Instytut Katalizy i Fizykochemii Powierzchni
im. Jerzego Habera PAN

Polski Klub Katalizy

Komitet Chemii PAN

European Research Institute of Catalysis

LVII OGÓLNOPOLSKIE KOLOKWIUM KATALITYCZNE

LVII POLISH ANNUAL CONFERENCE ON CATALYSIS

9-11.04.2025 Kraków

Zamek Królewski na Wawelu

LVII OKK

Kraków 9-11.04.2025

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Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera PAN
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Redakcja: A. Drzewiecka-Matuszek

Druk i oprawa: Drukarnia „Attyka”, Kraków

Zdjęcie na okładce: M. Ruggiero-Mikołajczyk

ISBN 978-83-60514-40-5

Materiały wydane przez Instytut Katalizy i Fizykochemii Powierzchni im. Jerzego Habera PAN
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IKiFP PAN, Kraków 2025

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Wykłady plenarne
Plenary lectures

PL-1

Beyond photocatalysis: how light and heat team up to boost heterogeneous catalysis

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The sun is the ideal renewable energy source (albeit intermittent) to be harnessed and integrated into catalytic reactions to make them more sustainable and cost-effective. Primary aims are to accelerate reaction rates to get shorter processing times and higher yields under fixed conditions, to soften the reaction conditions without lowering the yields, to enhance reaction selectivity and catalyst stability. In less than a decade, evidence of cooperative (synergistic) effects between thermal and photonic excitations gave rise to the fastly expanding area of photothermal catalysis with applications for a wide span of reactions [1,2].

As photothermal catalysis rapidly spreads across communities with diverse backgrounds, the term *photothermal* is often used as a broad umbrella encompassing various phenomena and descriptors (e.g. photothermo-, photo-assisted/driven thermal catalysis), and no unique definition has been established to date [3-5]. The key feature of a photothermal catalyst - regardless of how it is named - is that at least one of its constituents must be light-sensitive.

The dual-mode excitation strategies differ according to the way the thermal energy is supplied to the catalyst, as in any case photons are provided by external excitation. First, both photonic and thermal energies can be provided to the catalyst through a unique source, namely the sun or simulated solar light, low-energy photons (Vis-NIR) increasing the surface temperature, while high-energy photons (UV-Vis) interact with the catalyst for driving reactions. Second, distinct photonic and thermal energy sources rely on the introduction of photons within thermal (conventional) reactors heated following conductive/convective transfer modes. Third, the catalyst itself offers optical heating, where a unique photonic energy supplier provides local heat delivery through a light-to-heat conversion mechanism (self-heating catalyst).

Following an overview of the fundamentals of photothermal catalysis and its underlying mechanisms, the presentation will highlight a series of representative examples across various reactions of interest, drawn from recent literature and studies conducted at ICPEES lab in Strasbourg. The main synergistic (cooperative) effects under dual excitation will be discussed, including the delivery of heat at both macro and nano scales through light-to-heat conversion phenomena, enabling the driving of thermally-activated catalytic reactions. Additionally, electron-driven mechanisms will be explored, where photonic excitation establishes an alternative low-energy transition state, further controlling reaction kinetics through a new dark rate-determining step.

The challenges to overcome and the key strategies to envision in order to advance further the fundamental understanding, efficiency and applicability of photothermal catalysis, will be highlighted.

References

1. N. Keller, J. Ivanez, J. Highfield, A.M. Ruppert, Appl. Catal. B Environ. 296 (2021) 120320.
2. A. Iglesias-Juez, F.Fresno, J.M. Coronado, J. Highfield, A.M. Ruppert, N. Keller, Curr. Opin. Green Sust. 37 (2022) 100652 .
3. M. Ghoussoub, M. Xia, P.N. Duchesne, D. Segal, G. Ozin, Energy Environ. Sci. 12 (2019) 1122.
4. D. Mateo, J.L. Cerrillo, S. Durini, J. Gascon, Chem. Soc. Rev. 50 (2021) 2173.
5. R. Ma, J. Sun, D.H. Li, J.J. Wei, Int. J. Hydrogen Energy 45 (2020) 30288.

PL-2

Recent Advances in the Adsorption of Nanoporous Materials

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Nanoporous materials (e.g. carbons, zeolites, metal organic framework materials, ordered and hierarchically structured meso-macroporous oxides etc.) have been the subject of extensive research targeted towards a wide range of applications because of their unique textural properties such as increased surface area and the ability to customize the pore size and pore size distribution. In addition, unique nano-confinement effects, such as for instance enhancements in the adsorption capacity, reaction kinetics, ion selectivity and gas solubility can be observed within narrow nanopores. Moreover, confinement induces shifts in the phase diagram of pore fluids and alters their thermophysical properties. Hence, in order to utilize effects of nano-confinement in the various application areas (e.g.,separation, catalysis, gas-energy storage) a detailed understanding of the interplay between effective fluid-fluid and fluid-(pore) wall interactions on the one hand and the effects of confined pore space and pore geometry/pore network on the other hand is required. For this, a detailed characterization of the surface properties and pore network architecture is required.

Within this context, we focus on fundamental aspects associated with the adsorption-, phase- and wetting behavior of fluids in nanoporous materials and will link this with recent advances in the application of advanced and novel adsorption methodologies for assessing key aspects of their pore network characteristics and surface properties.

PL-3

Challenges in developing catalysts for CO_2 methanation

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The transformation of CO_2 into valuable chemical products and fuels has been of interest for many years. Today, CO_2 is used extensively in the chemical industry, e.g. in the production of urea, food and beverage, enhanced oil recovery. However, much attention is currently being paid to the development of new processes with a view to decarbonisation of the economy. Alongside more efficient use of fossil fuels, widespread utilisation of renewable energy sources and the introduction of a circular economy, the concepts of CO_2 capture and storage (CCS) or utilisation (CCU) have found widespread interest. Waste or biogenic CO_2 in the reactions with hydrogen obtained from water electrolysis by the application of surplus renewable or nuclear energy can be converted into a range of products, such as methane (synthetic natural gas, SNG), carbon monoxide, methanol, hydrocarbons. However, in order to scale up the use of CO_2, economic, regulatory and technological barriers need to be overcome.

The CO_2 methanation reaction is highly exothermic. Therefore, the development of active and selective catalysts for thermochemical conversion processes operating at low temperatures (250-350 °C) and at the same time characterised by high resistance to coking, poisoning and sintering at high temperatures is currently a major challenge. The catalysts should also demonstrate adequate mechanical strength and have a relatively low price. Several trends in catalyst development can be observed. These are linked to concepts that explain the elementary catalytic phenomena. The expensive ruthenium catalysts have been shown to have very high catalytic activity. The use of cheaper supported nickel or cobalt catalysts, but with a higher metal content is a commercially interesting alternative. Based on the concept that elementary catalytic processes take place exclusively on the surface of metallic nanoparticles, versatile methods of catalyst synthesis have been proposed to achieve a high nanoparticle dispersion or to modify the nature of the active centres, e.g. by changing the morphology of nanoparticles, increasing reducibility or by forming bimetallic or multimetallic systems. Other approaches assume that functional groups on the surface of the support or introduced modifiers can be actively involved in elementary surface reactions, e.g. the activation and subsequent transformation of CO_2 through the participation of the relevant acid-base or redox centres and hydrogen activated at nearby active sites. Hence, numerous catalytic systems containing, for example, Ni, Co or Ru nanoparticles, which are deposited on high-surface supports, often with specific acid-base or redox properties, such as Al_2O_3, SiO_2, ZrO_2, CeO_2, other rare earth oxides, zeolites, perovskites and carbon materials were proposed in the literature. Suitable modifiers with the above properties are also introduced into the catalyst formulation, including alkali and alkaline or rare earth oxides. Another interesting trend is the use of new materials based on MOFs, grafted metal complexes, functionalised polymers and carbon materials. The development of new processes, e.g. the electrocatalytic and photocatalytic reduction of CO_2, plasma-assisted conversion, the integration of CCS and CCU units, an application of membrane and new types of reactors are creating new challenges, including the need to reformulate catalysts composition and their intrinsic properties. Further progress in this field depends on a better understanding of catalytic phenomena. This can be achieved through the wider use of modern computational and advanced experimental methods, the development of new synthesis routes of the catalysts.

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Komunikaty ustne
Oral communications

O-1

Slowing the magic bullet: imatinib in FeMOFs enhances safety and efficacy

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Historically, patients with chronic myeloid leukemia (CML) were treated with busulfan, cytarabine, hydroxyurea, interferon, or a combination of them. Unfortunately, these types of therapies had limitations such as non-specificity, low efficacy, and multiple toxicities. A huge breakthrough in the fight against leukemia was the development of small molecule tyrosine kinase inhibitors (TKI). The primary representative of TKI is imatinib mesylate (Gleevec), which has a 10-year survival rate over 83%, hence earning its designation as a magic bullet. Nonetheless, one of its most severe adverse effects is congestive heart failure. The mitigation of drug toxicity can be accomplished using drug delivery systems.

Biocompatible metal-organic framework (MOF) compounds, FeMIL-100 and FeMIL-101-NH_2, were used as potential carriers for imatinib. They effectively administered the medication as an anticancer agent while reducing cardiotoxicity. The release of imatinib from FeMIL-100 occurred rapidly in acidic environment and more slowly in pH-neutral environments, facilitating targeted delivery to cancer cells.

