 July, 2025

Towards Direct Electro-Catalytic Production of Ammonia

Douglas R. MacFarlane

School of Chemistry, Monash University, Clayton, Victoria 3800, Australia

Abstract

In current discussions of new industries on the path to a zero net carbon future, "green hydrogen" – producing hydrogen and hydrogen carrying fuels using renewable energy – features prominently. The dream is capturing abundant but variable renewable energy by direct production of a storable and transportable form of the energy, for example as “green ammonia”.

This talk will begin by looking at the role of ammonia as a hydrogen vector, for conversion back into hydrogen at point of use, or for direct use as ammonia-fuel. Engine and turbine technologies for the latter application are developing rapidly for applications in marine transportation and power generation. Of course, green ammonia has a primary use in green fertiliser production.

Delving deeper, the talk will discuss progress and missteps in the search for electrocatalytic processes that can produce ammonia from renewable energy at ambient temperatures and pressures. While the reduction of N_2 in aqueous media seems possible, thermodynamically, with the right catalyst, the literature is littered with false positives. On the other hand, the lithium catalysed (mediated) approach, which involves lithium electrochemistry in an aprotic electrolyte, has recently emerged[1] [2] as a front runner, holding the promise of a genuinely practical and high efficiency process. We will discuss this in detail.

Biography

Doug MacFarlane is a materials chemist whose research focusses on materials based on room temperature liquid salts. Recent discoveries include electrocatalytic pathways that use renewable energy to produce green ammonia for fertilisers and fuels. He has published more than 800 papers and 30 patents during his career (92,000 citations, h-index 148) and has been a Highly Cited Researcher since 2020. He is a Fellow of the Australian Academy of Science and was awarded the Academy’s Craig Medal. His group won the 2023 Royal Society of Chemistry’s Horizon Prize. In 2024 he was elected Fellow of the Royal Society of London.

Biomass/waste valorisation into high-added value products: from energy vectors to pharmaceuticals

Rafael Luque

National University of Science and Technology Polytehnica Bucharest

Universidad ECOTEC, Km 13.5 Samborondon, Samborondon, EC092302, Ecuador

Abstract

The design of benign and environmentally sound methodologies has been the driving force of scientists in recent years towards more sustainable methodologies.

Attractive and innovative protocols that nowadays are even part of industrial ventures including biomass-derived porous carbonaceous materials, designer nanomaterials for catalytic applications and catalytic strategies for biomass/waste conversion into useful materials, chemicals and fuels have been recently developed in our group in recent years. These topics have extensively covered the preparation and design of (nano)materials, biocatalysts and photocatalysts and their utilisation in heterogeneously (bio)(photo)(electro)catalysed processes, flow chemistry as well as in biomass/waste valorisation practices. An important research avenue from the group deals with the search for novel and alternative reaction media in Organic Synthesis including mechanochemistry, organocatalysis and photo-redox processes as well as greener catalytic processes in Organic Chemistry (flow chemistry) for the synthesis of APIs.

In this lecture, we aim to provide an overview of recent efforts from our group in leading the future of global scientists in benign-by-design methodologies for biomass valorization including the “waste-to-pharma” concept.

Biography

Rafael Luque (PhD in 2005 from Universidad de Cordoba, Spain) has significant experience in biomass and waste valorization practices including nanoscale chemistry, green chemistry and catalysis as well as environmental remediation (>900 publications, h-index 118, >63,000 citations, 7 patents, >10 edited books).

Prof. Luque is currently Head of B4 group (Bioresources, Biopolymers, Biotechnology and Biorefineries) at National University of Science and Technology Polytehnica Bucharest (Romania), holding various positions as DFSP Chair Professor at King Saud University (Saudi Arabia), Distinguished Visiting Professor at University of Lahore (Pakistan) and International Distinguished Scientist at Universidad ECOTEC (Ecuador).

Green Methods for the Synthesis of Phosphonates, Phosphonates, and Phosphine Oxides

Gyorgy Keglevich

Department of Organic Chemistry and Technology, Faculty of Chemical Technology and Biotechnology,
Budapest University of Technology and Economics, 1521 Budapest, Hungary.

Abstract

The microwave (MW) technique is an important tool in organophosphorus chemistry. In this lecture, the advantages of MWs in different reactions are surveyed allowing green chemical accomplishments. The first case is the MW-assisted direct esterification of phosphinic-[1] and phosphonic acids,[2] along with phosphoric ester-acids[3] that all became more efficient in the presence of an ionic liquid catalyst. The O-alkylation of phosphonic acids and phosphoric ester-acid derivatives under MW irradiation is also a useful approach.[4] The interconversion of phosphinates and phosphinic amides was also elaborated.[5] Alcoholyses and hydrolyses of P-esters were also investigated and optimized.[6–8] A valuable finding of ours is that in the Hirao P–C coupling of >P(O)H reagents and bromoarenes applying $Pd(OAc)_2$ as the catalyst, the slight excess of the >P(O)H species may substitute the usual P-ligands in its tautomeric >POH form.[9] Ni-catalyzed cases will also be shown. The latter variation involves a brand new mechanism assuming a Ni(II) → Ni(IV) transition.[10] Heterocyclic derivatives were also involved in P–C couplings to provide P-functionalized species with cytostatic activity.[11] MWs may substitute catalysts, in certain reactions, such as in the Kabachnik–Fields condensations of amines, aldehydes and >P(O)H reagents. A series of new α-aminophosphonate derivatives were prepared that displayed significant anticancer activity on certain cell cultures.[12–16] β-Aminophosphonic derivatives were also prepared and derivatized.[17] The utilization of the Pudovik reaction in the synthesis of α-hydroxyphosphonates and their derivatization,[18] as well as the preparation of hydroxy-methylenebisphosphonates (dronic acid derivatives)[19] as biologically active substrates or drugs in the treatment of bone diseases will also be discussed. Phosphonoyl-functionalized hydroxyphosphonates were also synthesized.[20,21] The hydroxyphosphonates were converted to the mesyloxy derivatives.[22] Flow chemical accomplishments of a few reactions mentioned above, *e.g.* esterifications, alcoholyses and hydrolyses are also presented. It is also the purpose of this paper to elucidate the scope and limitations of the MW tool.[23]

References

1. Kiss N. Z., Keglevich G. Tetrahedron Lett. 2016, 57, 971–974.
2. Harsági N., Henyecz R., Ábrányi-Balogh P., Drahos L., Keglevich G. Molecules 2021, 26, 5303.
3. Harsági N., Kiss N. Z., Keglevich G. Synthesis 2022, 54, 3047–3054.
4. Keglevich G., Harsági N., Drahos L., Kiss N. Z. ChemPlusChem 2023, 88, e202200342.
5. Keglevich G., Harsági N., Szilágyi S. Green Chem. 2023, 25, 10372–10380.
6. Kiss N. Z., Henyecz R., Keglevich G. Molecules 2020, 25, 719.
7. Harsági N., Kiss N. Z., Drahos L., Keglevich G. Synthesis 2022, 54, 3899–3905.
8. Harsági N., Keglevich G. Green Process. Synth. 2022, 11, 176–183.
9. Keglevich G., Henyecz R., Mucsi Z. Molecules 2020, 25, 3897.
10. Keglevich G., Henyecz R., Mucsi Z. J. Org. Chem. 2020, 85, 14486–14495.

11. Huszár B., Szolga R., Bősze S., Oláhné Szabó R., Simon A., Karaghiosoff K., Czugler M., Drahos L., Keglevich G. Chemistry-A Eur. J. 2023, e202302465.

12. Varga P. R., Karaghiosoff K., Sári É. V., Simon A., Hegedűs L., Drahos L., Keglevich G. Org. Biomol. Chem. 2023, 21, 1709–1718.

13. Varga P. R., Dinnyési E., Tóth S., Szakács G., Keglevich G. Lett. Drug Des. Discov. 2023, 20, 365–371.

14. Varga P. R., Oláhné S. R., Dormán G., Bősze S., Keglevich G. Pharmaceuticals 2023, 16, 506.

15. Szalai Z., Bednárik J., Tóth B. S., Takács A., Tekula S., Kőhidai L., Karaghiosoff K., Drahos L., Keglevich G. Pharmaceuticals 2025, 18, 91.

16. Bircher M., Karaghiosoff K., Czugler M., Takács A., Kőhidai L., Drahos L., Keglevich G.:. Chemistry-A Eur. J. 2025, in press.

17 Keglevich G.,Varga P. R., Dinnyési E., Szalai Z., Bősze S., Oláhné Szabó R., Drahos L., Karaghiosoff K. *Org. Biomol. Chem.* **2024**, *22*, 3940–3950.

18 Varga P. R., Belovics A., Bagi P., Tóth S., Szakács G., Bősze S., Szabó R., Drahos L., Keglevich G. *Molecules* **2022**, *27*, 2067.

19-Nagy D. I., Grün A., Garadnay S., Greiner I., KeglevichG. *Molecules* **2016**, *21*, 1046.

