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PLENARY TALKS

Digital chemistry – A trip to the blue

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Abstract

The digital transformation of chemistry is redefining how molecules are designed, synthesized, and understood. Advances in data-driven tools, automation, and artificial intelligence are enabling a new research paradigm — one where chemical discovery is faster, more reproducible, and more accessible than ever before. This lecture will present perspectives on how digital technologies and autonomous systems are reshaping molecular science and its applications in health technologies. Examples will show how sophisticated materials, e.g., for applications in organic light-emitting diodes (OLEDs), can be designed and used in devices [3].

Stefan Bräse will take us on "A Trip to the Blue", highlighting how digital infrastructures can revolutionize the way chemists store, share, and analyse molecular data. Key initiatives include the Molecule Archive, a robust repository for the systematic capture and preservation of chemical knowledge; Chemotion, an open-source electronic lab notebook and repository platform [1]; and chemASAP [2], a self-driving lab for organic synthesis analysis. Together, these tools create an integrated ecosystem that enhances collaboration, supports reproducibility, and accelerates the chemical innovation cycle.

ChemASAP aims to provide chemical compounds that are designed to suit the diverse applications of researchers at KIT (and beyond). We want to accelerate science by straightforwardly synthesizing and analyzing molecular building blocks. ChemASAP is a modular system of functional components, each of which enables precisely tailored processes for chemical reaction control and analysis of the resulting compounds.

Keywords: Self-Driving Labs, Electronic Lab Journals, Digital Chemistry, OLEDs

Biography:

Stefan Bräse is the director of the Institute of Biological and Chemical Systems at the Karlsruhe Institute of Technology, where he is interested in automation and digital solutions. Software development and services within the group include, e.g., the Chemotion Electronic Lab Notebook (ELN) and Chemotion repository. Stefan Bräse has been a Professor in Chemistry at KIT since 2003.

Chemical and membrane engineering: the impact of process intensification and circularity principles in the net-zero CO_2 emission energy sector perspective

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Abstract

Today, most of the industrial hydrogen manufacture comes from natural gas steam reforming, responsible for massive emissions of CO_2 and further harmful compounds in the environment. The European Green Deal is promoting measures to create a future hydrogen energy infrastructure. In the transition from a carbon-based to a sustainable hydrogen economy, the European Clean Hydrogen Partnership agency is promoting research and innovative technologies on decarbonised hydrogen generation by the exploitation of renewable sources, such as biogas, which constitutes an option with respect to the natural gas utilisation. Membrane reactors may play a strategic role in the field of zero-net strategy [1], as they constitute an intensified solution presenting several benefits over the conventional processes to generate low impact carbon emissions hydrogen through biogas reforming [2].

This work deals with the recent developments on foam structured membrane reactors to generate decarbonised hydrogen with the intent of meeting the strict targets of the European Clean Hydrogen Partnership. Furthermore, a pioneeristic design and development of an electrically-driven foam structured membrane reactor will be presented, outlining the benefits of an electricity-to-heat (Joule heating) assisted membrane reactor in terms of depletion of collateral CO_2 emissions (conventionally due to the fossil fuel combustion heating), and higher energy efficiency, over other competing technologies.

Acknowledgement: The European Union – NextGeneration EU, POR H_2 project - AdP MASE/ENEA/CNR/RSE, PNRR M2C2, Inv. 3.5 "Research & Development on H_2" is particularly acknowledged to supporting this work.

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The Challenge of Developing Selective Drugs to Target the Endocannabinoid System

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Abstract

Endocannabinoids (eCBs) are the endogenous ligands to cannabinoid receptors 1 and 2 (CB_1 and CB_2), that are also target of the cannabis (C. sativa or C. indica)-derived phytocannabinoid Δ^9-tetrahydrocannabinol. The two main eCBs were identified in the 1990s as anandamide (N-arachidonoylethanolamine, AEA) and 2-arachidonoylglycerol (2-AG), an amide and an ester of arachidonic acid, respectively. Both molecules are metabolized by a complex array of biosynthetic enzymes, hydrolases and oxygenases, and are transported through the plasma membrane and intracellularly by distinct carriers. Altogether receptors, enzymes and transporters of eCBs form the "eCB system" [1].

The various components of the eCB system support and control the manifold actions of eCBs, both centrally and peripherally, thus representing remarkable targets for drug development. Yet, their number appears striking and makes the development of selective drugs very challenging.

Here, I shall discuss available tools to modulate CB_1, CB_2, and a few metabolic enzymes of eCBs, emphasizing the need of new chemical entities to target the other eCB system components in order to exploit their therapeutic potential.

Keywords: *endocannabinoids, enzymes, phytocannabinoids, receptors, therapeutic drugs, transporters*

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Biography:

Mauro Maccarrone is Dr. Enzymology and Bio-Organic Chemistry, Professor and Chair of Biochemistry at University of L'Aquila (Italy), and Head of the Laboratory of Lipid Neurochemistry at the European Center for Brain Research – IRCCS Santa Lucia Foundation, Rome. He published numerous highly cited papers (citations > 28,000; h-index = 90 according to Scopus). Invited speaker at more than 120 international congresses, Guest Editor of 16 theme-issues of scientific journals, holder of 10 granted patents. President of the International Cannabinoid Research Society (ICRS) in 2010-2011. Chair of the 2015 Gordon Research Conference on "Cannabinoid Function in the CNS". Visiting Professor at Leiden University in 2017, and University of Cambridge in 2019. Included in the Stanford University "World Top 2% Scientists' List", the ScholarGPS "Top Scholars" (top 0.5%), the AD Scientific Index "World Top 100 Biochemists", and the "Top Italian Scientists".

Digitalizing Materials Research: Insights from Designing Metal-Organic Frameworks for Advanced Optoelectronic Applications

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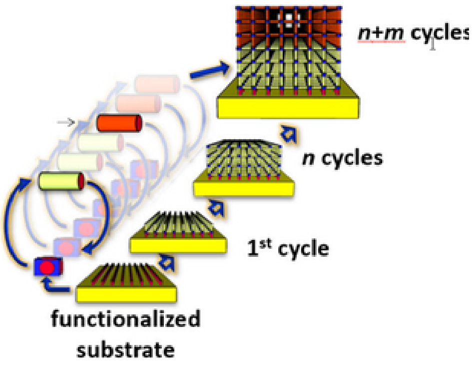
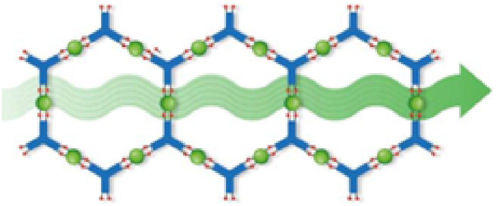
Abstract

The deliberate assembly of 'Designer Solids' from extensive libraries of prefabricated units is a compelling goal that has garnered significant interest, particularly within the domain of metal–organic frameworks (MOFs). This lecture will spotlight recent breakthroughs in MOF-based device development, encompassing electrochemical, photoelectrochemical, photovoltaic, and sensing technologies based on MOFs incorporating different types of organic linkers, such as porphyrins, phthalocyanines, naphthalene diimides, and triphenylene. Additionally, we will delve into the potential of internal interfaces in MOF heterostructures for photon upconversion and diode manufacturing.

Since the fabrication of reliable and reproducible electrical contacts to MOF-materials represent a major challenge, we have developed a layer-by-layer (lbl) deposition method to produce well-defined, highly oriented and monolithic MOF thin films on appropriately functionalized conducting substrates. The resulting films are referred to as SURMOFs [1,2] and have very appealing properties in particular with regard to optical applications.[3] The fabrication of hetero-multilayers is rather straightforward with this lbl method. In this talk, we will describe the principles of SURMOF fabrication as well as the results of systematic investigations of electrical and photophysical properties exhibited by empty MOFs. Band structure effects occurring in crystalline porphyrin arrays assembled using the SURMOF approach will also be discussed.[5] We close by presenting the first metallic MOF thin film [6], which shows clear evidence of Dirac-cone band transport from temperature-dependent measurements.