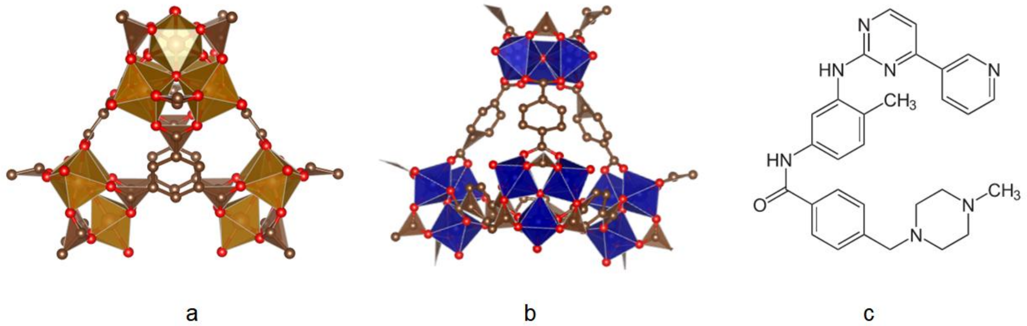

Fig. 1. Schematic structures of (a) MIL-100, (b) MIL-101, (c) imatinib.

The pH-dependent stability of the carriers controlled the drug release mechanism. Two release models: Korsmeyer-Peppas and Weibull were fitted to the experimental data and discussed in terms of drug release from rigid microporous matrix. Cytotoxicity assays were performed on two cell lines: HL60 (a model for acute myeloid leukemia) and cardiomyocytes (H9c2 cell line).

Our experimental results demonstrate that iron-based MOF carriers, specifically MIL-100 and MIL-101-NH_2, hold promise as desirable therapeutic agents.

O-2

Incorporation of zinc into the protic imidazolium-based ionic liquid: synthesis and application

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In this work, a novel acidic catalyst based on the protic ionic liquid (1-methylimidazolium triflate, [Hmim][OTf]) and zinc oxide (ZnO) was developed and evaluated for its catalytic performance. Structural analysis was conducted using various techniques including high-resolution mass spectrometry (HRMS), Fourier-transform infrared spectroscopy (FT-IR), Raman spectroscopy, nuclear magnetic resonance (NMR), and X-ray absorption spectroscopy. The results revealed an alternative structure and mechanism for the formation of the ionic liquid/ZnO adduct [Hmim][OTf] ZnO. The liquid system was synthesized with a molar ratio of [Hmim][OTf] to ZnO of 3:1 and demonstrated to be an effective acidic catalyst and solvent for the synthesis of alternative plasticizers.

Specifically, [Hmim][OTf]-ZnO catalyst (10 mol%) was utilized for the esterification of succinic acid, adipic acid, and lactic acid with two alcohols, 1-butanol and 2-ethylhexanol. Remarkably, the use of 2-ethylhexanol resulted in the complete conversion of succinic acid within 1 hour at 130 °C. The synergistic effect of the ionic liquid and ZnO was demonstrated by comparing the catalytic efficiency of the individual components when used separately. Moreover, [Hmim][OTf]-ZnO exhibited stable catalytic activity over six consecutive reaction cycles without a significant drop in efficiency.

This study underscores how structural studies can provide a basis for the rational design and development of acidic catalysts, thereby contributing to more environmentally friendly and economically feasible processes.

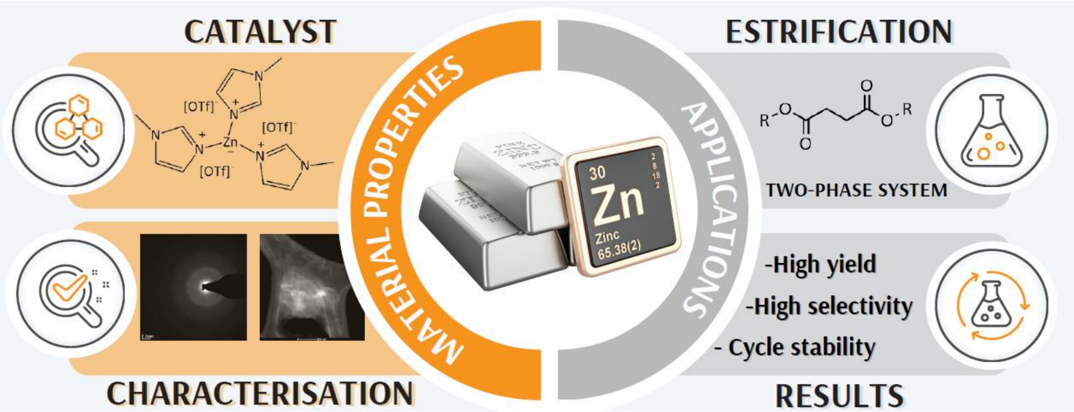

Fig. 1. Graphic illustration of the synthesis and application of incorporated of zinc into the protic imidazolium-based ionic liquid.

References

1. A.P. Abbott, G. Capper, D.L. Davies, H.L. Munro, R.K. Rasheed, V. Tambyrajah, Chem. Commun. (2001) 2010-2011.
2. J. Estager, P. Nockemann, K.R. Seddon, M. Swadźba-Kwaśny, S. Tyrrell, Inorg. Chem. 50 (2011) 5258–5271.
3. Z. Liu, S.Z. El Abedin, F. Endres, Electrochemistry Communications 58 (2015) 46–50.

Acknowledgements: This work was funded by the National Science Centre, Poland. Grant no. UMO-2022/45/B/ST8/02288..

O-3

Synthesis of fluorine-free lithium-salts for electrolytes for green and sustainable Li-based cells

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Transitioning to a carbon-neutral society introduces several challenges, particularly in the field of electrochemical energy storage. Since the 1990s, lithium-ion batteries (LIBs) have been the dominant commercial energy storage technology. However, current commercially available LIBs use fluorinated salts, solvents, and additives in their electrolytes [1]. The main risks associated with fluorinated compounds include toxicity, adverse environmental impacts, and the complexity of recycling [2,6].

In response to these challenges, our study presents the synthesis of a novel fluorine-free lithium salt and explores its application in aqueous-based LIBs with LFP as the cathode and synthetic graphite as the anode. The compatibility of this new electrolyte with commercial materials has been demonstrated, and its feasibility has been confirmed by scaling up the battery from coin cells to pouch cells. This work represents a significant step forward in the development of fluorine-free batteries, offering both technological advancements and a move towards a safer and more sustainable energy storage solution.

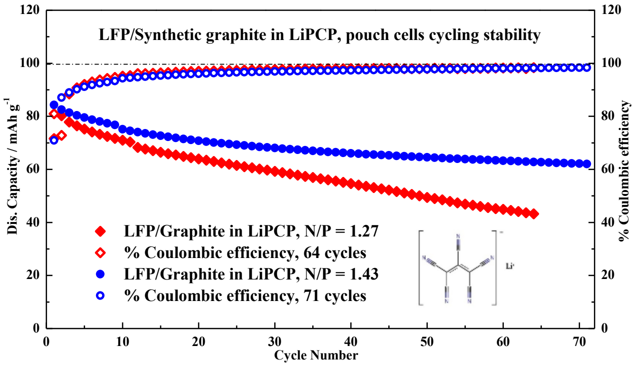

Fig. 1. Cycling stability and coulombic efficiency of LFP/synthetic graphite, pouch cell with a N/P ratio equal to 1.27 and 1.43 at 25 ℃

References

1. H. Zhang, et al., Fluorine-Free Noble Salt Anion for High-Performance All-Solid-State Lithium–Sulfur Batteries. Adv. Energy Mater., 2019. 9(25): p. 1900763.
2. H. Bae and Y. Kim, Technologies of lithium recycling from waste lithium-ion batteries: a review. Mater. Adv., 2021. 2(10): p. 3234-3250.
3. A. Rensmo, et al., Lithium-ion battery recycling: a source of per- and polyfluoroalkyl substances (PFAS) to the environment? Environ. Sci. Process. Impacts, 2023. 25(6): p. 1015-1030.

Acknowledgements: As a part of the DESTINY PhD programme, this research project is acknowledged by funding from the European Union's Horizon2020 research and innovation programme under the Marie Skłodowska-Curie Actions COFUND (Grant Agreement #945357). The financial support from the National Science Centre, Poland, grant OPUS 24 Project No. 2022/47/B/ST5/03077 is acknowledged.

O-4

Sustainable Imidazolium-Titanium Hybrid Material for Advanced Functional Applications

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In this study, we aim to advance esterification catalysts and address existing challenges by combining our expertise in catalyst design and activity analysis with the potential of tailoring the structure of ionic catalysts based on organic-inorganic hybrid material resulted in interaction of $TiCl_4$ and 1-methylimidazole.

The catalyst was synthesized by mixing $TiCl_4$ and 1-methylimidazole using various molar ratios (1:1 – 1:4). Based on Fourier-transform infrared spectroscopy (FT-IR), Raman spectroscopy, nuclear magnetic resonance (NMR), and energy dispersive X-ray fluorescence spectroscopy (EDXRF), two possibilities of the product structure were proposed.