20 Varga P. R., Hägele G., Keglevich G. *Tetrahedron Lett.* **2021**, *68*, 152902.

21 Varga P. R., Belovics A., Karaghiosoff K., Szabó R., Bősze S., Drahos L., Keglevich G. *Synthesis* **2024**, *56*, 561–566.

22 Szalai Z., Debrei M., Ábrányi-Balogh P., Bősze Sz., Oláhné Szabó R., Karaghiosoff K., Drahos L., Keglevich G. *ACS Omega* **2024**, **9**, 31043-31055.

23 Schindler J., Nagy D., Harján R., Keglevich G**.** *React Chem. Eng.* **2025**, *10*, 371-378.

Single Atom Catalysts for the Efficient and Selective Synthesis of Fuel Additives

M. Samy El-Shall

Department of Chemistry, Virginia Commonwealth University, Richmond, VA 23284-2006, USA

Presentation mode (Keynote)

Abstract

The catalytic conversion of isobutene into branched liquid hydrocarbons is of vital importance for the development of efficient fuel additives. Here, by developing a tungsten single-atom catalyst (W_{SAC}) atomically dispersed on a silica-doped alumina (SDA) support, we report that the W_{SAC}/SDA catalyst affords efficient conversion of isobutene selectively into highly branched C_8 and C_{12} liquid olefins while avoiding higher molecular weight hydrocarbons. The atomically dispersed tungsten single-atom catalyst was synthesized using a facile route based on the high-temperature pyrolysis of a sacrificial zinc metal-organic framework (Zn-MOF) in a nitrogen atmosphere followed by annealing in air. The results revealed the presence of W single-atom sites with an average size of 0.2 nm anchored on rod-like SDA elongated nanoparticles' support. The conversion of isobutene was investigated over the W_{SAC}/SDA catalysts at 1 atm and 150 - 250 ^oC using different W-loading of 1.6 - 6.0 wt.%. The 3.7% W-content catalyst demonstrated the highest catalytic activity for the conversion of isobutene into liquid branched dimers and trimers as determined by gas chromatography and NMR analyses. The selectivity of the catalyst can be tuned by controlling the temperature of the reaction. At 150 ^oC, the 3.7 wt.% W_{SAC}/SDA catalyst yielded liquid olefins containing >60% dimers and ~40% trimers. When the reaction temperature increased to 250 ^oC, the catalyst resulted in the formation of ~95% dimers and ~5% trimers. The W_{SAC}/SDA catalysts with promising activity, selectivity, and high stability in ambient conditions pave the way for a new family of single-atom catalysts for the selective synthesis of highly efficient fuel additives.

Biography

Samy El-Shall is the Mary Eugenia Kapp Endowed Chair in Chemistry and Commonwealth Professor at Virginia Commonwealth University, USA. He received his B.S. and M.S. degrees from Cairo University and a Ph.D. from Georgetown University. He did postdoctoral research in nucleation and clusters at the University of California, Los Angeles. His research interests include nanostructured materials, graphene, and nanocatalysis for energy and environmental applications, gas phase clusters and nucleation. He has published over 300 refereed papers and review chapters (Google Scholar h-index = 65, citations > 16,500), and he holds 11 US patents on the synthesis of nanomaterials, nanoparticle catalysts, graphene, and graphene-supported catalysts.

Iron Catalysis: Developing Reactions for Conjugated Material Synthesis

Rui Shang* and Eiichi Nakamura

Department of Chemistry, The University of Tokyo 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033.

Presentation mode (Oral)

Abstract

Because of the abundance and negligible toxicity, iron is ideal as a sustainable catalytic resource for producing organic functional materials. Through years of research on iron catalysis and conjugated materials, I have come to understand various unique properties of organic iron compounds, especially their low oxidation-reduction potentials in catalyst turnover and the mechanism of C-H bond cleavage. The speaker acknowledges that these characteristics give iron catalysis an advantage in synthesizing highly conjugated molecules, especially those with higher HOMO energy levels, fused rings, and large ring strains, that are difficult to obtain by other methods. We have successfully designed several iron-catalyzed reactions to obtain conjugated molecules. These include C–H/C–H coupling for polymerization, tandem cyclization to highly strained frameworks, efficient aza-p-extension, and spiro-cyclizations. These new methodologies facilitate the efficient synthesis of various conjugated polymers and small polycyclic conjugated molecules. Some new molecules have exhibited promising performance in solar cells, organic photodetectors, and promising applications for light-emitting diodes, demonstrating their potential for the organic electronics industry. Biography: Rui Shang works at the Department of Chemistry at the University of Tokyo. He received his B.Sc. and Ph.D. (2014) from the University of Science and Technology of China and had a joint-training Ph.D. at U-Tokyo (2012–2014) with Prof. Eiichi Nakamura. Then he served as a JSPS postdoctoral fellow there. In 2017, he was promoted to lecturer at U-Tokyo, as an associate professor in 2020, and to project professor in 2024. Rui's research interests cover catalytic reactions, conjugated molecules, and their material functions. Rui received the Young Chemist Award of the Chemical Society of Japan (2022), the Chemist Award BCA 2022, Thieme Chemistry Journals Award 2023, and the ACS Catalysis Lectureship Award 2025.

Biography

Rui Shang works at the Department of Chemistry at the University of Tokyo. He received his B.Sc. and Ph.D. (2014) from the University of Science and Technology of China and had a joint-training Ph.D. at U-Tokyo (2012–2014) with Prof. Eiichi Nakamura. Then he served as a JSPS postdoctoral fellow there. In 2017, he was promoted to lecturer at U-Tokyo, as an associate professor in 2020, and to project professor in 2024. Rui's research interests cover catalytic reactions, conjugated molecules, and their material functions. Rui received the Young Chemist Award of the Chemical Society of Japan (2022), the Chemist Award BCA 2022, Thieme Chemistry Journals Award 2023, and the ACS Catalysis Lectureship Award 2025.

Organic Nanoparticles for Biohybrid Photocatalysis

Haining Tian*

Physical Chemistry, Department of Chemistry-Ångström Laboratory, Uppsala University, 75120 Uppsala, Sweden

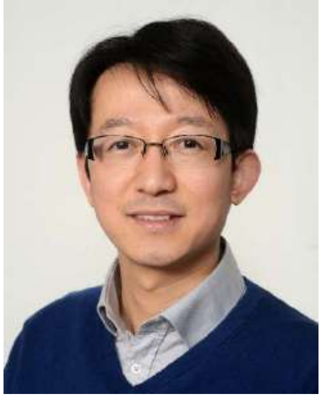
Presentation mode (Keynote)

Abstract

Organic nanoparticles including molecule nanoparticles and polymer nanoparticles have used for wide application in photocatalysis for solar fuel and solar chemical production, thanks to their excellent water dispersibility and tunable optical properties [1]. These nanoparticles, with their small size and adjustable surface charge via different surfactants, offer unique opportunities for integration with biological systems. Although organic nanoparticles have traditionally been used as fluorescent probes and in phototherapy [2], their potential in bio-integrated systems for solar fuel production remains largely untapped.

In our recent work, we explore innovative strategies employing organic particle-based biohybrid systems for solar fuel production. In this talk, I will present our lab's progress on developing organic–enzyme and organic–bacteria hybrid systems for the generation of solar fuels and solar chemicals [3-4]. This includes key advancements from our involvement in the EU Photo2Fuel project, with a particular focus on the development of biohybrid systems for CO_2 fixation.[5]

Biography



Haining Tian is a full Professor at Uppsala University, where he leads the Molecular Devices for Artificial Photosynthesis research group. He received his PhD from Dalian University of Technology in 2009, followed by postdoctoral and researcher positions at the KTH Royal Institute of Technology in Sweden. In 2014, he began his independent research career at Uppsala University and was promoted to full Professor in 2024. Professor Tian has received several prestigious awards, including Göran Gustafsson Prize for young researchers, Young Investigator Award from the European Photochemistry Association, and Wallenberg Academy Fellow. His research focuses on the development and investigation of sustainable soft materials for solar energy conversion and storage. He has published over 100 peer-reviewed articles and edited the book *Molecular Devices for Solar Energy Conversion and Storage*.

P-alkyl esters and methods to obtain them without the use of transition metals and halides

Jacek Nycz[1]*, Jakub Adamek[2], Piotr Latos[3]

[1] *Institute of Chemistry, Faculty of Science and Technology, University of Silesia in Katowice, ul. Szkolna 9, 40-006 Katowice, Poland*

[2] *Department of Organic Chemistry, Bioorganic Chemistry and Biotechnology, Silesian University of Technology, B. Krzywoustego 4, 44-100 Gliwice, Poland*

Department of Organic Chemical Technology and Petrochemistry, Faculty of Chemistry, Silesian University of Technology, 44-100 Gliwice, Poland

Abstract

Phosphate esters are vital constituents of various biologically active compounds such as nucleotides, glycolipids, nucleic acids, proteins, and steroids. These monoesters are actively involved in cell signaling and regulation pathways. They find potential applications in medicinal chemistry, such as water-soluble prodrugs. Phosphorylation is carried out in biological systems by ATP in the presence of kinases as catalysts; on the other hand, phosphatases catalyze the removal of a phosphate group in biological systems. Therefore, laboratory methods for synthesizing analogous compounds are mandatory to understand the biological pathways and develop therapeutic routes. The mono-substituted phosphate esters derived from alcohols are not commercially available due to their intrinsic instability, due to various decomposition pathways. Monoesters $(RO)P(=O)(OH)_2$ have hardly been used for this purpose due to the absence of established synthetic protocols to stabilize these unstable species. Multigram quantities of unstable and normally inaccessible phosphate monoesters $ROPO_3H_2$ (R = Me, Et, iPr, and tBu) have been synthesized by modifying an existing synthetic protocol known for the preparation of more stable ethyl phosphate. The methyl, ethyl, isopropyl, and tert-butyl monoesters were initially isolated as their corresponding cyclohexylamine salts and were characterized by single-crystal X-ray diffraction to establish the layered nature of these organic ionic phosphates. These monoesters are thermally labile and undergo facile thermolysis at low temperatures through β elimination.