This progress—metallic conductivity being a holy grail for MOFs—was enabled by unattended experimentation, for which SURMOFs are especially suited. Robot systems guided by machine learning efficiently optimize film properties such as orientation, crystallinity, and conductivity. We will highlight this in the context of SURMOF-based sensors and metallic MOF thin films.





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Biography:

Christof Wöll Senior Professor at the Karlsruhe Institute of Technology (since 2009). He studied Physics at the University of Göttingen and received his PhD in 1987 at the Max-Planck-Institute of Dynamics and Self-Organization. After several years of postdoctoral activity at the IBM Research laboratories in San Jose, USA, and at Heidelberg University, in 1996 he took over the chair for Physical Chemistry at the University of Bochum (until 2009) and founded the collaborative research center SFB 558. He has received several awards including the Max-Planck Medal for his PhD thesis (Max-Planck Society) and the van't Hoff Prize of the German Bunsen Association. He is a member of the German National Academy of Sciences, Leopoldina and was the Spokesperson of the German Physical Society (DPG) Surface Physics Division (2016−2018). His research activities focus on fundamental processes in Surface Physics and Surface Chemistry, in particular development and advancement of techniques for the characterization of molecular adsorbates, oxide surfaces, and surface-mounted meal-organic frameworks (SURMOFs).

Intensification and Electrification of Flow Chemistry

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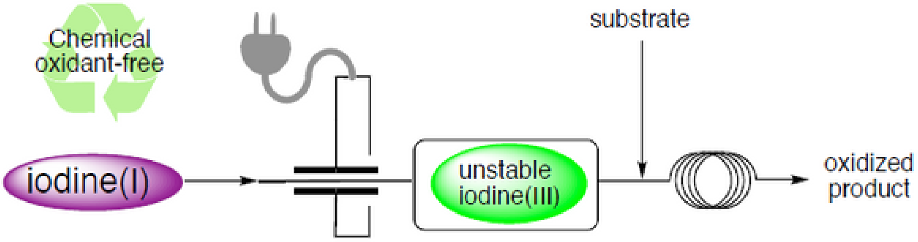
Abstract

The advantages of increased mixing of biphasic reaction mixtures in flow offers great potential compared to conventional flask techniques. The development of a microreactor for electrochemistry including several applications to modern synthesis will be discussed.[1,2]. The electrochemical generation of hypervalent iodine compounds using this technique will be highlighted.[3,4,5] Product generation in segmented flow systems is significantly faster than in traditional batch reactors, which is exemplified in high yield esterifications and in the sesquiterpene cyclase-catalysed synthesis of sesquiterpenes such as cubebol from farnesyl diphosphate as high-value natural products with applications in medicine, agriculture and thefragrance industry.[6]



Keywords: *electrochemistry, enzyme calatysis, flow synthesis, hypervalent iodine*

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Thomas Wirth is professor of organic chemistry at Cardiff University. After studying chemistry in Bonn, he obtained his PhD and at the Technical University of Berlin. After a postdoctoral stay at Kyoto University, he started his independent research at the University of Basel in 1994, before taking up his current position at Cardiff University in 2000. He was invited as a visiting professor to several places. Thomas Wirth was awarded the Werner-Prize from the New Swiss Chemical Society, the Wolfson Research Merit Award from the Royal Society and the Bader Award from the Royal Society of Chemistry (2016). In 2016 he was elected as a fellow of The Learned Society of Wales. His main interests of research concern stereoselective electrophilic reactions, oxidative transformations with hypervalent iodine reagents including mechanistic investigations and electrochemical synthesis performed in microreactors.

Multiple Ways to Inhibit tRNA-Guanine Transglycosylase: A Target to Fight Shigellosis

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Abstract

The target tRNA-guanine transglycosylase (TGT) plays an important role in the pathogenicity of Shigella, a gram-negative bacterium that is ingested with contaminated water or food and adheres to the epithelial cells of the intestinal mucosa. To gain access to these cells, the bacteria produce invasive virulence factors. The efficient biosynthesis of these invasins requires the incorporation of the modified preQ$_1$ base into the wobble position of tRNAs by TGT. First hits as active site inhibitors were discovered by de novo design. A virtual screening campaign revealed a variety of basic scaffolds for inhibitor design, among which a lin-benzoguanine scaffold served as a promising lead. Substitutions at its 2- and 4-positions led to two series of compounds. The addition of a 2-amino group provided the lead with two basic centers. Interestingly, the less basic center becomes protonated and charged in the protein due to the local polarity of the binding pocket inducing salt bridge-like interactions with two aspartate residues. However, the addition of the 2-amino group produces the more basic center, which remains uncharged but also shows an enormous increase in affinity. This surprising increase in affinity can be attributed to the formation of two parallel H-bonds that are not affected by secondary repulsive effects. Substitutions at the 4-position disrupt and partially replace a continuous water network buffering between two opposing aspartic acid residues. Remotely, the 4-substituents can access a small hydrophobic pocket. Thorough design revealed that significant potency enhancement can only be achieved by introducing a polar H-bonded linker connecting the parent lin-benzoguanine scaffold to a terminal hydrophobic group. Simultaneous attachment of 2- and 4-substituents results in sub-nanomolar inhibition. Surprisingly, the enzyme is only functional as a homodimer with an interfacial contact of more than 1600 Å^2. Several H-bonds and a cluster of aromatic amino acids were found to be critical. Since the interface is close to the catalytic center, active site inhibitors with very long spike-like substituents were able to disrupt the dimer contact and convert the dimer to a monomer. Remarkably, under the same crystallization conditions, ligands with more bulky, partially sugar-containing substituents at the 4-position serendipitously showed a new crystal form in which the monomer units packed together in such a way that the tRNA substrate could no longer be bound. This induced twisted, catalytically inactive form seemed promising for inhibition. Using ESR and ^{19}F-NMR spectroscopy, this ligand-induced dynamic rearrangement between the catalytically competent and the twisted inactive dimer form could also be detected in solution. A cysteine residue introduced into the dimer interface contact led to the formation of a new crystal form under oxidative conditions. A disulfide bridge is formed, exposing the former contact surface. In this "pseudomonomerized" enzyme, an interfacial loop assumes a geometry that no longer fits the original packing of the active homodimer. Below the loop, small fragments could be structurally characterized by crystallography and NMR, suggesting a different principle of inhibition. Finally, a transient pocket was detected near the active site, exposing a cysteine residue in the bacterial enzyme. Inhibitors that fill the transient pocket and potentially form an irreversible covalent bond to the cysteine thiol group suggest another inhibition strategy.