The performance of the designed material as catalyst was investigated in the esterification of oleic acid with 2-ethylhexanol, focusing on key catalyst parameters such as activity, catalyst stability and recyclability. The versality of the catalyst was presented in the esterification of oleic, octanoic, adipic and succinic acids with 1-butanol, 2-ethylhexanol. Tailoring of the catalyst structure provided the foundation for the rational design and development of an acidic catalyst, consequently leading to a more environmentally friendly and economically feasible process.

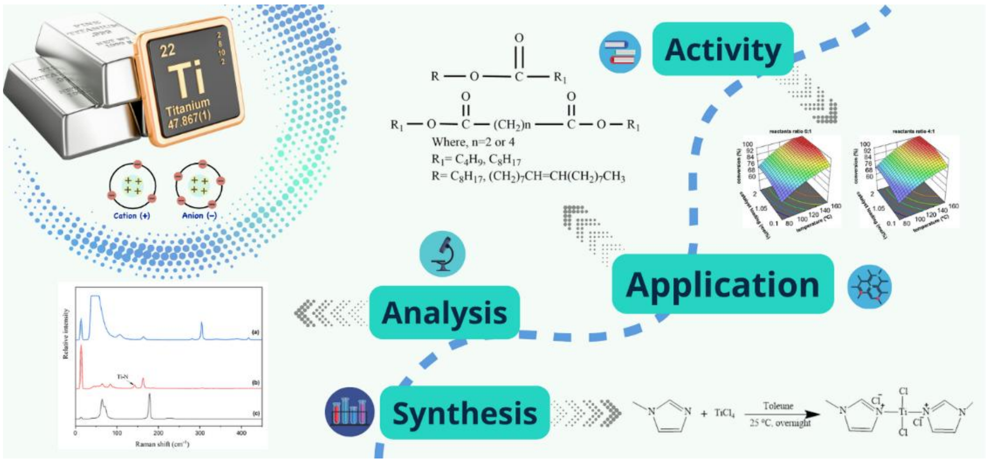

Fig. 1. Graphical illustration of synthesis, analysis and application of titanium-imidazolium catalyst

References

[1] D. Kim, Y. Moon, D. Ji, H. Kim, D. Cho, *ACS Sustain. Chem. Eng.* **2016**, *4*, 4591–4600.
[2] C. K. Lee, M. J. Ling, I. J. B. Lin, *Dalt. Trans.* **2003**, *1*, 4731–4737.
[3] P. Latos, J. Gabzdyl, S. Jurczyk, A. Chrobok, *Ind. Eng. Chem. Res.* **2024**, *63*, 8102–8110.

Acknowledgement: Project financing from National Science Centre, Poland. Grant no. UMO-2022/45/B/ST8/02288.

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O-5

Enhancing photocatalytic activity of carbon nitride with single copper atoms: insights from DFT and photoconductivity studies

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Photocatalytic reactions are driven by excited charge carriers; therefore, their performance inherently depends on photocarrier behavior [1]. Following our previous report [2], we investigate the relationship between photocarrier behavior and the photocatalytic activity of graphitic carbon nitride (g-C_3N_4) loaded with single Cu atoms. Using transient microwave conductivity, we find that the introduction of single Cu atoms enhances photoconductivity by increasing the mobility and extending the lifetimes of photoexcited electrons. This enhancement results in a greater population of mobile electrons. While pristine g-C_3N_4 exhibits no measurable photoconductivity, it is still capable of driving photocatalytic reactions. This suggests that in g-C_3N_4, photoexcited electrons are primarily trapped rather than recombined, yet they remain reactive. The product of photoconductivity and electron lifetime shows a linear correlation with photocatalytic activity, demonstrating its potential as a descriptor for catalyst design. Spatial separation between reduction and oxidation sites can be achieved within the intralayer of Cu-loaded g-C_3N_4. Each isolated Cu^+ cation is coordinated with two nitrogen atoms inside a cavity formed by three heptazine units. The Cu^+ cation acts as a hole-accumulation site, serving as an oxidation center alongside the two directly connected heptazine units.

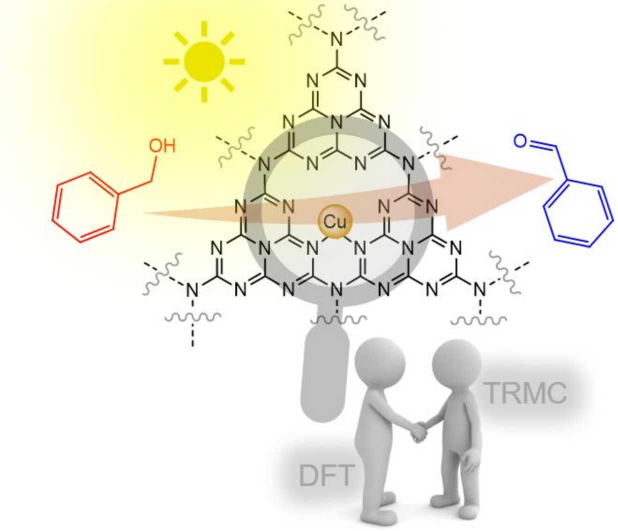

Fig. 1. Elucidating the role of single Cu atoms in enhancing carbon nitride performance.

References

1. H. Sudrajat, et al., J. Phys. Chem. C. 127 (2023) 21881
2. H. Sudrajat, et al., Nanoscale 16 (2024) 14813

Acknowledgements: This work was supported by Polish National Agency for Academic Exchange (Award No. BPN/ULM/2022/1/00009), National Science Centre (Grant No. 2020/39/B/ST5/00076), and Research Organization for Nanotechnology and Materials of BRIN (Grant No. 3/III.10.4/HK/2023).

O-6

Copper-based nanocomposite for efficient degradation of tetracycline in water: unraveling the origin of synergistic interactions between $CuWO_4$ and $Cu_3(PO_4)_2$

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Tetracycline (TC), one of the most widely used antibiotics, is frequently detected in wastewater and surface water due to its extensive medical and veterinary applications [1]. Conventional wastewater treatment methods are often ineffective in removing this pollutant, leading to its accumulation in the environment and contributing to the development of antibiotic resistance [2]. Advanced oxidation processes (AOPs), particularly Fenton-like and photo-assisted Fenton-like reactions, have emerged as one of the most promising approaches to the degradation of persistent pharmaceuticals [3]. This study explores the catalytic potential of a composite catalyst containing $Cu_3(PO_4)_2$ and $CuWO_4$ (1/1 weight ratio; CuPW-1/1) in the degradation of TC via H_2O_2-based AOPs.

A wide range of research techniques were used to characterize the synthesized materials, including XRD, XPS, FT-IR, DR UV-vis, TEM-EDS, and nitrogen physisorption. The activity of the catalysts was tested in the degradation of TC in the presence of H_2O_2 and/or UV light. The efficiency of TC degradation was followed by UV-vis spectroscopy. Pathways of antibiotic degradation were estimated based on LC-MS/MS analyses, while the efficiency of total organic carbon (TOC) removal was determined using a TOC analyzer.

Results of catalytic tests revealed that the CuPW-1/1 composite exhibited significantly higher activity in the degradation of TC via the Fenton-like process than $CuWO_4$ and $Cu_3(PO_4)_2$ used individually. In the photo-assisted Fenton-like process, CuPW-1/1 also outperformed $CuWO_4$ and $Cu_3(PO_4)_2$, achieving a much higher TC removal rate (Fig. 1). The origin of this enhanced activity will be discussed during the presentation. Radical scavenging tests and EPR measurements showed that hydroxyl radicals were the main strongly oxidizing species formed upon H_2O_2 activation, which were responsible for the efficient degradation of TC. Additionally, stability tests demonstrated that the CuPW-1/1 catalyst could be successfully reused in five consecutive cycles without significant loss of its activity.

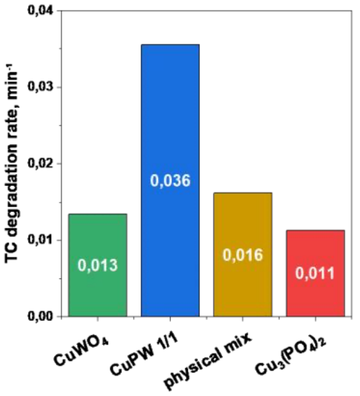

Fig. 1. Comparison of TC degradation rates in the presence of Cu-based catalysts in the photo-assisted Fenton-like process.

References

1. Carvalho, I. T, et al., Environ. Int. 2016, 94, 736–757
2. Sanganyado, E, et al., Sci. Total Environ. 2019, 669, 785–797
3. Ahmed, Y, et al., J. Environ. Chem. Eng. 2025, 13 (1), 115068

Acknowledgments: We thank the National Science Center in Poland (project no. 2023/51/D/ST5/00216) for the financial support of this work.

O-7

Work Function-Guided Design of Oxygen Evolution Electrocatalyst – Lessons from Thermocatalytic N2O Decomposition

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Guided by the work function-dependent interfacial electron transfer (IET) at the material-electrolyte interface, the design of monolithic catalysts primarily focuses on optimising catalytic performance by tuning the work function of the materials. In many studies, the relationship between the modulated work function and catalytic performance is determined using only two or three samples, which may lead to arbitrary conclusions. Employing a broad range of doping levels to modulate the work function of materials yields relatively accurate work function–catalytic performance correlation (e.g., linear or volcano plots) than that obtained from studies with only one or two doping levels. In the case of heterostructure design, the IET-mediated work function between different components facilitates the creation of active catalysts. Therefore, precise control over the work function of heterojunction components holds promise for optimising the overall performance of heterostructures by tailoring material–material IET. Researchers can develop high-performance electrocatalysts by identifying the IET-work function catalytic performance dependence [1].