It is much easier to convert the reagents possessing a P-halogen bond to appropriate esters, which is confirmed by numerous papers and methods described in the literature.

Phosphoric acid is produced from phosphate rocks through a so-called “wet process” in which the minerals are treated by sulfuric acid. Therefore, from an economic and green point of view, it is worth converting phosphoric acid into phosphoric acid esters. However, to date, relatively few methods have been developed for the direct conversion of phosphoric acid into its esters. It is generally believed that phosphoric acids, described with the general >P(=O)OH fragment, are difficult to convert in one synthetic step to the corresponding >P(=O)OR esters, especially when R is an aryl or tertiary carbon atom under thermal conditions. One interpretation could be that monoesters of phosphoric acids of the type $(RO)P(=O)(OH)_2$ are thermally labile and undergo easy thermolysis already at low temperatures. Keglevich et al. report successful esterifications of phosphinic acids under microwave (MW). For comparison, they presented the results of traditional heating, which resulted in a maximum of 12-15% conversion [1].

In this lecture, we will present alternative preparations of alkyl esters, especially phosphoric acid methyl esters.

References

[1] G. Keglevich, N. Z. Kiss, Z. Mucsi, T. Körtvélyesi, *Org. Biomol. Chem., 2012, 10, 2011*.

Mechanochemistry and Photochemistry: Novel Synthetic Strategies

Bartłomiej Furman

Institute of Organic Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

Abstract

Our research group has carried out extensive work in organic synthesis for many years, focusing on various challenges including the design of target molecules, the creation of high value compounds and the development of novel methods for the synthesis of heterocyclic compounds. Until recently, our primary approach was based on traditional methods - carrying out reactions in solution, using thermal energy to excite molecules, and studying different catalytic systems.[1] In essence, we were following the conventional synthetic chemistry paradigm.

While these methods produced satisfactory results, we decided it was necessary to move beyond established practices. We decided to explore new techniques, venturing into classical photochemistry ('photolysis')[2] and moving from solvent-based reactions to mechanochemistry.[3] In this talk, we will highlight some of the key findings and discuss the potential implications of these innovative approaches for the future of organic synthesis.

CURRICULUM VITAE – Bartłomiej Furman

Institute of Organic Chemistry Polish Academy of Sciences, Kasprzaka 44/52,

01-224 Warsaw, Poland

Email: bartlomiej.furman@icho.edu.pl

Homepage: www.ichopan2.pl

Research field

Bartłomiej Furman has been a full professor since 2014 and has led the 'Stereoselective Synthesis of Biologically Active Compounds' team at the Institute of Organic Chemistry, Polish Academy of Sciences for 15 years. As a synthetic organic chemist, Professor Furman focuses on the development of fundamentally new and practical synthetic reactions and methods for the efficient production of complex organic molecules of pharmaceutical interest.

Selected awards and Recognition

2001- Foundation for Polish Science Award for Young Scientists

2000- Polish Prime Minister Award for Ph.D. Thesis

Since 2022- Polish representative in EuChemS Division of Organic Chemistry

Representative Publications 1. P. J. Czerwiński and B. Furman Chem. Commun. 2019, 55, 9436-9439 2. A. Domżalska-Pieczykolan, I. Funes-Ardoiz, B. Furman and C. Bolm Angew. Chem. Int. Ed. 2022, 61, e202109801 3. P. Szcześniak and B. Furman Chem. Commun. 2022, 58, 1898-1901 4. P. J. Czerwiński, B. Grzeszczyk and B. Furman Org. Lett. 2022, 24, 9269–9274 5. M. Dolna, J. Narodowiec, O. Staszewska-Krajewska, P. Szcześniak and B. Furman React. Chem. Eng., 2023, 8, 784-789

6. P. J. Czerwiński, J. J. Najczuk and B. Furman ACS Sustainable Chemistry & Engineering 2022, 32, 10486-10492

7. K. Bartkowski, E. Masoumifeshani, U. Klimczak, M. Kotowska, B. Furman, C. Foroutan-Nejad and M. Lindner Angew. Chem. Int. Ed. 2025, e202423282

Operando NAP-XPS During Electrochemical Methane Formation on Ni(Cu)/YSZ: A Model Approach

Bernhard Klötzer*[,1] and Christoph W. Thurner[2]

[1]*Institute of Physical Chemistry, University of Innsbruck, Innrain 52c, 6020 Innsbruck, Austria*

[2]*Plansee SE, Metallwerk-Plansee-Strasse 71, 6600 Reutte, Austria*

Presentation mode: Oral

Abstract

Solid oxide cell technologies play a pivotal role in the realm of renewable energy storage, guiding us through the journey toward decarbonization. Understanding how electrocatalytic materials behave under high-temperature conditions is an absolute necessity to push these technologies forward. Operando spectroscopic investigations, such as near-ambient pressure X-ray photoelectron spectroscopy (NAP–XPS), offer insights into the chemical nature of active working electrodes, including the dynamic response of redox states and adsorbate chemistry to changing electrochemical conditions. Mixed ceramic–metallic electrodes exhibit a limited region with electrochemically active triple-phase-boundary (TPB) sites, which are located close to the electrolyte/electrode interface. To monitor this specific region spectroscopically, metallic (Ni) and bimetallic (NiCu) network-like structures are synthesized on a yttria-stabilized zirconia electrolyte and the electrochemical state and performance are studied by using operando NAP–XPS. In the experiments, the surface oxidation states under different polarizations are revealed, the gas composition dependent Nernst shift is confirmed, electrocatalytic activities are unraveled, and hydrogen evolution is correlated with the applied potential and local electrical field strength. Under H_2O/CO_2 co-electrolysis conditions, enhanced electrochemical methane formation is correlated to reactive carbon intermediates formed near the TPB. The findings demonstrate the effectiveness of thin-film model cells with spectroscopically accessible TPB regions for probing interfacial states and electrochemical processes. The obtained fundamental knowledge can provide valuable insights for the advancement of renewable energy storage technologies.

Biography

Since 2011: Associated Professor at the Institute of Physical Chemistry, University of Innsbruck

January 2011: Habilitation in Physical Chemistry, Venia Legendi

2011-2019: Principal Investigator of FWF-SFB F45 “Functional Oxide Surfaces and Interfaces”, Project Part F4503-N16 “Catalytic synergisms at (bi)metallic and oxidic phase boundaries and interfaces”

2010-2011: Tenure Track Position at the Institute of Physical Chemistry, University of Innsbruck, Austria

Since 2006: Group Leader of the "Nanostructured Model Catalysts" Group at the Institute of Physical Chemistry, University of Innsbruck, jointly with PD Dr. Simon Penner

1996-1998: Postdoc at University of Cambridge, UK, Group of Prof. David A. King

Photoassisted radical-mediated regeneration of saturated activated carbons

Conchi Ania[1*], Guilherme Bandinha[1,2] Benoit Cagnon[3]

[1]CNRS (CEMHTI, UPR 3079), Univ. Orléans, 45071 Orléans, France; [2]School Science and Technology, Univ. Nova de Lisboa, Lisboa, Portugal; [3]CNRS (ICMN, UMR 7374), Univ. Orléans, 45071 Orléans, France

Presentation mode (Invited Speaker)

Abstract

The increasing demand for activated carbon for water treatment applications is pushing the need to extend their lifetime through the development of efficient regeneration methods. In this study we investigate the oxidative radical-induced degradation of pollutants retained in the porosity of activated carbons, leading to the partial regeneration of the exhausted carbon adsorbents. Activated carbons with different saturation degrees have been exposed to UV light in aqueous environments, and the extent of the regeneration has been compared with that of conventional thermal regeneration. The irradiation of the aqueous suspensions of the saturated carbons resulted in a gradual regeneration, which efficiency depends on the saturation state of the activated carbon, the illumination time and the density of radical species formed. During the regeneration, a small fraction of the pollutants retained in the porosity of the carbon is released into the solution (desorption induced upon illumination), being subsequently photodegraded in the homogeneous phase thanks to the photogeneration of radical species. Data has also shown that for certain activated carbons, the carbon matrix itself can be oxidized during the photoassisted regeneration when long irradiation times are applied. For the thermal regeneration, the desorption rate strongly depends on the porosity of the pristine carbon, with high regeneration efficiencies when moderate temperatures are applied (minimizing the decomposition of the adsorbed fraction inside the pores, clogging the porous network).