Catalysis for Carbon Neutrality: CO_2 and SO_2 Conversion Using Non-thermal Plasma Coupled with Heterogeneous Catalysis

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Abstract

Capture and conversion of CO_2 from industrial flue gases are important for reduction of carbon emissions and for sustainable supply of chemicals and fuels. Integrated solution for CO_2 capture from flue gases also requires prior removal of SO_2 from flue gases. This presentation will highlight the new design approach to CO_2 capture using molecular basket sorbents (MBS) that show exceptionally high capacity with superior selectivity to CO2 in flue gases, and the synergy of non-thermal plasma with dielectric barrier discharge and heterogeneous catalysis in CO_2 hydrogenation to hydrocarbons, as well as SO_2 reduction to elemental sulfur using supported metal-based catalysts related to CCU. For removal of SO_2 from flue gas, currently flue gas desulfurization (FGD) is used worldwide in scrubbers to convert SO_2 with Ca-based sorbent to form $CaSO_3$ which is then disposed as solid waste. We present a new design approach based on non-thermal plasma-enhanced catalysis for direct one-step SO_2 reduction to elemental sulfur (SO_2 to S) over transition metal sulfide catalysts. We have developed SO_2-selective solid molecular basket sorbent that is regenerable for adsorptive separation of SO_2 from gas mixture. For low-temperature SO_2 reduction to elemental sulfur in a flow reactor, coupling non-thermal plasma with supported transition metal catalysts can significantly promote low-temperature reduction of SO_2 to elemental sulfur by up to 200%, with over 98% selectivity to elemental sulfur. Recent advance in synergy of non-thermal plasma and supported metal catalysts for CO_2 hydrogenation to hydrocarbon chemicals and fuels at low temperatures will also be briefly discussed.

Biography

Chunshan SONG is the Dean of the Faculty of Science and Wei Lun Professor of Chemistry at the Chinese University of Hong Kong (Shatin, HKSAR) since July 2020 and Distinguished Professor Emeritus at the Pennsylvania State University in the US where he was Director of Energy Institute, Distinguished Professor of Fuel Science and Chemical Engineering, and the founding Director of the University Coalition for Fossil Energy Research consisting of 15 major research universities funded by the US Department of Energy. He received PhD and MS in Applied Chemistry from Osaka University, Japan, and BS in Chemical Engineering from Dalian University of Technology, China. His research focuses on the catalysis and chemistry of energy and fuels including CO_2 capture, catalytic/plasma-catalytic CO2 conversion to chemicals and fuels; adsorptive desulfurization and catalytic processing of fuels; shape-selective catalysis; synthesis and application of nano-porous materials.

He has 550 refereed journal articles (with 57,000 citations and H-index of 115 in Google Scholar, Dec 2025), 8 patents, 15 edited books, and 35 book chapters. He held Guest or Visiting or Honorary Professorship at Imperial College London, University of Paris VI (now Sorbonne), Tsinghua University, Tianjin University, Dalian University of Technology, Taiyuan University of Technology, and Chinese University of Hong Kong (Shenzhen) and also served as advisor or consultant for BP, ExxonMobil, and Saudi Aramco and advisory board member for several State Key Laboratories at Xiamen University, Institute of Coal Chemistry and Dalian University of Technology. He has received many awards such as George A. Olah Award and Henry H. Storch Award from American Chemical Society (ACS), Fulbright Distinguished Scholar from US-UK; ACS Fellow; ACS Energy & Fuels Distinguished Researcher Award; Outstanding Achievement Award from the Chinese American Chemical Society; Chang Jiang Scholar Award from Ministry of Education of China; Fellow of RSC; within Penn State, the Faculty Scholar Medal, Distinguished Professor, Faculty Mentoring Award and Wilson Award for Excellence in Research. Recently he was recognized as the 2025 Pioneer in Energy Research (PIER) by the ACS journal "Energy and Fuels" in CCUS, the 2025 Michele Aresta Prize in CO_2 Utilization Research from the 22nd International Conference on Carbon Dioxide Utilization in Lisbon, Portugal, the 2025 Carbon Capture Outstanding Achievement Award from the 4th Inter. Conference on Carbon Capture Science and Technology (CCST2025), and was elected as 2025 Fellow of Hong Kong Academy of Engineering (HKAE).

Metal Hydrides from Nano to Macro: Disruptive Science for Materials-Based Energy Storage and Conversion.

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Abstract

Metal hydrides are widely used as reducing reagents in a variety of chemical reactions. They are also useful for hydrogen storage and can be economically attractive alternatives to compressed gas and liquid hydrogen. Their thermodynamic and kinetic limitations remain vexing problems, however. Material-based hydrogen storage is a classic Goldilocks problem [1]: thermodynamic stability is a requirement for long-term storage, but a material cannot be so stable that impractically high temperatures are required for hydrogen release. This presentation will describe strategies we developed using functionalized nanoporous hosts to overcome the chemical limitations of both stable and metastable metal hydrides. These hosts include porous carbon, Covalent Organic Frameworks (COFs) [2], Metal-Organic Frameworks (MOFs) [3], and reduced graphene oxide. We also achieved the surprising result that a metal hydride within nanoporous carbon can have a higher usable capacity than bulk material [4]. These conclusions motivate additional research, driven by the need for economically viable hydrogen storage for a wide range of use cases and by the potential of hydrogen as an energy vector with gravimetric capacity exceeding that of lithium-ion batteries.

Keywords: *Metal hydride, hydrogen storage, nanocluster, metastable materials*

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Biography

Dr. Mark D. Allendorf is Honorary Senior Visiting Researcher at Washington University in St. Louis and former Senior Scientist at Sandia National Laboratories in Livermore, California. He holds a Ph.D. in inorganic chemistry from Stanford University. His research focuses on hydrogen storage, fundamental science and applications of metal-organic frameworks (MOFs), and the chemistry of geologic hydrogen formation. His research has generated over 250 publications and fourteen patents. He is also Past President and Fellow of The Electrochemical Society and has received Sandia awards for research, leadership, and teamwork, as well as a 2014 R&D100 Award for a novel approach to radiation detection.

KEYNOTE TALKS

Reaction Optimization through Mechanistic Insight and Predictive Modelling

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Abstract

The ability to control and optimize chemical reactions is central to modern synthetic chemistry, underpinning advances in efficiency, selectivity, and sustainability [1]. This study traces the progression of reaction optimization strategies, from empirical one-factor-at-a-time (OFAT) methods to statistically rigorous approaches grounded in design of experiments (DoE). Such methodologies allow systematic mapping of reaction space and the development of quantitative models that expedite process optimization and deepen mechanistic insight [2]. The convergence of experimental and computational chemistry is presented as a transformative strategy for unraveling catalytic mechanisms and rationalizing selectivity in complex reactions. Recent advances in density functional theory (DFT) and electronic-structure analysis have enabled detailed descriptions of reaction intermediates and transition states, thereby supporting predictive mechanistic frameworks [3]. Moreover, the growing integration of machine learning (ML) into synthetic and mechanistic chemistry is highlighted as a promising frontier in predictive catalysis, offering powerful tools for reaction discovery, development, and implementation [4]. By combining experimental design, theoretical modeling, and data-driven approaches, this multidisciplinary paradigm sets the stage for autonomous reaction optimization and rational catalyst design.

Keywords: *Machine learning, reaction mechanism, DFT, predictive catalysis, selectivity*

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Biography

Dr. Albert Poater (b. 1979) earned his PhD in Chemistry in 2006 at the Universitat de Girona with Profs. Miquel Duran and Miquel Solà. Apart from research in Chile with Prof. Alejandro Toro-Labbé, in Montpellier with Prof. Odile Eisenstein, he undertook a long postdoctoral stay at the University of Salerno with Prof. Luigi Cavallo. In 2010, he became an independent researcher in Girona, with visiting researcher positions at KAUST (Saudi Arabia) and at LCC-CNRS-Toulouse

(France). In 2019, he was appointed Associate Professor, and since 2020 is Head of the Chemistry Department. He has supervised 7 PhD students (10 ongoing), co-authored 365 publications, accumulating more than 17,000 citations (h-index = 70), primarily in the field of DFT applied to the mechanisms of inorganic and organometallic catalysis. He serves as an editor and board member for several scientific journals, and in 2019 was awarded the ICREA Acadèmia and in 2025 ICREA Excel·lència.