Hydrogen is considered a game-changer in worldwide energy management and is starting to play a vital role in future mobile energy conversion devices. However, a kinetically limited anodic oxygen evolution reaction (OER) hinders water electrolysis for H_2 production. The solution is to use an appropriate catalyst to reduce overpotential and provide high current density for the inherently slow OER. The effective catalysts should also be synthesised from abundant and cheap reagents.

We have shown that the work function of the Bi-doped Co_3O_4 increases, leading to a weaker interaction with water molecules, which may facilitate the interaction of the active centres with the adsorbates. The substituted Bi is an active site in (OER) processes, enhancing oxygen desorption. At the same time, the activity of the neighbouring Co atoms is also substantially improved. This improvement leads to an increased intrinsic activity of Bi-doped Co_3O_4. The resulting optimised electrocatalyst achieved promising activity (350 mV@10 mA cm^{-2}) by reducing the value of the OER overpotential by 43 mV compared to the bare Co_3O_4. Incorporating Bi atoms into the Co_3O_4 lattice also improved long-term stability compared to an undoped sample in a 4-h test provided for the potential of 1.65 V vs RHE as well as a 6-h cyclic test examined by a measurement at 1.7 V vs RHE. Theoretical calculations revealed that atomically dispersed Bi dopants are more likely to replace octahedral Co^{3+} than tetrahedral Co^{2+}. An increased density of states below the Fermi level modifies the electronic structure of the Bi-doped spinel. Experimentally, Bi doping weakens the Co–O bond, improving the material's reducibility [2].

References

1. Z. Chen, T. Ma, W. Wei, W.-Y. Wong, C. Zhao, B.-J. Ni, Adv. Mater. 2024, 36, 2401568, https://doi.org/10.1002/adma.202401568
2. D. Gorylewski, F.Zasada, G. Słowik, M. Lofek, G. Grzybek, K. Tyszczuk-Rotko, A. Kotarba, P. Stelmachowski, ACS Catal. 2025, 15, XXX, 4746–4758, https://doi.org/10.1021/acscatal.4c07911

Acknowledgements: This study was financially supported by the National Science Centre, Poland, project number 2020/37/B/ST5/01876.

O-8

CuNi systems for electrocatalytic CO_2 hydrogenation

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We present a DFT and machine learning-assisted analysis of CO_2 reduction to C_2H_4 on bimetallic Cu-Ni catalysts, comparing their performance to pure Cu. Our study explores both extended surfaces and 13-atom nanoclusters with icosahedral geometry, emphasizing the role of Cu-Ni synergy in stabilizing reactive intermediates along the C_2 formation pathway. We observe that introducing Ni lowers the required reaction potential and alters the preferred reaction mechanism, despite Cu being the primary surface for intermediate interactions. In nanoclusters, the spatial distribution of Cu and Ni atoms significantly influences catalytic performance. To efficiently screen potential configurations, we developed a machine learning model trained on DFT-derived data, predicting cluster stability and interaction energies. While not providing exact energies, the model effectively identifies promising candidates for further optimization. Our findings highlight the crucial role of Ni in tuning reactivity, even when not directly interacting with intermediates, offering insights into the design of efficient bimetallic catalysts for CO_2 conversion.

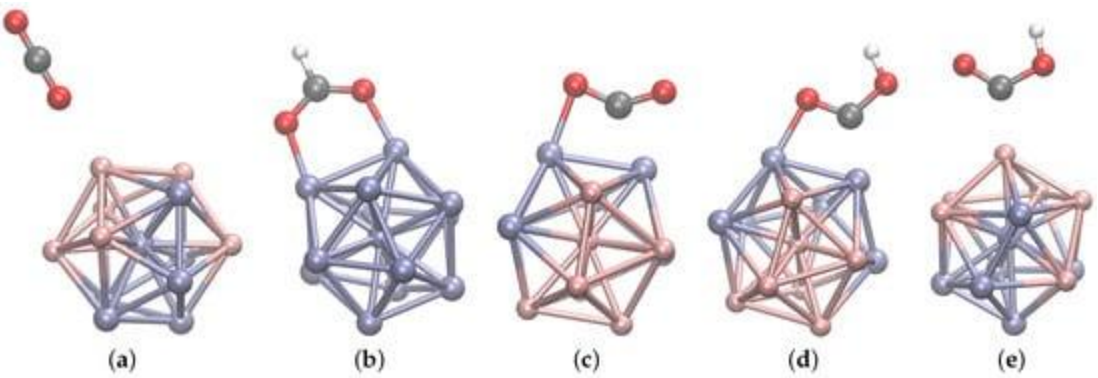

Fig. 1. Binding modes of the intermediates to the cluster: (a) MO, (b) MOCOM, (c) MOCM, (d) MOCM_H_n_bond, (e) MC. Letters indicate dominant interaction(s); M stands for metal, either Cu or Ni.

References

1. R. Stottko, E. Dziadyk-Stopyra, B.M. Szyja, Catalysts, 13 (2023) 1470.
2. E. Dziadyk-Stopyra, I. Tranca, D. Smykowski, B.M. Szyja, Materials, 16 (2023) 5138.

O-9

Operando FT-IR and UV-Vis spectroscopic studies untangle alcohol-to-hydrocarbons reaction's path

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Light olefins, which are used as substrates in a wide range of industrially important chemical reactions, can be derived from alcohols. It is well established that the conversion of methanol or ethanol over zeolites occurs through the hydrocarbon pool mechanism, leading to the formation of various olefinic, paraffinic, and aromatic compounds [1]. These transformations inevitably result in the production of "coke" species. This study provides a detailed examination of the methanol and ethanol conversion mechanisms over protonic chabazite (HSSZ-13, Si/Al = 11), using FT-IR and UV-Vis operando spectroscopic techniques alongside simultaneous mass spectrometry and gas chromatography analysis. The findings were supported by multivariate curve resolution – alternating least squares (MCR-ALS) analysis of the spectroscopic data, enabling the separation of spectra from different components and tracking their changes over time. The correlation maps (2D-COS) of the obtained spectra provided additional insights into the reaction mechanism. Post-reaction analysis of retained compounds was conducted using spectroscopic, chromatographic, and thermogravimetric methods. Methanol conversion produced a broad distribution of olefinic products, with a significant proportion of DME as the reaction time progressed. In the ethanol reaction, an excessive production of ethylene, primarily resulting from direct alcohol dehydration [2], was observed. Cyclopentenyl cations were identified as key intermediates in the formation of olefins in both methanol-to-hydrocarbons (MTH) and ethanol-to-hydrocarbons (ETH) reactions. In the MTH case, poly-alkylated benzene species played a more significant role as intermediates compared to ETH. This suggested that the hydrocarbon pool mechanism was more effectively activated during methanol conversion. The coke formed after the conversion of either alcohol consisted of similar compounds, mainly substituted benzene and naphthalene, differing in the branching of substituent groups. The sequence of events during the reactions was proposed based on MCR-ALS and 2D-COS analysis of the spectral data.

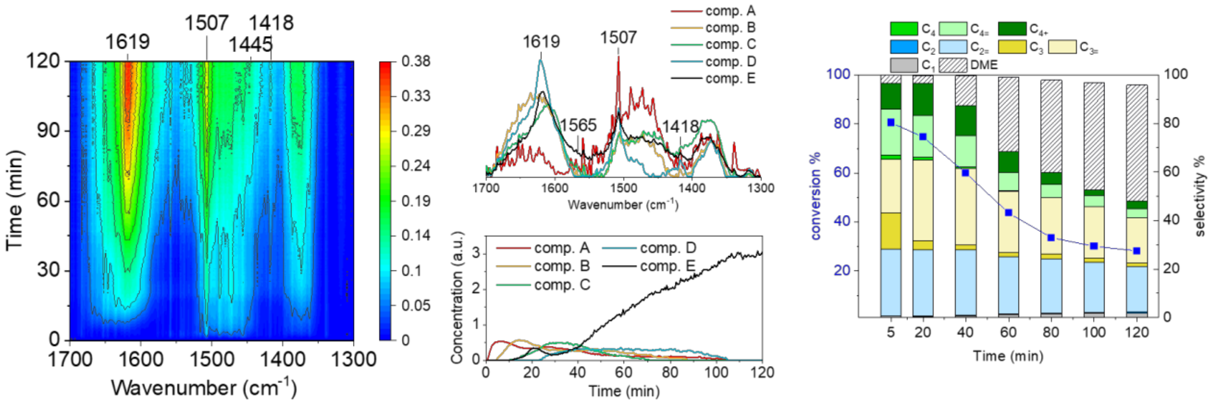

Fig. 1. Spectroscopic results (a) obtained during methanol conversion, MCR-ALS analysis of obtained IR spectra (b) and chromatographic results in the range of light olefins (c).