Acknowledgements: H2020 (Project Ô, 776816); region CVdLoire (ARD-MATEX), ANR (SACRE).

Biography

Dr. Conchi ANIA (PhD 2003) is a Research Director of CNRS (France) and Research Scientist of CSIC (Spain). She has a long-standing interest on nanoporous carbons with tailored surface chemistry and architectures for applications in energy conversion and storage and environmental remediation (adsorption, photocatalysis, electrocatalysis). She has coauthored over 170 scientific publications with over 9000 citations (H_{index} 53). In 2008 she received the national L'Oreal-Unesco Research Fellowship "For women in Science". In 2023 she has received the Silver Medal of CNRS. She is Editor of Carbon journal since 2020.

Recent advances in MBE-grown GaAsSb nanowires for near-infrared photodetector applications.

Priyanka Ramaswamy

North Carolina A&T State University, North Carolina, USA.

Presentation Mode: Oral

Abstract

Over the past decades, III-V nanowires (NW) have been extensively studied due to their excellent physical properties and the advantage of realizing various architectures enabling monolithic integration of III-V semiconductor-based devices on the Si platform for the application of nanoelectronics and nanophotonic-based devices from the defense to civilians. In recent years, $GaAs_{1-x}Sb_x$ NW has attracted significant interest in high-performance and high-speed near-infrared photodetector (NIRPD) applications owing to the critical telecommunication wavelength coverage of 1.3 µm and 1.55 µm. In addition, GaAsSb exhibits good crystal quality due to the surfactant nature of Sb, excellent carrier mobility, longer electron lifetime, suppressed auger recombination, and ability to tailor band gap by tuning Sb composition. These superior characteristics make GaAsSb a highly desirable Sb-based ternary III-V alloy for NIRPD. This presentation will discuss the fabrication of MBE-grown room-temperature hybrid axial core-shell GaAsSb NWs NIRPD. I will focus on the characterization of the nanowires as the assessment of dopant incorporation for realizing advanced high-performance NW-based IRPD is essential. Finally, an overview of the advancements in ternary III-V NWs for the next-generation optoelectronic applications will be provided.

Biography

Dr. Priyanka Ramaswamy is a Sr. Process Integration Engineer at Micron Technology, Boise, USA. Dr. Priyanka earned her M.Sc. Physics from the National Institute of Technology, Trichy, India, in 2015 and Ph.D. in Electrical and Computer Engineering from North Carolina A&T State University, Boise, USA, in 2022. Her research focused on the fabrication and characterization of MBE-grown GaAsSb nanowires for near-infrared photodetectors. Dr. Priyanka has published over nine research articles in highly eminent journals and is pending approval for one US patent.

Shaping the Future of Catalysis: AI and Molecular Modeling for Superior Selectivity

Izabela Czekaj*

Faculty of Chemical Engineering and Technology, Cracow University of Technology, Warszawska 24, 31-155 Kraków, Poland

Invited Talk

Abstract

This presentation will delve into the pivotal role of artificial intelligence (AI) and molecular modeling in selecting catalytic materials with enhanced selectivity for biomass valorization, catalytic biofuel production, and deNOx processes. It will explore the future of chemical technology through the integration of biorefineries and advanced molecular modeling, covering the electronic structure of lignocellulose and the nano-design of zeolite-based catalysts for selective biomass conversion into chemicals. The technological aspects of catalytic biomass valorization to carboxylic acids will also be discussed, along with innovative catalysts for biomass gasification and methanation, and modern aspects of selective catalytic reduction of NOx. Emphasis will be placed on the necessity of AI in computational chemistry, particularly for analyzing numerous reaction pathways under complex process conditions. The presentation will highlight the limitations of independently interpreting extensive DFT calculations and the need for AI tools, illustrated with examples of DFT results for various heterogeneous systems. These topics underscore the crucial role of advanced modeling in enhancing complex processes and its growing importance in future technologies.

Biography:

DSc Eng. Izabela Czekaj is a Professor at the Faculty of Chemical Engineering and Technology at Cracow University of Technology since 2015. With over 20 years of experience, she specializes in heterogeneous catalysis, theoretical modeling, and AI applications in chemical engineering. Her work focuses on catalytic biomass valorization, NOx reduction, and innovative environmental solutions. DSc Eng. Czekaj has collaborated with leading institutions like the Paul Scherrer Institute and ETH Zurich, and has published in prestigious journals such as Nature Catalysis and Angewandte Chemie. She actively contributes to the scientific community and industrial advancements through her research and expertise.

Poster Presentations

Efficient oxidation of organic pollutants using Ni(II)@SiO_2–PDS: A study on reaction pathway and kinetics

Justinabraham Romiyo Vijayakumar1*, Amir Mizrahi2 , Dan Meyerstein1,3 1

Department of Chemical Sciences and The Radical Research Center, Ariel University, Ariel, Israel 2 Chemistry Department, Nuclear Research Centre Negev, Beer-Sheva, Israel 3 Department of Chemistry, Ben-Gurion University, Beer-Sheva, Israel Presenter

Abstract

In recent years, numerous Fenton-like reactions have been employed in the degradation of organic pollutants through various advanced oxidation processes (AOPs) involving hydrogen peroxide (H_2O_2), peroxymonosulfate (PMS), and peroxydisulfate (PDS). In this context, the present work investigates the kinetics and reaction mechanism between the catalyst and PDS for the degradation of the organic pollutant methylene blue at different reaction conditions. The Ni supported wrinkled silicon oxide (SiO2) was used as catalyst for the degradation of methylene blue. The rapid kinetics elucidates the efficiency of the catalyst and the role of PDS in the degradation mechanism. The proposed reaction mechanism consists of persulfate activation by the Ni/SiO2 surface active sites, which generates highly efficient sulfate radicals. The catalyst loading, methylene blue concentration, PDS concentration, and pH studies were analysed to clarify the reaction pathway for the degradation process. The crystallinity, structural morphology, oxidation states, and elemental composition of prepared Ni/SiO2 nanocomposite were analysed by X-ray diffraction (XRD), Transmission electron microscopy (TEM), and X-ray photoelectron spectroscopic (XPS) analysis. UV-Vis spectroscopy and HR-MS 3rd International Conference on Catalysis Science and Chemical Engineering (CatScience 2025) July 21 - 23, 2025| Budapest University of Technology, Hungary spectroscopic techniques are used to investigate the degradation and its products for methylene blue degradation. The findings indicate that the excellent catalytic activity of Ni/SiO2 and highly active sulfate radicals enhanced the degradation of methylene blue for environmental remediation. Due to its remarkable catalytic performance, cost-effective and eco-friendliness, the developed Ni/SiO_2–persulfate system represents a promising advancement in catalytic oxidation, contributing valuable insights toward the evolution of nextgeneration catalytic technologies.

Keywords

Fenton-like reactions, Advance oxidation process, persulphate radical anion, wrinkled SiO2

Biography

Dr. Justinabraham Romiyo Vijayakumar is currently working as a Postdoctoral fellow in department of chemical sciences at Ariel University, Israel. He holds a background in material science with a strong interest in catalysis. His research primarily focused on developing nanomaterials and their derived nanohybrids/composites for applications in catalysis based water remediation. Dr. Justin has actively participated in many national and international conferences, workshops and is passionate about translating scientific knowledge into practical solution.

A Magnesium-Catalyzed Fenton-Like Process: Radical Pathways in Peroxymonosulfate Oxidations for Environmental Remediation

Gayathri Jeevanandham[1]* and Dan Meyerstein[1,2]

[1]*Ariel University, Chemical Sciences Department and The Radical Research Center, Ariel, Israel*

[2]*Ben-Gurion University, Chemistry Department, Beer-Sheva, Israel*

Abstract

Transition-metal-free Fenton-like systems are gaining interest for sustainable advanced oxidation processes (AOPs). The effective activation of peroxymonosulfate (PMS) by magnesium ions (Mg^{2+}) is reported. To follow the kinetics the oxidation of Rhodamine B (RhB), a representative xanthene dye, under near-neutral pH (7.5) was studied. Unlike conventional Fe-based systems, this Mg^{2+}/PMS system operates efficiently without pH adjustment or iron sludge generation. The reaction was performed with 5 mM Mg^{2+}, 3 mM PMS, and 0.01 mM RhB. An increase in RhB (0.01 to 0.5) concentration leads to slower degradation kinetics due to higher pollutant loading, whereas increasing the concentrations of Mg^{2+} and PMS (1 to 5mM) accelerates the reaction, maintaining a pseudo-first-order kinetic profile with significantly faster reaction rates. UV- Vis spectroscopy was used to monitor degradation kinetics, showing rapid conversion following pseudo-first-order behavior. Reactive oxygen species (ROS) including sulfate radicals ($SO_4{\bullet}^-$) and hydroxyl radicals ($OH{\bullet}$) were identified as the dominant oxidants through scavenging experiments with ethanol and tert-butyl alcohol. The synergistic effect between Mg^{2+} and PMS significantly improves ROS generation compared to PMS alone. Degradation intermediates were identified using liquid chromatography–mass spectrometry (LC-MS) and high-resolution mass spectrometry (HRMS), enabling proposed degradation pathways. The system offers a green, efficient, and scalable alternative for the removal of dye pollutants, expanding the applicability of non-transition-metal AOPs in environmental remediation.