Innovations to Improve Rare Earth Elements Separations

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Abstract

Rare earth elements (REEs) are critical to many important items we use daily. REEs are difficult to separate due to their inherent chemical properties. Innovations that utilize magnetic susceptibility, chemical properties, and engineered materials can be used to enhance REEs separations in water. In addition, transport properties and carefully controlled use of time can be effectively applied in combination with magnetic forces, chemical attraction, and engineered materials to enhance separation capabilities. This presentation will discuss related principles and present results for enhanced REEs separations based on these methods.

Essential per- and polyfluoroalkyl substances (PFAS) in our future society

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Abstract

Per- and polyfluoroalkyl substances (PFAS) are man-made compounds involved in compositions of many industrial processes and consumer products. The largest volume man-made PFAS are made up by refrigerants and fluoropolymers. Major concerns for our society related to these substances are their contribution to global warming as greenhouse gasses and the potential for adverse effects on living organisms, particularly by long-chain perfluoroalkyl acid derivatives. Restrictions on manufacturing and applications will increase in the near future. Full remediation of historical and current contaminations of air, soil and water remains problematic, especially for ultra-short PFAS, such as trifluoroacetic acid. Future monitoring of PFAS-levels and their impact on ecosystems remains important. PFAS have become integrated in the lifestyle and infrastructures of our modern worldwide society and are likely to be part of that society for years to come in essential applications by closing the fluorine loop .

Keywords: *Per- and polyfluoroalkyl substances , essential uses, closing the fluorine loop*

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Biography

Dr. Rudy Dams got his PhD from the University of Antwerp in 1982 before joining 3M Company at their Technical Center in Zwijndrecht, Belgium. He spent 5 years at the corporate R&D campus of 3M USA. He is co-author of 13 scientific publications , 133 patent families and 2 book chapters and gave many lectures at international Fluorine Conferences. He retired from 3M in 2021 as Corporate Scientist and since then is active as consultant on PFAS for industrial companies and universities.

Intensified Processes for Renewable Hydrogen Production

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Abstract

Energy and environmental issues are now at the forefront of concerns; the rapid increase in the use of fossil fuels to meet growing energy needs has led to major negative environmental impacts. Energy-intensive industries such as iron and steel, refineries, power plants, cement, and petrochemicals are responsible for most anthropogenic CO_2 emissions. The global atmospheric CO_2 levels surpassed 425 ppm in 2025, a dramatic increase from 315 ppm in 1960. According to the Paris Agreement, governments around the globe prioritize urgent reductions in CO_2 emissions to minimize global warming. Sustainable strategies include the use of alternative fuels (e.g., hydrogen and renewable sources) and the application of carbon capture, utilization, and storage (CCUS) technologies. While the valorization of CO_2 via catalytic hydrogenation is a promising strategy for transforming waste into value-added compounds, its viability depends on the availability of hydrogen. Except for its use as a chemical feedstock in numerous processes (e.g., alcohols, dimethyl ether, formic acid, ammonia), hydrogen has also attracted considerable interest in many other applications, such as carbon-free energy carrier with high energy density, as a reducing agent in metallurgy, and in fuel cell applications. To circumvent the traditional use of fossil fuels, the conversion of abundant, renewable biomass, as well as its processing derivatives, becomes a promising approach to renewable hydrogen production [1-6]. On the other hand, with the implementation of environmentally friendly policies to address serious waste-related problems, much attention has been paid to the use of solid industrial waste in the development of catalysts for various reaction processes. Our presentation will highlight different strategies we have developed over the last few years to produce high-purity renewable hydrogen by integrating CO_2 capture and reforming reactions via intensified sorption-enhanced processes.

Keywords: *Renewable hydrogen production; Intensified processes; Sorption-enhanced process; CO2 capture; Waste valorization; Bifunctional materials.*

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Biography

Maria C. Iliuta is a professor in the Department of Chemical Engineering at Université Laval (Quebec, Canada). She received her PhD in Chemical engineering from Université Catholique de Louvain (Belgium) and performed postdoctoral fellowships in phase equilibria thermodynamics, separation technologies, and heterogeneous catalysis at the Technical University of Denmark (DTU) and Université Laval. Her research interests are especially directed towards process intensification, catalysis, capture and catalytic conversion of CO2, waste valorization, alternative fuels/hydrogen production, and process modeling. She co-authored more than 150 refereed publications (107 Q1 papers as corresponding author), 5 books/book chapters, and one patent as principal inventor. She was awarded 24 Best Teacher and Star Professor awards, the Summa 2021 (Université Laval), a prestigious award that recognizes professional achievements, and was recognized among the World's Top 2% Scientists based on Stanford and Elsevier Data.

Recovery of Pure H_2 and Other Valuable Gases Using Membrane Separation: A Techno-Economic Analysis

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Abstract

Hydrogen is a clean fuel, energy carrier, raw material for electricity generation by fuel cells, reactant for synthesis of ammonia, methanol, dimethyl ether etc. Depending on its application, H_2 requires different levels of purity. Membrane technology is well known to be suitable for H_2 concentration and recovery from multicomponent mixtures. Different kinds of inorganic and organic membranes can be used for this purpose. Pd and Pd-alloys allow an ultrapure H_2 stream (> 99.9999%) to be achieved [1]. On the other hand, cheaper polymer membranes are often synthesized in large-scale applications, performing concentration rather than purification due to their limited H_2/gas selectivity (especially for the H_2/CO_2 pair). Small pore zeolite structure can offer a good selectivity, even if they present problems in terms of reproducibility, defects into the layer and high cost, which limit their large-scale adoption [2].

Here, a simulated single stage CHA membrane module, treating an equimolar $H_2/CO_2/CH_4$ ternary mixture and based on the experimental binary permeances obtained in [3], is found to concentrate moderately H_2 (up to 44% at 20 bar), with a recovery close to 90%. A significant improvement in H_2 purity up to 65% is estimated in a two-stage process, which also allows CO_2 and CH_4 purification up to 92 and 95%, respectively, even if their recovery is just above 70%. A hybrid multistage membrane plant, combining zeolite membrane units with a single Pd-alloy stage, allows the simultaneous purification of all the components, as already demonstrated [4]. Based on that work, a four-stage simulated process, treating variable feed flow rates of a ternary equimolar mixture, is performed here to achieve an ultrapure H_2 stream (H_2 recovery higher than 95%) coupled with two additional streams, each containing CO_2 and CH_4 at purities of almost 98 and 96%, respectively, when retentate pressure is set at 20 bar. A techno-economic assessment on the plant shows that membrane cost is less significant than raw material (72%) and compression (18%), being about 6% of the total (installation + utilities) when feed price is set to 0.15 $/Nm^3. Assuming a plant flow rate of 50 kmol/h, the economic potential is positive when the feed gas price is below 0.35 $/Nm^3, showing that this solution can generate profit.

Keywords: *H_2 purification, membrane separation, CO_2 capture, economic assessment.*

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Biography

Pasquale Francesco Zito graduated in Chemical Engineering at the University of Calabria in 2010. After graduation, he obtained two second level university Masters in "Industrial Plants, Engineering and Technologies" and "Quality control Manager of the agri-food, biological and biotechnological supply chain" at the University of Genoa and University of Calabria, respectively. He obtained his PhD in Science and Engineering of the Environment, of Building and Energy (SIACE) at the University of Calabria in 2020. Since 2013, he started his research activity at the University of Calabria and the Institute on Membrane Technology as a fellowship and then as a research fellow. Since November 2023, he has been a researcher at the Institute on Membrane Technology. He is co-author of more than 20 scientific papers in peer-reviewed journals, 3 book chapters, various contributions in international congresses and he serves as a reviewer for several international scientific journals.