References

1. S. Ilias, A. Bhan, Mechanism of the Catalytic Conversion of Methanol to Hydrocarbons, ACS Catalysis, 3 (2013) 18-31
2. S. Zeng, W. Zhang, J. Li, S. Lin, S. Xu, Y. Wei, Z. Liu, Journal of Catalysis, 413 (2022) 517-526

Acknowledgements: The work was financed by Grants No 2020/37/B/ST4/01215, 2021/41/B/ST4/00048 and 2023/49/B/ST4/02340 from the National Science Centre, Poland.

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O-10

Investigating reactive intermediates in CO_2 hydrogenation catalyzed by Ni/Al_2O_3 using Modulation Excitation Spectroscopy

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The uncontrolled growth of modern civilization has led to critical CO_2 levels in the atmosphere, posing a significant threat to climate disaster. One promising solution is CO_2 hydrogenation via the Reverse Water-Gas Shift (RWGS) reaction and/or methanation (the Sabatier reaction). Despite progress, finding more efficient and cost-effective catalysts remains crucial, requiring a comprehensive investigation of key structural parameters and a detailed understanding of reactive surface intermediates [1,2].

In this study, we prepared three archetypical Ni/Al_2O_3 catalysts that showed significantly different catalytic activity and selectivity for CO_2 hydrogenation, depending on the calcination and reduction temperature. After thorough characterization (N_2 physisorption, chemisorption, XRD, XPS, SEM, TEM), we applied the combination of Modulation Excitation-Phase Sensitive Detection-Diffuse Reflectance Infrared Fourier Transform Spectroscopy (ME-PSD-DRIFTS) and Steady State Isotopic Kinetic Analysis (SSITKA) to identify key reactive intermediates and spectator species.

Our experiments revealed that even slight modifications in the pretreatment procedure significantly impact the catalytic performance in CO_2 hydrogenation. Additionally, we identified bicarbonates and formates as key reactive intermediates, which undergo various transformations based on the size and the location of the metal active phase nanoparticles (Fig. 1). The results confirmed that CO_2 hydrogenation with Ni/Al_2O_3 catalysts follows an associative and consecutive reaction pathway that is highly sensitive to structural variations [3].

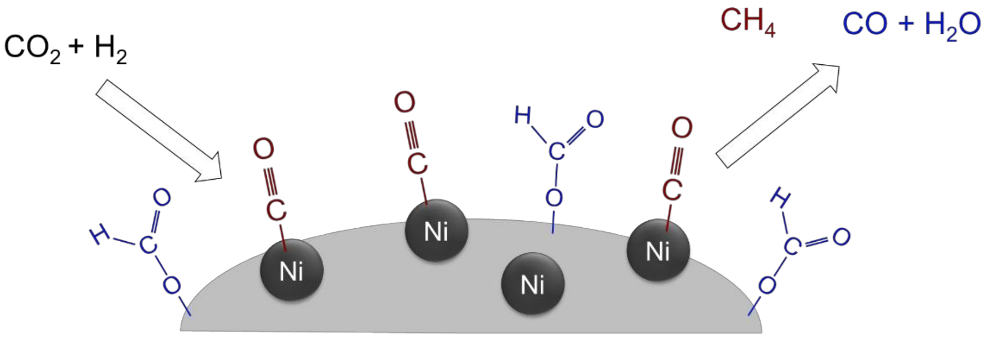

Fig. 1. Structure-sensitive CO_2 hydrogenation pathway with Ni/Al_2O_3 catalysts.

References

1. A. Saravanan et al., Chem. Eng. Sci. 236 (2021) 116515
2. D. Iltsiou, J. Mielby, S. Kegnæs, J. CO_2 Util. 69 (2023) 102396
3. M. Kock, E. Kowalewski, D. Iltsiou, S. Kegnæs, ChemCatChem 16 (2024) e202301447

Acknowledgements: This work was supported by Independent Research Fund Denmark (grant no. 6111–00237 and 0217–00146B), Villum fonden (Grant No. 13158) and Technical University of Denmark (DTU).

O-11

Wpływ dodatku neodymu na właściwości katalizatorów niklowych w reakcji uwodornienia CO_2

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W dobie dążeń do neutralności klimatycznej szczególnie istotne staje się opracowanie skutecznych metod redukcji emisji dwutlenku węgla. Jedną z obiecujących strategii jest reakcja uwodornienia odpadowego CO_2, która pozwala m.in. na otrzymanie metanu, tlenku węgla lub wyższych węglowodorów. Proces ten, zwłaszcza przy wykorzystaniu wodoru pochodzącego z odnawialnych źródeł energii, umożliwia zarówno produkcję cennych surowców chemicznych, jak i magazynowanie nadwyżek energii. Wysoką aktywnością w reakcji metanizacji CO_2 cechują się nośnikowe katalizatory niklowe. Poprawę ich właściwości katalitycznych można osiągnąć poprzez zastosowanie nowych metod syntezy, dobór nośnika lub dodatek odpowiednich modyfikatorów [1, 2].

Celem niniejszych badań było określenie wpływu niewielkich ilości neodymu wprowadzanych do katalizatorów niklowych z nośnikiem krzemianowym na ich właściwości fizykochemiczne oraz aktywność, selektywność i stabilność pracy w reakcji uwodornienia CO_2. Katalizatory otrzymano zmodyfikowaną metodą impregnacyjną. Zawierały one 10% wag. niklu oraz zmienne ilości neodymu (0.5-20% wag.). Ich właściwości fizykochemiczne badano przy zastosowaniu różnorodnych technik, m.in. temperaturowo-programowanej redukcji (TPR), transmisyjnej mikroskopii elektronowej (TEM), chemisorpcji wodoru, spektroskopii w podczerwieni (in-situ DRIFTS). Aktywność katalizatorów w reakcji metanizacji CO_2 badano w zakresie temperatur 200-600°C z wykorzystaniem mikroreaktora przepływowego. Wykonano również testy stabilności ich pracy (20 h) w temperaturach 350°C oraz 500°C.

Uzyskane wyniki wskazują na złożony wpływ neodymu na fizykochemiczne i katalityczne właściwości badanych układów. Dodatek neodymu wpływał na właściwości redukująco-utleniające katalizatorów, co wiązano ze zmianą oddziaływań pomiędzy niklem a nośnikiem oraz pomiędzy niklem a tlenkiem neodymu. Wraz ze wzrostem zawartości neodymu obserwowano spadek liczby centrów aktywnych na powierzchni nanocząstek niklu oraz zmianę ich natury. Jednocześnie wyniki badań spektroskopowych uwidoczniły, że neodym wpływał na zwiększenie adsorpcji CO_2 oraz ułatwienie przemian powstających powierzchniowych cząstek w reakcji uwodornienia. Badania katalityczne ujawniły, że zwiększenie zawartości neodymu do ok. 15% wag. prowadzi do wzrostu aktywności katalizatorów w niskich temperaturach oraz wpływa na poprawę selektywności w kierunku metanu. Badania zmian aktywności katalizatorów w czasie wykazały pozytywny wpływ dodatku neodymu na ich stabilność w wysokich temperaturach. Dalsze zwiększanie zawartości neodymu skutkowało jednak pogorszeniem ich właściwości katalitycznych.

Literatura

1. W. Gac, W. Zawadzki, M. Kuśmierz, G. Słowik, W. Grudziński, Neodymium promoted ceria and alumina supported nickel catalysts for CO_2 methanation reaction, Appl. Surf. Sci. 631 (2023) 157542.
2. K. Karpińska-Wlizło,W. Zawadzki, G. Słowik, W. Gac, Does the active surface area determine the activity of silica supported nickel catalysts in CO_2 methanation reaction? Chem. Eng. J. 502 (2024) 157827.

O-12

Tuning the shape of $SrTiO_3$ crystals: a pathway to enhancing the efficiency of photocatalytic reduction of nitroaromatic compounds

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Using photocatalysis in organic synthesis *e.g.* for selective reduction of nitroaromatic compounds has emerged as a promising alternative to traditional methods, which often generate significant amounts of waste and are not an environmentally friendly approach [1]. This type of reaction has been demonstrated to achieve high, nearly 100% selectivity in the presence of TiO_2 [2].

In this work, selective photocatalytic reduction of nitroaromatics to amines was carried out on tailored $SrTiO_3$ crystals. Investigating the role of exposed facets highlights their significant impact on the efficiency and selectivity of this type of reduction reaction. A series of uniform $SrTiO_3$ crystals with systematically varied morphologies, differing only in shape and type of exposed facets, were synthesised. Photoelectrochemical measurements and photodeposition experiments demonstrated that reduction reactions preferentially occur on the {001} facets, while oxidation predominantly takes place on the {110} facets. Furthermore, the {110} facets play a key role in enhancing charge separation, thereby significantly boosting photocatalytic activity. The changes in the efficiency of photocatalytic oxidation of terephthalic acid follow the same pattern as photocurrent generation. The reduction of nitroaromatic compounds was successfully achieved with high efficiency using tailored $SrTiO_3$. This remarkable photocatalytic performance of the modified $SrTiO_3$ crystals is attributed to the synergistic effects of enhanced charge separation and the presence of the reductive {001} facets.