Keywords

Magnesium catalysis, Peroxymonosulfate, Fenton-like reaction, Rhodamine B, Sulfate radicals, Advanced oxidation processes

Biography

I am Dr. Gayathri Jeevanandham, a Postdoctoral Research Fellow at Ariel University, Israel, working under the mentorship of Prof. Dan Meyerstein. I completed my B.Sc. in Chemistry from Seethalakshmi Ramaswamy College, followed by an M.Sc. from Cauvery College for Women, an M.Phil. from St. Joseph's College, and a Ph.D. from SRM Institute of Science and Technology. My research focuses on radical-based Fenton-like advanced oxidation processes for environmental remediation, alongside the development of nanomaterials for electrochemical sensing and sustainable hydrogen production. I am passionate about green chemistry, sustainable technologies, and empowering women in science

B/Co/Carbon-Catalyzed Pyrolysis of Plastic Waste for Enhanced Hydrogen Generation

M. Calero1* , L. Jiménez-Rodríguez1 , M.A. Martín, R. Rodríguez-Solís, A. Pérez, S. Pérez-Huertas, G. Blázquez1 ,
M. J. Muñoz-Batista1

1 Department of Chemical Engineering, University of Granada, 18074 Granada, Spain

Abstract

The study explores the development of novel catalytic materials and their application in the valorization of real plastic waste through a catalytic pyrolysis process designed to produce a gas stream with a high H_2 content and other non-condensable gases. The materials consist of cobalt oxide and boron (as a minor component) supported on carbon. Pyrolysis experiments were conducted on a horizontal laboratory-scale fixed-bed tubular reactor (ID: 4 cm and L: 34.25 cm Nabertherm R 50/250/12 Model) made of stainless steel 316 integrated with a flowmeter to regulate the inert nitrogen drag. Pyrolysis tests were performed using 20 g of plastic waste placed in a closed 316 stainless steel tube (internal diameter of 27.25 cm and 30.6 cm of length) with a heating rate of 10 ºC/min from room temperature to 550-650 ºC, which was maintained for 60 min with a constant flow rate of 0.8 L/min of nitrogen. In addition to significantly enhancing the H_2 yield during the reaction with the B/Co/C systems, the catalysts exhibit magnetic properties, enabling their efficient recovery and separation from the carbonaceous solid fraction (with a separation efficiency exceeding 95% by weight). The study is complemented by a comprehensive characterization scheme, which includes the analysis of the materials' chemical, electronic, structural, and morphological properties using various techniques, such as magnetic susceptibility measurements, X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), nitrogen adsorption-desorption (BET analysis), and transmission electron microscopy with energy-dispersive X-ray spectroscopy (TEM-EDS), among others. This work has received funds from the project PID2022-139014OB-I00/SRA (State Research Agency)/10.13039/501100011033

Biography

Full Professor of Chemical Engineering at the University of Granada, Spain and responsible of the Research Group "Waste Recovery Technologies and Catalytic Processes (RNM-152). Its main lines of research focus on the characterization and valorization of waste from diverse sources to obtain compounds of interest. Some of the main technologies studied focus on thermochemical recycling processes, such as pyrolysis and gasification, and the development of catalysts for the different technologies. Finally, she collaborates in environmental impact studies through life cycle analysis.

Development of Non-Critical Metal-Based Electrocatalysts for Enhanced OER Activity in Anion Exchange Membrane Water Electrolyzers

Mireya Carvela*, Jesús Barranco, Daniel Mesas, Leticia Antequera, María José Torres

Industrial Technology Center of Castilla-La Mancha (ITECAM), Tomelloso (Ciudad Real), Spain

Abstract

In recent years, hydrogen production through water electrolysis has great potential to become a major energy source, particularly in the context of reducing carbon dioxide emissions. Anion Exchange Membrane Water Electrolysis (AEMWE) has emerged as a promising alternative to traditional low-temperature electrolysis technologies, reducing capital costs and addressing issues related to critical materials. However, lowering manufacturing costs is essential for competitiveness in the market. To accelerate development, research has focused on electrocatalysts based on non-critical metals, especially for the Oxygen Evolution Reaction (OER), which is key for designing high-performance, durable AEMWE electrolyzers. Two main challenges persist: first, current synthesis methods are not optimized for industrial applications, and second, while Ni/Fe-based materials have been explored as OER catalysts, their stability remains insufficient. This study aims to develop new electrocatalytic materials that improve both OER catalytic activity and hydrogen production efficiency in AEM electrolyzers. Conventional synthesis methods were tested, using sodium borohydride, formic acid, and ethylene glycol as reducing agents. Several synthesis parameters were modified to reduce operation times and enhance efficiency. Bimetallic and trimetallic catalysts based on Ni, Fe, and Co were developed to improve stability. These materials were characterized using physicochemical and electrochemical techniques. The results showed that transition metal-based materials enhance OER activity, achieving current densities of up to 2 A cm^{-2} at cell potentials below 2.3 V. This work is part of the AEMIOS project (SBPLY_23_76300_000001), co-financed by the European Union through the ERDF under the Castilla-La Mancha FEDER Program 2021-2027 and the Government of Castilla-La Mancha through INNOCAM.

Biography

Dr. Mireya Carvela Soler (ITECAM) is a specialist technician in the Department of Hydrogen Technologies at ITECAM since 2023. Her research focuses on electrochemical technologies for hydrogen production and energy storage. She specializes in the design of photo- and electrocatalytic reactors for hydrogen generation and CO_2 capture, as well as the development of catalysts for PEM and AEM technologies.

Engineering High-Performance PTLs for Next-Generation AEM Electrolyzers

María José Torres, Jesús Barranco*, Daniel Mesas, Leticia Antequera, Mireya Carvela

Industrial Technology Center of Castilla-La Mancha (ITECAM), Tomelloso (Ciudad Real), Spain

Abstract

Anion Exchange Membrane Water Electrolysis (AEMWE) is a promising approach to addressing the global energy crisis. However, this technology remains in development and requires further investigation. AEMWE cells consist of an anode and a cathode compartment separated by a membrane, which is integrated with two porous transport layers (PTLs) to form the Membrane Electrode Assembly (MEA). Each compartment contains a catalytic layer composed of an electrocatalyst and an ionomer binder. While research has primarily focused on enhancing membranes, ionomers, and PGM-free catalysts to improve AEMWE performance, PTLs also play a crucial role in system efficiency by minimizing ohmic and concentration overpotentials, which significantly influence total cell voltage. For this reason, this study aims to optimize PTLs in an AEM electrolyzer to reduce system resistance, decrease energy consumption, and enhance hydrogen production efficiency. The impact of PTL materials based on transition metals (Ni, Ti, stainless steel) was examined, along with different structural designs (foam and mesh) and porosities. Optimizing porosity is critical, as inadequate gas removal can lead to bubble formation, blocking active sites and increasing overpotential. Furthermore, the effect of catalyst layer deposition was assessed using an airbrush spraying technique, comparing membrane (CCM) and substrate (CCS) deposition. Results indicated that Ni foam with smaller pores exhibited superior electrochemical performance, reducing ohmic resistance by up to 72% compared to Ti-based PTLs. This work is part of the AEMIOS project (SBPLY_23_76300_000001), co-financed by the EU (ERDF) and the Government of Castilla-La Mancha under the 2021-2027 FEDER Program through INNOCAM.

Biography:

Dr. María José Torres Gómez-Calcerrada (ITECAM) is the Head of the Department of Hydrogen Technologies at ITECAM since 2021. In this role, she leads research and development (R&D) projects, with a particular focus on hydrogen production technologies. Throughout her career, she has demonstrated a strong commitment to advancing innovative solutions in chemical and environmental engineering, particularly in hydrogen production and CO_2 recovery through photo- and electrocatalytic technologies.

DAY – 3, 23 July, 2025

Battery Innovation Empowered by Lithium Bond and Artificial Intelligence

Xiang Chen, Chen-Zi Zhao, and Qiang Zhang*

Beijing Key Laboratory of Complex Solid State Batteries,
Tsinghua Center for Green Chemical Engineering Electrification (CCEE),
Department of Chemical Engineering, Tsinghua University, Beijing 100084, China

Plenary Talk

Abstract

Lithium bonds, analogous to hydrogen bonds, exhibit unique properties due to lithium's weak metallic nature, offering exciting potential for lithium battery applications. This talk will delve into the concept of lithium bonds, exploring their underlying chemistry and how they can be harnessed to design new battery material combining with emerging artificial intelligence, and further improve battery performance. Specifically, solid electrolytes combined with high-voltage Li-rich Mn-based cathodes and anode-free cell designs hold significant promise for high-energy-density and high-safety systems. However, challenges such as interfacial oxygen escape and unstable anode morphology continue to hinder their widespread applications. To address these issues, we have developed a fluoropolyether-based solid polymer electrolyte featuring a novel anion-rich solvation structure, which stabilizes the interface and enhances cycling stability. The resulting pouch cell demonstrates an ultra-high energy density (>600 Wh/kg) and excellent safety under a nail penetration at a full charge condition, advancing solid-state battery technology and paving the way for safer, higher-energy systems.