Fluorescent Biosensor-Guided Engineering of Metabolic Enzymes for Electrochemical Applications

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Abstract

A bottleneck for directed evolution of enzymes remains the activity screening step. In this study, we describe a high-throughput screening assay enabled by a fluorescent biosensor that was performed in cell lysates to identify enzyme fusions with enhanced substrate channeling. Critically, the improved enzyme fusion exhibited 29% higher current densities on electrodes with a bilayer architecture, highlighting utility in bioelectrocatalysis. Furthermore, recent advances in de novo protein design have enabled the creation of new biocatalysts with tailored activity. We demonstrate that de novo protein design can be applied to redesign multimeric enzymes into functional monomers. The simplified enzyme architecture enhanced stability and still retained substrate channeling.

Keywords: *Directed evolution, enzyme engineering, bioelectrocatalysis, fluorescent biosensor*

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Biography

Dr. Ming Chen Hammond is a Professor in the Department of Chemistry and Henry Eyring Center for Cell & Genome Science at the University of Utah. Her research group was one of the first to develop RNA-based fluorescent biosensors to study signaling and metabolism in living cells, and her research interests span the fields of chemical biology, synthetic biology, and microbiology. She received a B.S. in chemistry at Caltech, Ph.D. in chemistry as an HHMI predoctoral fellow at UC Berkeley, and was a BWF CASI postdoctoral fellow at Yale University. She is a recipient of the NIH Director's New Innovator Award and a Kavli Fellow.

INVITED TALKS

Manufacturing of metallic micro process devices and corrosion aspects - view of a material scientist considering different aspects

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Abstract

Micro process engineering allows intensification of chemical reactions by enhanced mixing of educts, effective heat transfer, save handling of hazardous chemicals and superior pressure resistance of devices due to microchannels.

Metallic materials can be microstructured e.g. by chemical etching of micromachining. However, due to small scale dimensions, corrosion resistance and fouling are critical prerequisites against failure, and the joining of devices keeps challenging.

An overview is given, underlined by practical examples and applications in different fields of micro process technology.

Keywords: *micro process device, corrosion resistance, micromachining, diffusion bonding, laser cutting*

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Development of Pentlandite-Based Electrocatalysts for Acidic Hydrogen Evolution Reaction: Composition–Structure–Activity Relationships

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Abstract

Finding efficient and stable electrocatalysts for the hydrogen evolution reaction (HER) in acidic environments remains one of the central challenges in the development of large-scale water electrolysis technologies. While platinum-group metals represent benchmark catalysts for this process, their cost and limited availability make the search for alternative materials increasingly important.

This work focuses on pentlandite-type chalcogenides as a promising class of non-precious metal catalysts for acidic HER. A set of multicomponent pentlandites with systematically varied metal composition (Co, Fe, Ni, Mn) and chalcogen content (S, Se) was investigated. Additionally, the influence of catalyst form – i.e., powdered, bulk ingots, and highly consolidated pellets – on catalytic performance was evaluated. Structural and morphological features were correlated with electrocatalytic behavior using a combination of electrochemical measurements and materials characterization techniques. To support the experimental data and gain insight into the structural aspects of the reaction mechanisms, DFT calculations focusing on hydrogen adsorption energetics and electronic structure were carried out. By combining compositional and morphological tuning with theoretical insight, the material exhibiting the highest HER activity, fast kinetics, and excellent long-term stability under acidic conditions was identified. These findings contribute to the growing interest in pentlandite-based systems as realistic, scalable alternatives to noble metal catalysts in green hydrogen production.

Keywords: *pentlandite, hydrogen evolution, metal chalcogenides, catalysis, DFT*

Acknowledgement

This work was financially supported by the National Science Centre, Poland, under grant no. 2022/45/B/ST8/03336.

Biography

Andrzej Mikuła, DSc Eng., Assistant Professor at the Faculty of Materials Science and Ceramics, AGH University of Krakow, Vice-dean for Student Affairs. Research focuses on the transport properties of metal chalcogenides, thermoelectric materials, and heterogeneous catalysis, particularly the hydrogen evolution reaction. Author of numerous peer-reviewed publications and active contributor to scientific projects related to functional materials foe energy conversion applications.

New Generation of Carbon Materials as Amendments and Adsorbents for Contaminated Water and Soil: Sucrose-based Carbon Foams

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Abstract

The use of new sustainable materials for eco-friendly applications, climate change control or health care is a combination that carries undeniable benefits for the wellness of the planet and the human kind. This could be achieved if the precursors of such materials, in particular carbon foams, are environmentally friendly and renewable, securing continuity in the future. Sucrose is identified as suitable precursors for the preparation of carbon foams. They are ultralight carbonaceous materials, consisting of a structure of interconnected macroporous cells, highly adaptable to typical adsorption applications by controlling the texture: size of macropores, incorporation of micropores, etc. In addition, they have high adsorption capacity that can favour the nanodispersion of iron species on their surface, when they are provided with microporous texture. In fact, these materials are excellent supports of metal and metal oxide nanoparticles [1,2].

This study explores the remediation of contaminated soils and adsorption of metal(loid)s in aqueous media using sucrose-derived carbon foams impregnated with iron nanoparticles. The results provide valuable insights into the practical application of carbon-based materials for environmental applications.

Keywords: *carbon foams, sucrose, metals, PAHs, remediation, adsorption*

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Biography

M. Antonia Lopez-Anton's main line of research focuses on pollution reduction from industrial processes. Currently Tenured Scientist position at Institute of Science and Technology of Carbon (INCAR), in Oviedo (Spain) belongs to CSIC (Spanish National Research Council) and Head of the Department of Sustainable Chemical Processes (h-index 35, 81 articles with IF, 7 book chapters, 1 patent).

Integrating CO_2 Capture with Electrolysis within the Electrode

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Abstract

Background. The electrochemical CO_2 reduction reaction (CO_2RR) is a promising route to mitigate CO_2 emissions because it operates under ambient conditions, can be powered by renewable electricity, and produces a range of value-added products. However, most studies use pure CO_2, whereas practical sources (flue gas/biogas) typically contain ≤40% CO_2. This mismatch undermines feasibility because upstream purification (e.g., CO_2/N_2 separation) can cost $70–100/tonne CO_2 and increase the carbon footprint. In situ purification within advanced electrodes could remove several process steps (Fig. 1a) [1,2].

Materials and methods. We developed a concept to integrate adsorption and membrane separation into gas-diffusion electrodes (GDEs) and demonstrate CO_2 conversion using an ionic-liquid-mediated CO_2-selective GDE [1]. The GDE includes a CO_2-purifying interlayer coated on a PTFE substrate (Fig. 1c). The interlayer is a polymer of intrinsic microporosity incorporating a CO_2-philic ionic liquid. CO_2RR was tested in an MEA-type cell (Fig. 1b).

Results and discussion. As shown in Fig. 1c, a uniform porous interlayer was deposited on PTFE and sputter-coated with a thin Ag layer for CO/syngas production. SEM confirms high porosity (Fig. 1d), indicating minimal resistance to gas transport, while the porous matrix acts as a local CO_2 reservoir due to high CO_2 adsorption. Preliminary CO_2RR results show maintained performance under dilute CO_2 feeds (50% or 15% CO_2 with 5% O_2, flue-gas-like). In contrast, the untreated electrode exhibited a sharp decline (from 92% to 22% in CO selectivity when switching from pure CO_2 to 15% CO_2), whereas the treated electrode retained essentially the same CO selectivity. Further improvements were achieved by reinforcing the layer with ionic liquid and by engineering the anodic conditions and membrane configuration.

Keywords: *CO2 capture-reduction integration, Electrode design, Gas-diffusion electrode*

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Biography

Dr. Hesam Rabiee is a SNSF Swiss Postdoctoral Fellow at the University of Bern, specializing in CO_2 capture and electrocatalytic conversion, and innovative electrode/electrolyzer design. He has so far published >65 papers in peer-reviewed journals.