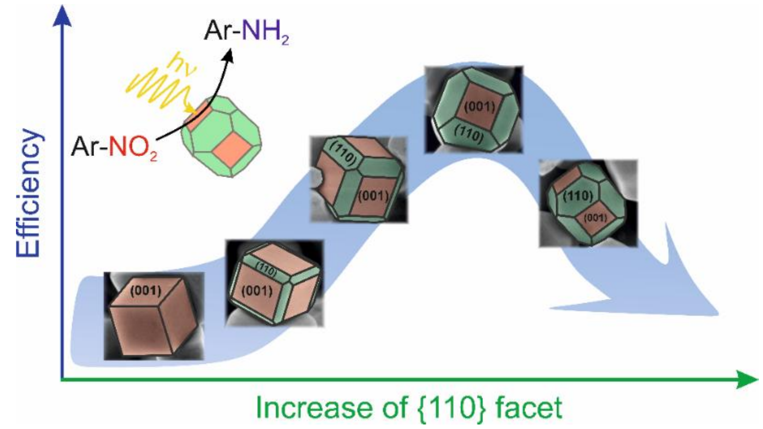

Fig. 1. Effect of tailored $SrTiO_3$ crystal on the efficiency of photocatalytic reduction of nitroaromatics.

References

1. W. Adamowicz, K. Yaemsunthorn, M. Kobielusz, W. Macyk, ChemPlusChem 89 (2024) e202400171
2. W. Adamowicz, M. Kobielusz, P. Mikrut, W. Macyk, Catal. Today 448 (2025) 115171

Acknowledgements: The authors acknowledge the support of the National Science Centre within the OPUS23 project (2022/45/B/ST5/04087) and the Faculty of Chemistry under the Strategic Programme Excellence Initiative at Jagiellonian University.

O-13

Advanced copper-containing carbon-based photocatalysts by sonication: sustainable friendly organic transformations

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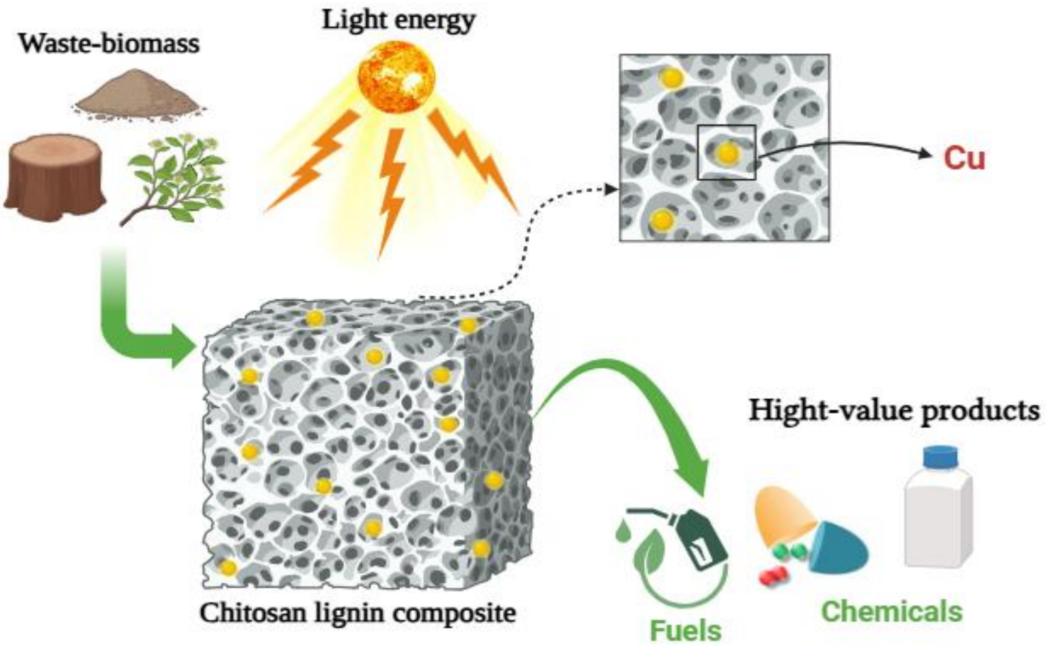

Abstract

This study optimizes an ultrasound-assisted solvo-hydrothermal method for synthesizing carbon-based materials and enhancing the selective oxidation of coniferyl alcohol (ConOH) into ferulic acid. The influence of ultrasound parameters specifically frequency 22 kHz and duration of 2 hours, was systematically investigated in relation to the yield, selectivity, and morphology of chitosan/lignin (C/L) composites. Structural and morphological analyses (XPS, FTIR, SEM) confirmed the successful synthesis and stability of the materials, while photocatalytic activity was assessed under visible light irradiation in acetonitrile. Ultrasound cavitation improved mass transfer and oxidation pathways, thereby enhancing overall efficiency. Moreover, the incorporation of copper into the C/L matrix, as verified through structural analysis, significantly boosted oxidation performance by promoting photocatalytic activity and selective reaction pathways. This study underscores the potential of advanced ultrasound-assisted techniques for synthesizing chitosan-lignin composite and highlights the synergistic effect of Cu integration through simple photo-deposition, enabling efficient biomass valorization into high-value aromatic compounds using eco-friendly conditions.

References

1. Chen, L. et al. (2009). Chinese Journal of Polymer Science.
2. Wu, H., et al. (2020). Instrumental and Experimental Techniques.
3. Oliveira, Rafael L., et al. (2022). Chemcatchem.

This study was financially supported by the National Science Centre: in Poland under the **OPUS 20** research project **No. 2020/39/B/ST5/00076.**

O-14

Deposition of Transition Metal Oxide Nanoparticles on Polypropylene for Photocatalytic Applications

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A key advantage of photocatalytic materials is their potential application in antibacterial and self-cleaning surfaces, as well as in the purification of water and air—an increasingly relevant challenge in today's world. This functionality arises from the excitation of electrons in the photocatalyst, leading to the generation of reactive oxygen species that could initiate a cascade of photocatalytic reactions [1].

Among the well-known photocatalysts are transition metal oxide nanoparticles, such as TiO_2, ZnO, and Fe_2O_3. However, for their photocatalytic properties to be effectively utilized in practical applications, these nanoparticles must be stably attached to a substrate. Polymers, widely used in various environments, including public spaces, could be promising candidates. Polypropylene is a commonly used polymer due to its stability, durability, and chemical inertness. However, these very properties cause challenges for the effective attachment of nanoparticles onto its surface.

This study focuses on the functionalization of polypropylene surfaces using low-temperature oxygen plasma, followed by nanoparticle deposition via ultrasound-assisted methods. The key objectives include evaluating the deposition efficiency, dispersion, stability, and photocatalytic activity of the attached nanoparticles. Oxygen plasma treatment introduces functional groups onto the polypropylene surface, analyzed using X-ray photoelectron spectroscopy (XPS) and water contact angle (WCA) measurements. The ultrasound-assisted deposition method enhances nanoparticle dispersion and adhesion, as observed through microscopic techniques. The photocatalytic activity of the resulting systems was measured the degradation of methyl orange and the reaction with terephthalic acid [2].

The developed method enables the effective and durable attachment of nanoparticles on polypropylene substrates, imparting photocatalytic properties to the material. Moreover, this approach is versatile and can be applied to various types of nanoparticles and substrate materials.

References

1. Tong H et al., Adv Mater. 2012, 24(2), 229-51
2. K. Zajac et al., Nanomaterials 2024, 14(16), 1372

Acknowledgements: We would like to thank the Polish Ministry of Science for financing this work within the Implementation Doctorate program 'Funkcjonalne powłoki nanokompozytowe,' project number DWD/6/0257/2022.

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O-15

Copper active sites in chabazite–type zeolites in reactions of selective catalytic reduction of NO_x with ammonia – insight into structure and reactivity using spectroscopic methods and DFT modelling

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Nitrogen oxides are one of the most environmentally dangerous groups of atmospheric compounds and generation of these substances can be attributed mostly to internal combustion engines. In diesel engines, the selective catalytic reduction of NO_x with ammonia (NH_3–SCR) is the most promising solution, with copper–exchanged small pore zeolites, mainly from the chabazite (CHA) family as the catalyst. The objective of this work was to establish the relation between structure and reactivity of copper active sites in chabazite–type zeolites. This aim has been achieved using a combination of spectroscopic (*EPR, IR, Raman, XRF, UV–VIS/NIR, NMR*), diffraction (*XRD*), microscopic (*SEM, TEM*), catalytic activity measurements in temperature–programmed and isothermic conditions, and other research techniques (*TPD, TPSR, SQUID)* in conjunction with extensive DFT molecular modelling (*VASP, ORCA*) supported by numerical simulations of thermodynamic parameters.

The initial stage of the study focused on characterising selected zeolites and identification of the various copper active sites on a molecular level – experimentally and by building a library of periodic (VASP) DFT–optimised structures. Utilisation of EPR spectroscopy, in conjunction with ORCA calculations of spin–Hamiltonian parameters, allowed for a highly accurate description of paramagnetic intrazeolite active centres (Cu^{2+}, $Cu^{2+}OH^{-}$). First principle thermodynamics (FPT) methodology was employed to construct stability phase diagrams of copper–ammonia adducts of various stoichiometry. At low temperatures (LT), copper species stay solvated by NH_3 and are unbound to the zeolite backbone. With increasing temperature, they release gas molecules and become located in specific aluminosilicate rings. Further studies revolved around interactions with nitric oxide and oxygen (oxidation half–cycle/OHC). Nitric oxide was found react with $Cu^{2+}OH^{-}$ and reduce them by generating HONO. In the presence of O_2 and NO, copper(I) species are instantly oxidised, forming nitrates considered to be the catalyst poison, however their reactivity is evidenced through synproportionation, leading to the formation of nitrites and NO_2. The FPT model, was adjusted to account for partial reactions, has predicted the experimentally observed NO_2 generation temperature windows of nitric oxide selective catalytic oxidation (NO–SCO).