Biography:

Prof. Qiang Zhang is a full professor at Tsinghua University. He is the director of Department of Chemical Engineering, Tsinghua University. His current research interests are advanced energy materials and energy chemistry, including dendrite-free lithium metal anode, lithium sulfur batteries, and electrolyte, especially the structure design and full demonstration of advanced energy materials in working devices. His h-index is 170 now. He is the Editor-in-Chief of EES Batteries, Advisor Editor of Angew. Chem. He is sitting on the advisory board of Joule, Chem Soc Rev, Matter, Adv Funct Mater, ChemSusChem, J Mater Chem A, Chem Commun, Energy & Fuels, and so on.

Design of core-shell catalysts for CO_2 /syngas conversion and hydrogen production

Chen Luwei*

*Institute of Sustainability for Chemicals, Energy and Environment ($ISCE^2$), Agency for Science, Technology and Research (A*STAR), 1 Pesek Road, 627833, Singapore*

Presentation mode (Oral)

Abstract

Global population and economic growth have led to a corresponding tremendous increase in CO_2 emission. CO_2 is well-known as a climate destroyer but it can be transformed into a source of economic benefit with the help of new technologies and business ideas. Utilising CO_2 as a carbon resource for the large-scale production of sustainable synthetic fuels would reduce fossil-fuel dependence. On the other hand, green hydrogen is critical to achieve zero or negative CO_2 emission for the CO_2 conversion process. Catalyst plays an important role to make the chemical process successful and efficient. In this talk, the design of core-shell structure catalysts for H_2 production and CO_2 /syngas conversion to methane, hydrocarbons and methanol will be discussed [1-6].

References

[1] Kelvin Mingyao Kwok, Luwei Chen and Hua Chun Zeng, J. Mater. Chem. A, 8 (2020) 12757.

[2] Kelvin Mingyao Kwok, Sze Wei Daniel Ong, Luwei Chen, and Hua Chun Zeng, ACS Appl. Mater. Interfaces, 11 (2019)14774.

[3] Hiroyuki Kamata, Zhi. Qun. Tian, Yoshinori Izumi, Catherine. K. S. Choong , Jie Chang, Martin Schreyer , Luwei Chen, Armando Borgna, Catal. Today 299(*2018)* 193.

[4] Kelvin Mingyao Kwok, Sze Wei Daniel Ong, Luwei Chen and Hua Chun Zeng, , ACS catal. 8 (2018) 714-724.

[5] Catalyst for CO_2 to methanol, PCT patent application, Tan Mingwu, Chen Luwei, Chang Jie et. Al. .

[6] Technology disclosure , Electrocatalytic Ammonia Oxidation Reaction with Nano Nickel-Copper Hydroxide Catalysts, Wang Jinquan, Chen Luwei

Biography

Dr. Chen Luwei is a Senior Principal Scientist at the Institute of Sustainability for Chemicals, Energy and Environment ($ISCE^2$), A*STAR, where she leads the Carbon Conversion and Future Energy Carriers (CCFEC) division. She also holds a joint appointment as an Adjunct Associate Professor at the Department of Materials Science and Engineering, National University of Singapore (NUS). Dr. Chen earned her PhD from NUS and brings over 20 years of expertise in catalysis. Her research focuses on catalyst and materials development for renewable and alternative energy, biomass valorisation, and carbon dioxide capture and utilization.

The atomically precise Au-Ag nanoclusters catalyzed chemical conversion of CO_2

Haizhu Yu,* Ling Chen and Ruru Qiang

Anhui University, Hefei, Anhui 230601, China.

Presentation Mode: Invited Speaker

Abstract

As the medium sized material in between metal complexes and metal nanoparticles, the ultrasmall nanoclusters has recently attracted extensive research interest, predominant for their high performance and the value in mechanistic elucidation at the sub-nanometer scale. Starting from the size-controllable synthesis of the atomically precise group IB metal nanoclusters (with 6 to 100 of Au/Ag/Cu atoms, protected by organic ligands) and the kinetic analysis on their structural conversion, our group recently endeavors to explore their application in carboxylation of simple organic molecules with CO 2 . This talk mainly covers the application of a series of thiolate/phosphine/halide protected Au/Ag nanocluster with no more than 30 metal atoms in the cyclization of epoxide and CO 2 , and the identification of the key reaction sites therein.

Biography

Haizhu Yu is a professor at Anhui University. She has received her Ph. D. degree in Chemistry from University of Science and Technology of China in 2011. Her research interests include the synthesis of the atomically group IB metal nanoclusters, their catalytic applications in biomass conversion, and the inherent structure-property correlations. She has been supervisor of postdocs, Ph. D. students, master students and undergraduate students.

Preparation, Modification and Performance of Low-Temperature SCR Catalysts

Jyh-Cherng Chen[1]*, Chi-Feng Lin[1], Yi-Jie Lin[1]

[1]*Department of Environmental Engineering and Science, Feng Chia University, Taiwan*

Presentation mode (Oral)

Abstract

To significantly reduce NOx emissions, improve the air quality, and comply with the stricter emission standards for stationary pollution sources in Taiwan, many factories are opting to use selective catalytic reduction (SCR) equipment as their air pollution control devices. However, the most commonly used vanadium-tungsten-titanium SCR catalysts often exhibit shortcomings, such as insufficient deNOx efficiency at low flue gas temperatures and easily been poisoned and deactivated by SO_2 and H_2O in practical applications. There is a pressing demand for the development of efficient, economical, and durable low-temperature SCR catalysts.

This study developed a novel SCR catalyst and investigated its denitrification efficiency and anti-poisoning performance under various operating conditions. Experimental results indicate that the SCR catalyst, composed of a modified zeolite support and manganese as the active metal, exhibited excellent low-temperature deNOx efficiency. As the SCR catalyst was modified with cerium at a molar ratio of 0.05, its deNOx efficiency at a low temperature of 150°C reached 95%, and its anti-poisoning performance was outstanding. The results from long-term durability tests were also highly favorable. The physical and chemical characteristics of the Mn-Ce/zeolite catalyst were analyzed and confirmed to outperform the commonly used commercial V-W/TiO_2 catalyst at low temperatures, as well as demonstrate greater tolerance to SO_2 and H_2O. This low-temperature SCR catalyst shows significant potential for practical applications and further development.

Biography

Dr. Jyh-Cherng Chen is a Professor at the Department of Environmental Engineering and Science, Feng Chia University, Taiwan. He holds a Ph.D. from National Chung Hsing University. His expertise includes thermal treatment and incineration engineering, waste treatment and resource circulation, air pollution control, catalyst synthesis and applications, waste-to-energy and fuel conversion, net zero emission and carbon capture technologies.

Atomically Precise Size-and Composition-Selected Subnanometer Cu, Pd and CuPd clusters in Oxidative Dehydrogenation Reactions

Stefan Vajda

Department of Nanocatalysis, J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Prague, Czech Republic

Abstract

The presentation will address the identification and the exploitation of tuning knobs available at the subnanometer scale to control the performance of catalyst made of monometallic and bimetallic clusters, specifically Cu and Pd and bimetallic CuPd clusters. These clusters, containing a handful of atoms are supported on technologically relevant oxide- and carbon-based supports. The potential of controlling catalytic activity and selectivity by atomic precision control of the size-and composition of the clusters, along with leveraging metal-support interactions and optimizing reaction conditions will be demonstrated on the examples of the oxidative dehydrogenation of propane and cyclohexene, under realistic conditions of pressure and temperature.

As support material for the clusters, two type of supports, oxide and carbon-based ones are used. Thin films of amorphous alumina, tin oxide, titania and zirconia are prepared using atomic layer deposition are used. The nano- and microcrystalline diamond films are prepared in various modification, including as made, oxygen treated and boron-doped and combined. Next, the atomically precise clusters of copper (single atoms to seven-atom clusters), palladium (single atoms, dimers, four- and five-atom clusters) and bimetallic four and five-atom CuPd clusters (all $Cu_{4-x}Pd_x$ combinations and select $Cu_{5-x}Pd_x$ clusters) are generated in molecular beam in vacuum, utilizing a magnetron sputtering cluster source. And deposited on the supports at controlled metal loading [1]. Catalytic testing is performed at atmospheric in a custom flow reactor with mass spectroscopic analysis of the reaction products.