Use of Iron-Based Materials and Engineered Persulfate Systems Toward Industrial Effluent Treatment: A Circularity Approach

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Abstract

This work presents a streamlined and circular approach to treating industrial effluents using iron-based materials and engineered persulfate systems. Our laboratory has shifted from traditional zero-valent and multi-metallic iron reductive systems toward oxidation-driven processes that pair hydrogen peroxide or persulfate with targeted activation strategies. The rationale behind this transition and its advantages over classical reductive pathways will be highlighted [1].

Examples include pesticide removal using earlier iron-based systems, rapid antibiotic degradation achieved by moving from micro- to nanoscale iron, and enhanced AOP performance through ultrasonication, which improves carbamazepine degradation and Fe(II) release in Fenton reactions. We also developed rapid oxidant-quantification tools that revealed significantly higher reaction stoichiometric efficiency in thermally and photochemically activated persulfate systems [2,3], compared with chemically activated systems such as ranitidine degradation [4].

Homogeneous UVC- and thermally activated persulfate systems effectively degraded several pharmaceutical active ingredients due to the strong selectivity of sulfate radicals [5]. More recently, iron-based MOFs such as MIL-88A were examined as sunlight-responsive persulfate activators for additional PAIs, although recyclability remains a challenge [6]. Continuous-flow AOP configurations were also developed to support future scale-up [7].

Overall, persulfate-based systems achieved high mineralization across tested contaminants. Future work in our laboratory focuses on strengthening circularity by converting winery wastes (e.g., grape-pomace–derived materials) and iron-scrap residues from car workshops into low-cost catalysts for AOP applications. These waste-derived materials aim to reduce treatment costs, enhance resource recovery, and expand the environmental and economic value of the process.

Keywords: *AOPs, Persulfate, Iron, Industrial Effluents, Remediation, Circularity*

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Biography

Dr. Antoine Ghauch is a Professor of Chemistry at the American University of Beirut (AUB) and a leading expert in advanced oxidation processes, environmental analytical chemistry, and sustainable industrial practices. He is ranked among the top 2% most-cited researchers worldwide, according to the Stanford–Elsevier global citation rankings. His research has significantly advanced the understanding of persulfate activation, reaction stoichiometric efficiency (RSE), and the degradation of pharmaceuticals, antibiotics, and pesticides in complex effluents. He has also pioneered rapid analytical methods and contributed to innovative approaches in cultural heritage conservation and surface analysis. Dr. Ghauch leads numerous national and international collaborations, including major projects with UNIDO, the IAEA, and the EU, focusing on resource efficiency, circularity, and technology transfer to industry. He is widely recognized for his creativity and innovation in anti-counterfeiting technologies as the inventor of SACOS. His current work explores converting winery wastes and iron-scrap residues into catalysts for AOPs and developing scalable systems for real-world environmental treatment.

POSTERS

Techno-Economic Evaluation of Integrated Zero Liquid Discharge systems for Seawater Desalination

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Abstract

Seawater desalination brine discharge has become a major environmental concern due to its high salinity and diverse ionic composition. Zero liquid discharge (ZLD) strategies have therefore received growing attention to valorize dissolved ions and enhance freshwater recovery. However, achieving ZLD requires additional concentration steps, where early precipitation of sparingly soluble ions such as Ca2+ and Mg2+ causes severe scaling. Softening-based selective removal of these ions prior to high-salinity concentration is thus essential [1]. Assessing the practicality of a ZLD pathway composed of desalination, softening, concentration, and crystallization further requires a comprehensive system-level evaluation. In this work, we develop an integrated process model to quantify the economic performance of the proposed strategy.

Across the three evaluated pathways that combine Reverse Osmosis, Multi-Effect Distillation, or Multi-Stage Flash desalination with Mechanical Vapor Compression-based concentration, the levelized cost of freshwater reached 0.93, 1.05, and 1.15 USD/m3. In the softening step, NaOH(aq) demand for pH swing dominated operating costs and exceeded revenue from CaCO3(s) and Mg(OH)2(s) recovery, highlighting the importance of chemical requirements in upstream ion management. In contrast, crystallization showed strong potential to offset costs through Na2SO4(s) and NaCl(s) recovery. Overall, the results indicate that reducing softening chemical consumption and leveraging salt recovery are key to economically viable ZLD implementation.

Keywords: *Seawater Desalination, Zero liquid discharge, Brine treatment, Economic analysis*

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Techno-Environmental Evaluation of Hydrogen Production in Australia under Net Zero Policy Frameworks

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Abstract

As the role of clean hydrogen becomes increasingly emphasized for achieving global carbon neutrality goals, this study conducted an integrated economic and environmental assessment of green (PV, wind), blue (SMR+CCS), and gray (SMR) hydrogen production in Australia. Based on the net zero scenario, the analysis set 2030, 2040, and 2050 as target years. In particular, this study enhanced the precision of the life cycle assessment by including the embodied carbon emissions of renewable energy generation facilities. For the economic assessment, Australian policies specifically Australian Carbon Credit Units and the Hydrogen Production Tax Incentive were applied to calculate the carbon-costed levelized cost of hydrogen. The analysis results indicated that the median LCOH in 2050 was 1.43/kgH2 for green hydrogen (PV), 2.14/kgH2 for green hydrogen (wind), 2.63/kgH2 for blue hydrogen, and 1.78/kgH2 for gray hydrogen. Regarding the C-LCOH reflecting policy effects, the cost of gray hydrogen rose to 1.97/kgH2 due to carbon costs, whereas green hydrogen (PV and wind) costs decreased to 1.42/kgH2 and 2.09/kgH2, respectively, confirming strengthened price competitiveness. This study quantitatively demonstrates the impact of Australia's hydrogen policies on the phase-out of gray hydrogen and the deployment of clean hydrogen, highlighting the importance of managing whole-life carbon emissions of renewable energy in future policy formulation.

Keywords: *Levelized Cost of Hydrogen, Life Cycle Assessment, Australian Carbon Credit Units, Hydrogen Production Tax Incentive*

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Multi-Period Optimization of Liquefied Hydrogen Supply Chain: Infrastructure Expansion and Distribution Strategy

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Abstract

As the global energy transition accelerates toward carbon neutrality, hydrogen has emerged as a key clean energy carrier due to its high energy density and zero-emission characteristics. South Korea's "2050 Carbon Neutrality Scenario" and "2030 Nationally Determined Contributions (NDC)" aim to meet approximately 80–82% of hydrogen demand through overseas imports [1]. Consequently, optimizing supply chain design and infrastructure deployment for imported liquefied hydrogen distribution is essential. This study proposes a multi-period optimization model for a long-term liquefied hydrogen supply chain spanning 25 years with three candidate import terminals: Incheon, Tongyeong, and Samcheok. The model incorporates five-year interval FCEV demand forecasts and boil-off gas (BOG) generation during unloading [2-3]. Three hydrogen conditioning states (100-bar, 200-bar compressed gas, and liquefied hydrogen) and multiple transport modes (pipelines, liquid hydrogen trucks, and compressed gas tube trailers) are optimized to minimize total annual cost and determine optimal terminal location and infrastructure expansion strategy. Optimization results indicate that the Incheon terminal is the most economically viable option due to its proximity to high-demand areas, achieving the lowest levelized cost of hydrogen (LCOH) at 2.91$/kg, followed by Samcheok (3.09/$/kg) and Tongyeong (3.19/$/kg). This framework provides quantitative evidence for national-level decision-making on hydrogen infrastructure investment priorities and phased expansion planning.