Finally the complete SCR reactivity was scrutinized, and the overall NH_3–SCR over Cu–CHA samples was proposed. The reaction was found to be accompanied by several competing processes, most notably ammonia oxidation (AMO). Copper–based catalytic cycle has been separated into four primary quadrants based on the Cu oxidation state and thermodynamically most stable adducts; with ammines for Cu^{2+} and nitrates/nitrites for Cu^{+} interlaced with redox steps accompanied with nitrosamine formation/decomposition.

O-16

Gold-decorated zeolites as promising catalysts for base-free glucose oxidation

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For decades, scientists have leveraged the great potential of zeolites in catalytic applications, thanks to their advantageous properties, including high surface area, outstanding (hydro)thermal stability, unique shape selectivity, and strong acidity [1,2]. Zeolites can also serve effectively as supports for composite catalysts, such as metal catalysts.

Since the ground-breaking discoveries of Haruta and Hutchings in the mid-1980s, gold nanoparticles (Au NPs) deposited on various supports (e.g., oxides, silicas, polymers, carbons) have been widely acknowledged as effective catalysts for many oxidation reactions [3]. However, although there have been some reports on the use of zeolites as supports for gold catalysts, their number remains limited.

To date, heterogeneous gold catalysts have been recognized as promising materials for base-free catalytic oxidation of glucose. Glucose, perceived as a bio-derived platform molecule, can be converted into a wide array of valuable chemicals, such as gluconic acid, which finds widespread use in the food, cosmetics, and pharmaceutical industries [4]. Notably, to the best of our knowledge, zeolite-based gold catalysts had not been previously explored for glucose oxidation prior to our studies on this topic.

The talk will provide an overview of our research on the synthesis of zeolite-based gold catalysts, their in-depth characterization, and their use in the selective oxidation of glucose [5–7]. The presentation will cover various factors that influence the activity, selectivity, and stability of the investigated catalysts, including: (*i*) the type of zeolite structure (microporous Beta zeolite vs. hierarchical, micro-/mesoporous MCM-36); (*ii*) the method of Au NPs introduction (ion exchange, deposition-reduction, impregnation, and grafting using aminosilane); (*iii*) the addition of modifiers (e.g., Nb/Ce/B) to the zeolitic support; and (*iv*) reaction conditions and the type of oxidant employed (O_2 vs. H_2O_2).

We have established that the method used for modifying zeolite Beta with gold species significantly influenced the efficiency of metal loading, the size of Au nanoparticles, and the acidity of the support. Among the zeolite Beta-based gold catalysts, the highest catalytic performance in base-free glucose oxidation was exhibited by the sample containing the smallest Au nanoparticles, prepared via the aminosilane-assisted grafting method. Moreover, gold catalysts deposited on layered MCM-36 zeolite demonstrated higher glucose conversions compared to their zeolite Beta-based counterparts.

References

1. W. J. Roth, P. Nachtigall, R. E. Morris, et al., Chem. Rev., 114 (2014) 4807–4837
2. Z. Magyarová, M. Králik, T. Soták, Monatshefte Für Chemie – Chem. Mon., 154 (2023) 815–835
3. T. Ishida, T. Murayama, A. Taketoshi, M. Haruta, Chem. Rev., 120 (2020) 464–525.
4. X. Meng, Z. Li, D. Li, Y. Huang, J. Ma, C. Liu, X. Peng, Green Chem., 22 (2020) 2588–2597.
5. A. Walkowiak, L. Wolski, M. Ziolek, Molecules, 25 (2020) 5781.
6. J. Wolska, A. Walkowiak, I. Sobczak, L. Wolski, M. Ziolek, Catal. Today, 382 (2021) 48–60.
7. A. Walkowiak, J. Wolska, A. Wojtaszek-Gurdak, I. Sobczak, L. Wolski, M. Ziolek, Materials, 14 (2021) 5250.

Acknowledgements: A.W. extends his gratitude to the Ministry of Science and Higher Education (project “Diamentowy Grant” no. DI2018 002248) for the financial support of this work.

O-17

Tailored design of silanols on zeolitic supports for efficient metal species anchoring

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Metal nanoparticles supported on zeolites constitute a crucial class of heterogeneous catalysts, benefiting from high surface area and excellent dispersion due to their nanoscale dimensions. However, achieving stable and well-dispersed metal species remains a challenge, particularly under harsh reaction conditions.

In this study, we explore the synergy between hierarchical zeolite architectures and supported metal nanoparticles, focusing on how the design of surface silanols influences nanoparticle stabilization. A series of catalysts with varying porosity, acidity, metal type, and loading were synthesized to investigate metallic and bimetallic nanoparticles supported on hierarchical zeolites. The zeolitic supports were tailored into different architectures, including layered, pillared, and nanosponge structures [1], in both pure-silica and acidic forms.

A key strategy for stabilizing metal nanoparticles involves leveraging silanols—surface hydroxyl groups that interact with metal atoms via hydrogen bonding and electrostatic forces. These silanols serve as anchoring sites, effectively preventing nanoparticle aggregation and leaching during catalytic processes [2]. To harness this effect, we utilized silanol-rich supports, derived through controlled dealumination of commercial USY zeolite, for the immobilization of Pd nanoparticles. The dealuminated USY zeolite exhibited a significantly increased silanol density, which facilitated strong metal-support interactions and enhanced catalyst stability.

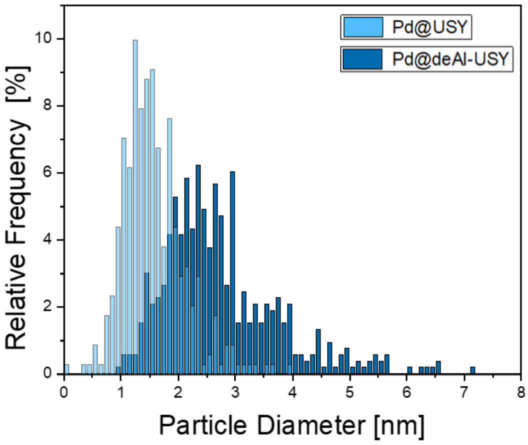

Fig. 1. Difference in the size of supported Pd nanoparticles with relation of the type of support: commercial and dealuminated USY zeolites.

Additionally, we employed a gallosilicate MFI zeolite nanosponge, synthesized hydrothermally, as an alternative support. This material features an interconnected, disordered network of MFI nanolayers [1], offering a highly accessible surface for nanoparticle immobilization. Post-synthetic degallation was applied to generate silanol nests—highly reactive hydroxyl groups that further improved nanoparticle anchoring [2].

The prepared catalysts were evaluated in hydrogenation reactions, including the selective conversion of eugenol, a model compound for lignin valorization. Our findings highlight the critical role of silanol engineering in tuning metal-support interactions, paving the way for more efficient and sustainable metal catalysts.

References

1. C. Jo et al., Chem. Commun. 50 (2014) 4175.
2. A. Li et al., Angew. Chem. Int. Ed. 62 (2023) e202213361.

Acknowledgements: We acknowledge the support of the Czech Science Foundation for the project no. 25-14521L.

O-18

Boosting oxygen evolution reaction of cobalt-carbon composites by post-synthetic plasma treatment

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Carbon-based materials are widely investigated for electrocatalytic applications; however, their weak interaction with metal oxides limits their effectiveness. To address this challenge, oxidative treatments are employed to introduce anchoring sites for the active phase.

In this study, we employed low-temperature plasma oxidation to modify graphitic ordered mesoporous carbon, which acts as a support for a cobalt-based catalyst in the oxygen evolution reaction (OER). Our results indicate that plasma pre-treatment significantly increases the concentration of carboxyl-type oxygen groups, thereby improving cobalt dispersion and catalytic activity.

Further, to evaluate the role of the carbon support, catalysts were subjected to post-synthetic oxygen plasma treatment. Post-synthetic plasma oxidation significantly enhanced their performance in OER (Fig. 1A). To understand this phenomenon, both the initial and modified catalysts were characterized using X-ray photoelectron spectroscopy (XPS), and transmission electron microscopy (TEM). XPS analysis showed that the elemental composition and Co 2p spectra remained unchanged after plasma treatment (Fig. 1B). However, TEM analysis (Fig. 1C) indicated the presence of another cobalt species, which might act as a more effective precursor for the active phase formed in situ, enhancing OER activity.