Alumina-supported Cu_n (n=1-7) reveals Cu_4 as the most active catalysts, being also the most active on alumina in comparison with the other oxide supports [1] Mixed CuPd and Pd tetramers exhibit support and composition-dependent performance in the dehydrogenation of cyclohexene, up to switched selectivity between benzene vs cyclohexadiene formation. [2]. Next, the size of Pd and CuPd clusters is increased to five atoms, leading to a further increase of activity by about an order of magnitude. Finally, when these same pentamers are deposited on variously treated and doped diamond supports of nanocrystalline and microscopic morphology, the activity increased by additional over an order of magnitude again, moreover with the activity of mixed CuPd pentamers exceeding twice that of the pure five-atom Pd custer. [3] Notably, the combustion channel is practically entirely suppressed on these catalysts.

As time shall allow, the performance of these clusters in the selective dehydrogenation of propane and direct propane oxidation to propylene oxide will be highlighted.

1. Valtera, S.; Jašík, J.; Vaidulych, M.; Olszówka, J.E.; Zlámalová, M.; Tarábková, H.; Kavan, L.; Vajda, Š. Atom by Atom Built Subnanometer Copper Cluster Catalyst for the Highly Selective Oxidative Dehydrogenation of Cyclohexene. *J. Chem. Phys.* **2022**, *156*, 114302-114310. DOI: 10.1063/5.0065350, link
2. Jašík, J.; Valtera, S.; Vaidulych, M.; Bunian, M.; Lei, Y.; Halder, A.; Tarábková, H.; Jindra, M.; Kavan, L.; Frank, O.; Bartling, S.; Vajda, Š. Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer $Cu_{4-n}Pd_n$ ($0 \leq n \leq 4$) tetramer clusters: The effect of cluster composition and support on performance. *Faraday Discuss.* **2023,** *242*, 70-93. DOI: 10.1039/D2FD00108J, link
3. in preparation

4. Halder, A.; Warburton, R.E.; Sun,G.,; Lei Cheng, Assary, R.S.; Seifert, S.; Homer, M., Greeley, J.; Alexandrova, A.N; Sautet, P.; Curtiss, L/A.; Vajda, S. "Low-Temperature Direct Oxidation of Propane to Propylene Oxide Using Supported Subnanometer Cu Clusters", *ACS Catal* **2025, 15**, 5760*,* DOI: 10.1021/acscatal.4c07577, link

Catalytic CO Oxidation and Photocatalytic Methylene Blue Degradation Using ZIF-8 Materials

Khaled Mohammad Saoud[1*], Rola Mohammad Al Soubaihi[1], and Shaheen A. Al-Muhtaseb[2]

[1]*Virginia Commonwealth University in Qatar, Liberal Arts and Sciences Program, P.O. Box 8095, Doha, Qatar.*

[3]*Department of Chemical Engineering, Qatar University, P.O. Box 2713, Doha, Qatar*

Presentation mode (Oral)

Abstract

Zeolitic Imidazolate Framework-8 (ZIF-8) and its derivatives have emerged as multifunctional materials with promising catalytic and photocatalytic properties. This study explores the performance of pristine, metal-doped (Co, Fe), and bare ZIF-8 in two key applications: catalytic carbon monoxide (CO) oxidation and photocatalytic degradation of Methylene Blue (MB) under visible light. Catalytic CO oxidation tests revealed that metal-doped and carbonized ZIF-8 materials exhibited significantly enhanced activity due to improved redox properties and oxygen activation. For MB degradation, photocatalytic efficiency increased with structural modifications that promoted better light absorption and charge separation. However, CoZif-8 stands out as having the highest CO oxidation conversion at low temperature (less than 50 °C) and the MB degradation (degrades 90% of MB to less than 60 nm). The results demonstrate that both the catalytic and photocatalytic behaviors of ZIF-8 can be effectively tuned by changing the metal center and thermal treatment, making these materials attractive candidates for air and water purification technologies. This work highlights the potential of ZIF-8-based platforms for dual-function environmental catalysis.

Biography

Dr. Khaled Saoud is a full Professor of Physics in the Liberal Arts and Sciences Program at Virginia Commonwealth University in Qatar (VCUarts Qatar). He has over 26 years of research, industrial, and teaching experience, including his previous positions at major American companies such as Philip Morris USA and Intel Corporation. His broad research interests encompass the development of nanomaterials for environmental and healthcare applications, including wastewater treatment, catalysis, and photocatalysis. Professor Saoud serves on the editorial boards of three international journals and is a reviewer for over 30 peer-reviewed journals. He holds three US patents and was the Lead Principal Investigator on a recent patent titled “Methods of Forming Aerogels.” He has published over 60 refereed papers and book chapters and delivered over 60 talks, including keynotes, invited talks, and conference presentations.

CO adsorption and H_2 dissociation at supported single-layer graphene

Luca Vattuone*

University of Genoa & IMEM- CNR Italy

Presentation Mode: (Oral)

Abstract

Adsorption and surface reactivity of 2D Materials such as graphene and h-BN is essential to understand at the fundamental level their sensing and catalytic properties as well as their functionalization. The interaction with the support is an important and not usually considered factor in applications. To study the effect of the substrate (Ni(111) in the present study) on the adsorption of test simple molecules such CO and H_2.

Single layer graphene is grown on Ni(111) by exposure to C_2H_4. Adsorption at liquid nitrogen temperature (LT) under Ultra High Vacuum conditions (UHV) is monitored by X ray Photoelectron Spectroscopy (XPS) and by High Resolution Electron Energy Loss Spectroscopy (HREELS) while adsorption at room temperature (RT) in the mbar range is monitored by Near Ambient Pressure (NAP) XPS in beamtimes at Soleil and PSI Light Sources.

We demonstrate that:

- CO adsorbs on monolayer graphene on Ni(111) both under LT/UHV and at RT/NAP conditions while no adsorption was detected under LT/UHV on a monolayer grown on Cu.

- Molecular H_2 can dissociate on graphene on Ni(111) when exposure is performed under NAP conditions. Theoretical DFT calculations show that this is possible thanks to a substantial reduction of the activation barrier in presence of the Ni substrate.

The strong interaction with the Ni(111) substrate substantially increases the reactivity of single layer Graphene with CO and H_2 This paves the way to the use of supported 2D materials as active supports and possibly even as catalysts.

Biography

L.V. got his PhD in Physics at the University of Genoa in 1994. After a post-doc stay at the University of Cambridge (UK) with Sir D.A. King he returned to Genoa. Since 1999 he is a staff Researcher at Unige, and since 2012 Associate Professor of Condensed Matter Physics.

L.V. research covers experimental studies of gas-surface interaction using vibrational spectroscopy, single crystal calorimetry, supersonic molecular beams and XPS as well as the measurement of surface plasmon dispersion using Electron Energy Loss Spectroscopy.

Recently his activity focused on the chemical reactivity of graphene and 2D materials and on confined chemistry.

Imagine! A World Free from Fossil Fuels

Jyri-Pekka Mikkola1,2*, Ajaikumar Samikannu2, William Siljebo2

1Åbo Akademi University, Finland; 2Umeå University, Sweden;

Presentation mode Oral

Abstract

Bio-ethanol production and ethanol transformation to gasoline has raised considerable interest in recent years concerning the demand for bio-renewable alternatives to petroleum-based fuels and chemicals. Ethanol cannot be directly used as a motor fuel, posing several technical difficulties such as low energy efficiency, cold start up and engine corrosion etc., but there is the possibility of converting it to gasoline range hydrocarbons. One of the major threats to the human life in the 21st century is the demand for the energy and the worldwide energy consumption is mainly derived from the fossil based non-renewable resources. For the reason of growing population and the increased energy consumption, there is the threat ahead that is the current petroleum crude oil reservoirs become depleted in the near future. Moreover, the use of non-renewable fossil reservoirs is a serious threat to the environment because of releasing large amount of CO2 to the environment that leads to the global warming. In this context, the current science community is much focused on finding the alternative and renewable resources for future energy. In this context, bio-ethanol considered to be the one of renewable resources that can be derived from biomass. We prepared transition metal modified mesoporous ZSM-5 by desilication method followed by metal loading by impregnation method. The prepared catalysts were tested on ethanol conversion to gasoline under gas phase. Mesoporous ZSM-5 loaded with several metals gives excellent performance in our pilot scale process yielding high-octane gasoline with very low benzene content, pure water and LPG gas.