Keywords: *Liquefied hydrogen, Supply chain optimization, Multi-period planning, Terminal location, Infrastructure expansion, Hydrogen economy*

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Domain-Informed Machine Learning Modeling for Predicting CO_2 Absorption Properties of Blended Amines

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Abstract

Improving the performance of amine absorbents is essential for achieving efficient wet CO_2 capture, particularly through optimizing blended amine formulations to reduce regeneration energy. However, complex reaction mechanisms and limited experimental data make conventional thermodynamic modeling difficult. This study proposes a machine-learning-based framework for quantitatively predicting CO_2 absorption performance in blended amine systems. The model integrates two single-amine prediction modules into a domain-informed architecture that forecasts CO_2 loading as a function of blend composition. Using 616 data points from three blended amine pairs (DEA/AMP, MDEA/AMP, and AMP/PZ), the model was trained and evaluated with R^2 as the primary metric. Results indicate consistently higher accuracy compared to existing approaches, demonstrating improved prediction of vapor–liquid equilibrium without additional complex experiments. This framework provides a reliable tool for designing and optimizing next-generation high-performance CO_2 absorbents.

Keywords: *Carbon Capture Process, Machine Learning, Artificial Neural Network, Amine Absorbent, Vapor-Liquid Equilibrium*

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Hybrid-Quantum Neural Network for Enhancement of Generalization Ability in Lubricant Recipe Feature Prediction

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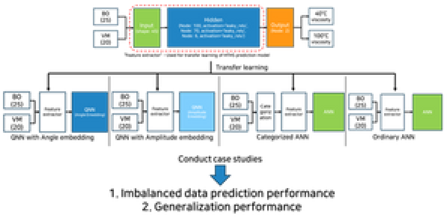
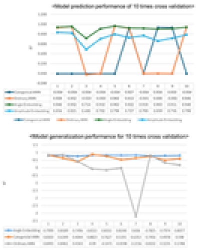
Abstract

Lubricants are critical for operation in various conditions. Since composition determines features, choice of recipe is critical. Conventionally, selection of recipes is by repetitive sample design and measurement, but it requires significant time and hardship in measuring. Since various machine learning methods used to predict features[1][2][3], they have also been used predict properties. But, due to data imbalance, performance of models and their generalization ability for unseen lubricants not satisfying. Therefore, quantum neural networks (QNN), which are known for imbalanced data treating power[4] and generalization ability[5] are used in this study. 2,182 data were used for training two deep neural networks (DNN) models and two hybrid QNN models. Then compared their prediction performance 10 times with 1,277 high temperature high shear stress (HTHS) viscosity. With Pearson correlation (R^2), stratified DNN showed 0.4572±0.4217, while angle QNN suggested 0.9673±0.0621. Then, generalization performance validated with 100 new data. With R^2, Stratified DNN showed 0.6510±0.1535 while QNN suggested 0.8082±0.0272. Therefore, we expect improvement of lubricant property prediction and appropriate recipe suggestions if suggested QNN property prediction model is applied to the process.

Keywords: *Lubricants, Machine learning, Quantum computing, Quantum neural network, Generalization performance*





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Online neutralization promotes water dissociation equilibrium forward in bipolar membranes to achieve 9.2 mol/L NaOH production

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Abstract

The bipolar membrane electrodialysis is a promising caustic soda production technique by taking advantage of the water dissociation under a reverse voltage bias. However, dissociation equilibrium is easily reached when forward water dissociation is equivalent to the back diffusion of acid and base into the salt chamber. Here, we propose manipulating the water dissociation equilibrium by introducing an online neutralization reaction for acid or base products. The results indicate that the online neutralization of the acid product could promote water dissociation forward in bipolar membranes, leading to an increase in the base yield of 27.7 % and a saving of 43.7 % in time in parallel with conventional operation. The boosting water dissociation via online acid neutralization results in the production of 9.2 mol/L NaOH, the highest recorded base concentration produced by bipolar membrane electrodialysis. The present study provides a simple and unique approach for manipulating the water dissociation equilibrium, suggesting the increasingly crucial role of bipolar membranes in base production.

Keywords: *Bipolar membrane, Electrodialysis, Water dissociation, Chlor-alkali, Clean production*

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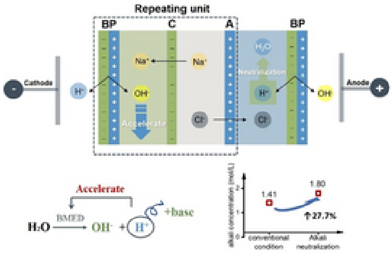

Biography

I’m Shuang Wu, a Ph.D. candidate in Chemical Engineering and Technology at the University of Science and Technology of China. My research focuses on functional membranes, particularly on acid–base production via bipolar membranes and the structural optimization and design of advanced functional membranes. I have published two research articles in the Chemical Engineering Journal and the Journal of Membrane Science.

Alkaline-resistant covalent organic framework membranes for selective hydroxide ion separation

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Abstract

Alkali holds a pivotal role in the chemical industry, however, the substantial discharge of alkaline wastewater causes a severe waste of resources and environmental pollution. Conventional polymer membranes have ether bonded backbones and form randomly assembled nanochannels, suffering from a weak alkali resistance and a low hydroxide ion selectivity. Covalent organic frameworks (COFs), known for their robust framework structure, highly ordered channels, and tunable channel chemistry, have been considered as the competent candidate for alkaline-resistant membranes for selective hydroxide ion separation. Herein, we fabricate a β-ketoenamine COF (TpTAPB) membrane with a high alkaline resistance via the interfacial growth strategy. After post-sulfonation, the negatively charged channels of sulfonated TpTAPB membrane allows OH^- with smaller size and lower charges to pass through while repulsing WO_4^{2-} ions, achieving a selectivity of OH^-/WO_4^{2-} up to ~60 and surpassing commercial and most reported polymeric membranes. This work expands the application scope of COF membranes in selective alkali separation.

Keywords: *Covalent organic framework membranes; alkali resistance; hydroxide ion selectivity; ion separation*

Biography

Yuan Xia is currently a Ph.D. candidate in the School of Chemistry and Materials Science, University of Science and Technology of China. Her research focuses on ion-selective separation membranes. She has authored a paper (Y. Xia, T. Xu*, et al., Chem. Eng. J. , 2024, 498, 155458) in a peer-reviewed journal. Her current work involves the application of covalent organic framework (COF) membranes in monovalent and multivalent ion separation.

Formation of TM_3Se_4 Multi-Metallic Selenide Thin Films via Electrophoretic Deposition

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Abstract

The hydrogen evolution reaction (HER), a key half-reaction in water splitting, enables the production of hydrogen – an eco-friendly and renewable energy carrier. However, HER is limited by sluggish reaction kinetics, requiring efficient electrocatalysts to enhance hydrogen evolution. While noble metals remain the benchmark for HER catalysis, especially under acidic conditions, their cost and scarcity hinder large-scale application. Recently, bulk multi-metallic selenides with the general formula TM_3Se_4 and a monoclinic C2/m structure have emerged as promising, cost-effective alternatives to noble metal-based catalysts. Particularly attractive is the use of such materials as thin films deposited on flexible, conductive substrates. This opens new possibilities for integrating them into modern electrolyzers – especially in compact, zero-gap configurations.

In this work, a procedure for obtaining TM_3Se_4 thin films was developed using a simple and easily scalable electrophoretic deposition (EPD) method. The synthesis route, along with the optimization of the deposition process, is presented and described in detail. The resulting coatings were structurally characterized and tested as HER catalysts using a standard three-electrode setup, allowing evaluation of their energy-conversion performance and operational stability. These findings show that TM_3Se_4 thin films not only outperform their bulk counterparts but also offer a realistic path toward more sustainable and cost-effective hydrogen production. The ability to directly coat lightweight supports with active films could help bring practical hydrogen technologies a step closer to everyday use.