Biography

Prof. Jyri-Pekka Mikkola received his M.Sc. in Chemical Engineering from Åbo Akademi University. After spending a few years at the industry he returned to the Åbo Akademi and completed his PhD (1999). In 2004 he was appointed as Academy Research Fellow and received 'The Incentive Award' in 2006. Since 2008 he is a professor at both Umeå University, Sweden and Åbo Akademi University, Finland. He has co-authored more than 400 papers, dozens of text books and holds a number of patents. The principal areas of interest are green chemistry; heterogeneous catalysis; ionic liquid technologies; chemical kinetics; biorefining; novel materials

Experimental Setups for Electrocatalysis in Magnetic Fields

Henrik Haspel[1,2]*, Áron Klonka[2], Ayoub Kaaouass[2], Fouad Alloun[2], Gergő Ballai[2], Zoltán Kónya[1,2]

[1]*HUN-REN-SZTE Reaction Kinetics and Surface Chemistry Research Group, University of Szeged, Szeged, Hungary*

[2]*Department of Applied and Environmental Chemistry, University of Szeged, Szeged, Hungary*

Presentation Mode: Invited Talk

Abstract

Hydrogen, a critical feedstock for the chemical industry, is predominantly generated via steam methane reforming (SMR) of natural gas, a process associated with a substantial carbon footprint. A more sustainable approach involves the electrochemical decomposition of water, powered by renewable energy, to produce carbon-neutral 'green' hydrogen. Research has demonstrated that applying an external magnetic field impacts the kinetics of water electrolysis through the reduction of overpotential of the oxygen evolution reaction (OER), which in turn decreases the energy required to achieve a specific hydrogen output. Moreover, the presence of a magnetic field has been shown to enhance the oxygen reduction reaction (ORR) activity, which improves H_2/O_2 fuel cell efficiency. Harnessing either the intrinsic magnetism of electrocatalysts or external magnetic fields offers potential for creating novel reaction pathways and substantially boosting electrocatalytic activity. Various experimental setups have been developed to apply magnetic fields to a working electrode, including permanent magnet slabs, electromagnets, magnetized electrodes, and magnetic coatings. After an overview of the current solutions specifically designed to study the effect of strong external magnetic fields on electrocatalytic reactions, experimental setups developed in our research group are presented: a horseshoe magnet assembly that uses NdFeB slabs to create a highly homogeneous and uniform magnetic field over several cm^2, a magnetic rotating disk electrode (RDE) setup for understanding the mechanisms of electrochemical reactions and a flow cell configuration for continuous, high-rate electrolysis under magnetic field.

Biography

Henrik Haspel holds an MSc in chemistry and physics and a PhD in chemistry from the University of Szeged, Hungary. He was a visiting researcher at Rice University's Department of Materials Science and NanoEngineering, specialized in 2D materials and heterostructures. Later, he dedicated almost five years to the KAUST Catalysis Center at King Abdullah University of Science and Technology (KAUST), involved in projects on photocatalytic and photoelectrochemical water splitting, as well as continuous-flow electrochemical CO_2 reduction. He is currently a senior research fellow at the University of Szeged, where his research is dedicated to electrocatalysis for environmental and energy applications.

Semiconductor Photocatalysts in Advanced Reduction Processes

Joanna Kisała*

Institute of Materials Engineering, Faculty of Exact and Technical Sciences,
University of Rzeszow

Presentation mode (Oral)

Abstract

Advanced Reduction Processes (ARPs) include techniques able to achieve degradation of contaminants by producing highly reactive reducing species such as, electron, or $CO_2^{\bullet -}$. Semiconductor photocatalysis is a highly effective and sustainable process leverages the unique redox properties of semiconductor materials under light irradiation to break strong carbon-halogen bonds, leading to detoxification and mineralization of these compounds. Semiconductor photocatalysts include metal oxides (TiO_2, ZnO, SnO_2, etc.), metal chalcogenides (CdS, ZnS, MoS_2), spinel ferrites ($CoFe_2O_4$, $ZnFe_2O_4$, $FeFe_2O_4$, etc.), perovskites ($BiFeO_3$, $SrTiO_3$). The photocatalytic dehalogenation reaction can proceed through two pathways: (a) direct pathway - in which the photogenerated electrons are separated and captured by the contaminant molecules; and (b) the indirect path, in which photogenerated holes are used to produce reducing radicals by reaction with molecules such as $HCOO^-$, $C_2O_4^{2-}$. The overall efficiency of a semiconductor is dictated by three key intrinsic characteristics of the material: (i) small band gap allowing harvesting visible light, (ii) absolute potentials of the E_{CB} and E_{VB}, (iii) the rate of charge recombination. A small bandgap is desirable regarding a broad light absorption band. The band-edge positions play crucial role in conducting the corresponding oxidation and reduction reactions. However, when redox ability is considered, the catalyst should have a high CB position and a low VB position, resulting in a large bandgap. These two prerequisites are not compatible. To achieve higher light absorption and appropriate band potentials, the materials design strategies are used such as introducing point defects in semiconductors, or forming heterostructures with multiple semiconductors and other materials.

Biography

Dr. Habil. Eng. Joanna Kisała is a Polish scientist affiliated with the Institute of Materials Engineering at the University of Rzeszów, where she conducts research and academic activities. Her scientific interests are focused on the study of nanomaterials, including their synthesis, characterization, and application, especially in photocatalytic degradation of POPs. She has contributed to research on the development and optimization of semiconductor photocatalysts—such as metal oxides, chalcogenides, and ferrites—for the degradation of organic pollutants, including halogenated compounds. Her work involves exploring the mechanisms of photocatalytic reactions, the design of advanced materials, and the study of their surface and electronic properties.

Pt clusters stabilized on 2D MoS2 for ultrafast hydrogen evolution

Tamás Ollár[1*], Antal A. Koós[1], Péter Vancsó[1], Péter Kun[1], Péter Nemes-Incze[1], Miklós Németh[1], Béla Pécz[1], Chanyong Hwang[2], József S. Pap[1], and Levente Tapasztó[1]

Affiliation (Institution/organization name, Country) {For Ex: [1]XXX University, China; [2]YYY Organization, Spain; [3]ZZZ Institute, USA)} [Should be in Italics]

1. *Centre for Energy Research, Institute for Technical Physics and Materials Science & Institute for Energy Security and Environmental Safety, Hungary*
2. *Korea Research Institute for Standards and Science, Republic of Korea*

Abstract

While platinum exhibits unmatched activity in catalysing hydrogen evolution, due to its scarcity, extremely atom-efficient solutions are needed, to enable large-scale applications, such as the cost-efficient, mass-production of green hydrogen. Here, we show that the intrinsic activity of Pt can be further improved by boosting its interaction with van der Waals crystals, inducing dramatic changes in the atomic and electronic structure of small (~1 nm) Pt clusters that acquire a bilayer structure (~3 Å height) and a sizeable bandgap (E_g~250 meV). Such semiconducting, bilayer Pt clusters display exceptionally high hydrogen production efficiency (~1400 H_2 s^{-1} @ 100 mV), with the most active sites (DG_H ~ -1 meV) located in the bottom Pt layer strongly adhering to the MoS_2 support. Such catalysts can reach the activity of commercial Pt/C catalysts at three orders of magnitude lower Pt loadings of ~10 nanograms/cm^2, utilizing Pt a hundred times more efficiently than Pt single atom catalysts.

Biography

1. Spontaneous doping of the basal plane of MoS2 single layers through oxygen substitution under ambient conditions J Pető, T Ollár, et al. Nature chemistry 10 (12), 1246-1251
2. Transition metal chalcogenide single layers as an active platform for single-atom catalysis P Vancsó, et al. ACS Energy Letters 4 (8), 1947-1953
3. Semiconducting Pt Structures Stabilized on 2D MoS2 Crystals Enable Ultrafast Hydrogen Evolution T Ollár, et al. Advanced Materials, 2025, 2504113--

Direct Methane Aromatization over Mo/HZSM-5 Zeolites: Significance of Nickel and Magnesium as Co-Promoters

Authors: Themba E. Tshabalala[1], Michael S. Scurrell[2]

[1]*Advanced Materials Research Group, Department of Physical and Earth Sciences, Sol Plaatje University, Kimberley 8300, South Africa*

[2]*Department of Civil and Chemical Engineering, University of South Africa Themba.tshabalala@spu.ac.za, +27 72 030 6325*

Presentation mode: Oral

Abstract:

Natural gas primarily consists of methane, which has the potential to be converted into valuable hydrocarbons through a process called catalytic aromatization. Recent studies have shown that using Mo/H-ZSM-5 zeolite catalysts can directly convert methane into aromatic compounds like benzene, toluene, naphthalene and hydrogen under a non-oxidative environment. However, an issue arises as these catalysts tend to deactivate due to coke formation. To address this challenge, we will investigate the effect of adding nickel (Ni) and magnesium (Mg) as co-promoters to Mo/H-ZSM-5 catalysts to improve their stability and overall performance. The catalysts were prepared using sequential impregnation methods with varying Ni (0.5–4 wt.%) and Mg (0.01–0.1 wt.%) loadings and were subsequently characterized using XRD, BET surface area analysis, NH_3-TPD, H_2-TPR, and TGA. The dehydroaromatization of methane was conducted in a fixed bed reactor at 700 oC under atmospheric pressure.

The characterization results showed that the presence of nickel enhances methane dissociation and molybdenum carbide formation while magnesium minimized the agglomeration of nickel particles on the surface of the zeolite catalysts. The addition of magnesium also altered the acidity properties of the Mo/HZSM-5 zeolite catalysts. The catalytic activity results demonstrated an increased methane conversion and improved resistance to deactivation with Ni addition. Mg further contributed to catalyst longevity by reducing coke deposition through modifications in acidity and enhanced nickel dispersion.

Keywords: Methane Aromatization, Mo/H-ZSM-5, Nickel, Magnesium, coke