Keywords: *metal chalcogenides, hydrogen evolution, thin film, catalysis*

Acknowledgement

This work was financially supported by the National Science Centre, Poland, under grant
no. 2022/45/B/ST8/03336.

Biography

Tomasz Kurek, MSc Eng., PhD student at the Faculty of Materials Science and Ceramics, AGH University of Krakow. Research focuses on transition metal chalcogenides for energy conversion applications. Currently, working on deposition procedures and optimization of thin films on various substrates for catalytic purposes. Research interests include synthesis, structural characterization, and evaluation of materials for electrocatalytic performance, particularly in hydrogen-related reactions.

Photocatalytic Degradation of 3 Ubiquitous Plastics in Batch Reactor

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Abstract

Microplastics in aquatic environments pose an increasing concern due to their persistence, ubiquity, and uncertain ecological and human health effects. TiO_2-based photocatalysis has been proposed as a potential strategy for microplastic degradation, though its effectiveness outside controlled laboratory conditions remain limited [1]. In this study, the photodegradation of low-density polyethylene (LDPE), polypropylene (PP) and polyethylene terephthalate (PET) was examined in a 1 L batch reactor containing distilled water and irradiated with a UV-C lamp. Each polymer was tested at a concentration of 300 mg/L. Experimental conditions varied in TiO_2 dosage and the addition of H_2O_2, with a total exposure time of seven days. Fourier-transform infrared spectroscopy (FTIR), optical microscopy and weight loss analysis were performed before and after treatment.

FTIR analysis revealed increases in carbonyl index for PET (44%), PP (900%) and LDPE (400%), indicating photo-oxidation across all polymers. However, neither TiO_2 nor H_2O_2 produced measurable enhancements, suggesting that degradation was dominated by direct UV-C photolysis. Slow reaction rates with photocatalytically-generated radicals—or their rapid scavenging—may account for this outcome [2, 3]. Microscopy showed minimal surface alteration, and weight-loss data were inconclusive due to measurement limitations. Challenges with slurry-phase TiO_2 recovery and reduced efficiency of immobilized catalysts further constrain applicability. Given the considerably long irradiation time and high energy demand of UV-C systems, these findings underscore the substantial resistance of common plastics and the significant hurdles they pose for water treatment technologies, particularly to highly sensitive ones like photocatalysis.

Keywords: *Photocatalysis; Titanium Dioxide; Water Treatment; Microplastics; Advanced Oxidation Processes*

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Biography

Danilo Bertagna Silva is a chemical engineer with international research experience in water treatment and environmental chemistry. In 2024 he was awarded an EU Horizon ERA individual postdoctoral fellowship for the REALIMP project at the Instituto Superior Técnico (Lisbon), focusing on the photocatalytic degradation of microplastics in water.

Material Recovery from Composite Waste in a Circular Economy Framework

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Abstract

In line with circular economy goals, this study investigates the solvolytic recycling of end-of-life composite pipe wastes reinforced with glass (GF) and carbon fibres (CF).

Composite samples underwent solvolysis at 190 °C for 180 minutes. Post-reaction, fibres were filtered, rinsed with isopropanol, dried at 105 °C, and weighed. Complete (100%) matrix removal was achieved in all tested systems. The recovered fibres retained high structural integrity, with typical lengths of 50–60 mm and maximum lengths up to 650 mm. SEM/EDS analysis confirmed the preserved morphology and elemental composition of the GF and CF bundles, with GF diameters around 20 µm and CF bundle diameters of ~8 µm.

Among the tested systems, ethylene glycol with 1% KOH emerged as the most effective and environmentally friendly. Increasing KOH concentration to 5% reduced process time to 2 hours while maintaining fibre quality.

The results demonstrate that solvolysis enables selective, efficient, and sustainable recovery of high-value fibres from composite waste, with strong potential for reintegration into circular manufacturing and material systems.

Keywords: *composite waste, solvolysis, recycling, glass fibres, carbon fibres*

Acknowledgements

This work was carried out within the HORIZON-CL4-2021-RESILIENCE-01 project European recycling and circularity in large composite components (EuReComp), under the call “A Digitized, Resource-Efficient and Resilient Industry 2021”, HORIZON Research and Innovation Actions, Contract Number 101058089.

Biography

Employee of the Faculty of Environmental Engineering and Energy (Department of Thermal Engineering) at the Silesian University of Technology. Vice-Rector for Science and International Cooperation, Head of the Renewable Energy Laboratory.

His research interests include thermal and biochemical utilization of biomass and waste in anaerobic digestion, gasification and pyrolysis processes (including solar pyrolysis), the use of composite materials and waste biomass in liquefaction, hydrothermal treatment and solvolysis processes, as well as the use of renewable energy sources and hydrogen production based on RES technologies.

Principal investigator of research projects funded from various sources. Currently leads two projects financed under Horizon Europe and the National Science Centre.Bibliometric indicators (according to Scopus): h-index 26; 133 publications; 2,542 citations. Supervisor of three completed PhD theses, including one industrial PhD. Currently supervising three doctoral projects.

Enhancement of Modelling and Testing Capabilities for Hydrogen Storage

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Abstract

The specificity of hydrogen storage research at LSPM, which recurrently secures high-level partnership conducive for project-based funding, stems from its historical core skills and resources in the field of high pressure. In terms of Technology Readiness Levels, the innovation-driven research ranges from TRL1 (predictive storage of functionalised graphene) [1,2] to TRL6 (test bench of pipe sections under real service conditions) [3,4]. On the one hand, the buffer storage of intermittent renewable energies has benefitted from the implementation of a test bench suitable for full scale-up which has been designed for testing pipe sections under monotonic or cyclic testing as required, for instance, for studying the dispatchability of a wind farm. On the other hand, solid-state hydrogen storage has benefitted from the implementation of high-pressure sorption devices up to 700 bar and of multi-scale modelling, including a revised intermolecular-hydrogen Hirschfelder model combining van der Waals's and Coulomb's forces [5] which has proved fully comprehensive and highly transferable to activity fields such as the oil sector, the exploration of natural 'white' hydrogen resources, the hydrogen geological storage as well as the carbon capture and storage [6-9].

Keywords: *hydrogen storage, renewable energy, high pressure.*

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Macromolecular Engineering Approaches Towards Advanced Polymer Mixed Ionic/Electronic Conductors For Solid-State Li-Metal Batteries

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Abstract

To enable *safer-by-design* post-Lithium-ion solid-state Lithium-metal batteries (LMBs), polymers with both high ionic conductivity and oxidative stability are sought-after as solid-state electrolytes (SSE)s 2.0 and advanced binders for high-voltage positive electrodes, respectively. Accordingly, we will present in this communication backbone**[1]** vs end-group**[2]** macromolecular engineering strategies applying to hemitelechelic polymeric host matrices for Li+ cations modified by catechol derivatives. Pristine vs. end-group modified poly(*n*-alkyl ester)s**[1]** and methoxy-PEG (mPEG) host matrices were selected to generate polymeric mixed ionic/electronic conductors (PMIECs) when mixed with LiTFSI. We will present the synthetic routes, chemical & thermal characterizations as well as electrochemical performances (sionic vs. sLi+, t+Li & ESW) of PMIECs featuring metal coordination capability and improved ionic conductivity (> 0.1 mS/cm @ 80°C) while preserving electrochemical stability windows (ESW) of their pristine counterparts.

Keywords: *Polymer Electrolyte, Lithium Metal Battery, PMIEC, Binder, Ionic Conductivity*

Acknowledgements

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