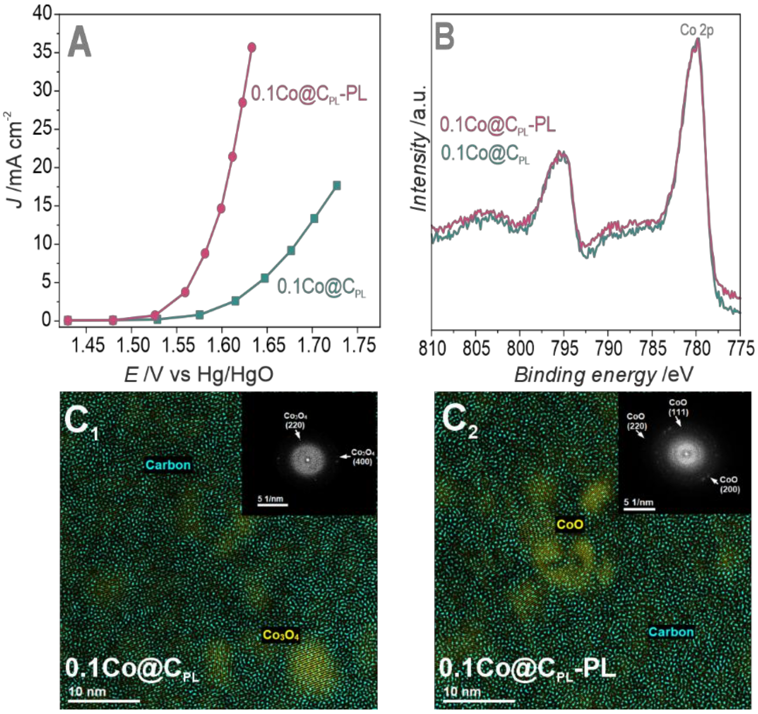

Fig. 1. Comparison of the initial and plasma-treated catalyst: (A) chronoamperometry, (B) XPS of Co 2p spectra, (C) TEM images with phase analysis.

This work demonstrates that oxygen plasma can serve not only as a tool for functionalizing carbon supports but also as an innovative approach for modifying metal oxides, significantly enhancing their activity in the oxygen evolution reaction.

Acknowledgements: This study was financially supported by the National Science Center, Poland, project number 2020/37/B/ST5/01876.

O-19

Szkła potasowe domieszkowane metalami redoksowymi jako katalizatory utleniania zanieczyszczeń powietrza

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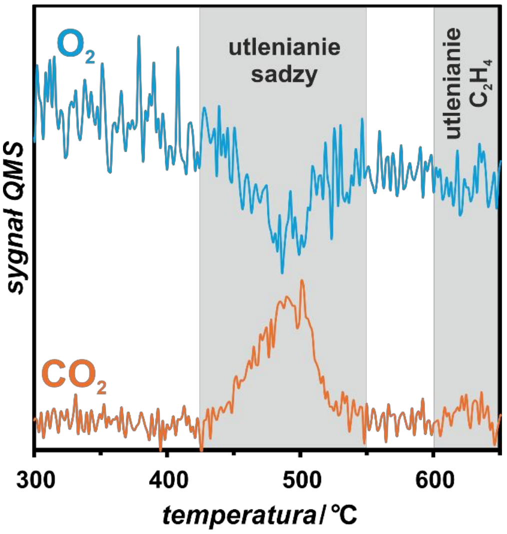
Zanieczyszczenie powietrza przyczynia się do rozwoju wielu chorób cywilizacyjnych i może być przyczyną przedwczesnych zgonów. Ma również negatywny wpływ na środowisko i może intensyfikować zmiany klimatu. Katalityczne usuwanie jest skuteczną metodą usuwania takich zanieczyszczeń jak sadza, lotne związki organiczne (LZO) czy NO_x. Układy katalityczne oparte na szkłach są ciekawą alternatywą dla często stosowanych faz metalicznych czy tlenków krystalicznych. Celem niniejszej pracy było opracowanie efektywnego katalizatora do jednoczesnego usuwania sadzy i LZO opartego na domieszkowanych metalami szkłach potasowych.

Synteza podstawowego szkła potasowego obejmowała topienie odpowiednich prekursorów (SiO_2, K_2CO_3, $CaCO_3$) w temp. 1345°C przez 1h. Szkło o składzie molowym 25%K_2O-59%SiO_2-16%CaO było następnie domieszkowane metalami (Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zr, Ce, Pb, Bi) na poziomie 5%. Domieszki wprowadzano przy tym na dwa sposoby – przez przetapianie szkła z prekursorem metalu oraz poprzez impregnację matrycy szklistej roztworem soli metalu i następczą obróbkę termiczną. Uzyskane preparaty zostały następnie scharakteryzowane wieloma metodami (XRD, RS, FTIR, NMR, UV/Vis-DR, DRIFT, TPR, XPS, XRF, SEM, SR-TAD). Aktywność katalityczna uzyskanych układów została zbadana w reakcjach dopalania sadzy (kontakty ścisły i luźny, w atmosferze 10%O_2 i 0-500ppm NO) oraz utleniania etylenu, jako modelowego LZO (3.5% C_2H_4, 10%O_2), a także jednoczesnego utleniania obu tych zanieczyszczeń.

Amorficzny charakter uzyskanych preparatów został potwierdzony przy pomocy technik analizy strukturalnej. Sposób wprowadzenia domieszek istotnie wpłynął na ich dostępność dla reagentów, specjację, stabilność i redukowalność. Wszystkie otrzymane układy wykazywały znaczną aktywność w dopalaniu sadzy, co przejawiało się wartościach konwersji $T_{50\%}$ = 430-490°C dla kontaktu luźnego i $T_{50\%}$ = 350-380°C dla kontaktu ścisłego (Rys. 1). Układy, dla których domieszki lokalizowały się na powierzchni obniżały ponadto temperaturę utleniania etylenu o 100-150°C.



Rys. 1. Temperaturowa ewolucja sygnałów QMS CO_2 i O_2 podczas jednoczesnego utleniania sadzy i C_2H_4 na szkle potasowym domieszkowanym manganem.

Podziękowania: Niniejsza praca została sfinansowana ze środków Priorytetowego Obszaru Badawczego *Anthropocene* w ramach programu *Inicjatywa Doskonałości – Uczelnia Badawcza* w Uniwersytecie Jagiellońskim.

O-20

Hierarchiczne cząstki tlenku ceru o architekturze wykazującej symetrię ikozaedryczną: wpływ hierarchii strukturalnej na utlenianie sadzy i propanu

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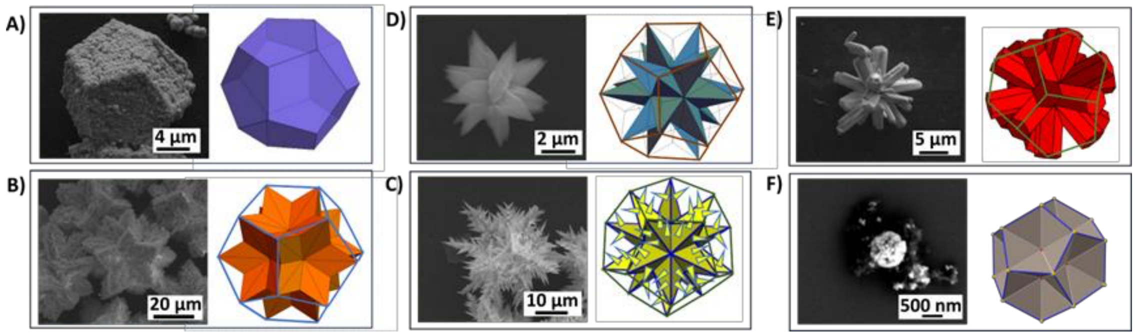
Hierarchia strukturalna jest cechą materiałów składających się z bloków budulcowych zorganizowanych w struktury wieloskalowe. Materiały takie dzięki swojej budowie (architekturze) wykazują lepsze właściwości transportowe, wyższą stabilność termiczną, większą ekspozycję miejsc aktywnych w porównaniu do materiałów nieustrukturyzowanych lub litych. Ścisła kontrola architektury katalizatorów jest zadaniem niełatwym ze względu na wzajemne powiązania zmiennych fizykochemicznych: wielkości ziaren, rozmiarów porów, morfologii jednostek budulcowych [1].

Prezentowane wyniki badań przedstawiają wpływ architektury tlenkowych katalizatorów cerowych i cerowo-gadolinowych na reaktywność układów w utlenianiu propanu i dopalaniu sadzy. Na zmienną niezależną wybrano trzeci poziom struktury hierarchicznej cząstek odnoszący się do morfologii agregatów krystalicznych. Pozostałe zmienne charakteryzujące niższe poziomy hierarchii strukturalnej poddawano kontroli celem uzyskania maksymalnego podobieństwa między testowanymi układami.

Odpowiedni dobór parametrów syntezy solwotermalnej - skład mieszaniny reakcyjnej, temperatura, czas syntezy - pozwala na otrzymanie cząstek o zadanej architekturze przejawiającej symetrię ikozaedryczną (rys. 1). Mechanizm odpowiadający za formowanie się agregatów krystalicznych o tak skomplikowanych morfologiach oparty jest o wielokrotne bliźniakowanie kryształów mrówczanu ceru zgodnie z orientacją krystalograficzną {101}. Potwierdzają to modele geometryczne skonstruowane w oparciu o zaproponowany mechanizm.

Trzeci poziom hierarchii strukturalnej odgrywa istotną rolę w katalitycznym dopalaniu sadzy. Odpowiada za to zwiększenie geometrycznego dopasowania cząstek sadzy i katalizatora. Próbka o najkorzystniejszych właściwościach geometrycznych obniża T_{50} o 143°C w porównaniu do nieustrukturyzowanych hierarchicznie nanocząstek CeO_2. Powierzchnia właściwa materiałów nie jest liniowym predyktorem aktywności katalitycznej, a istotnym modulatorem aktywności jest architektura cząstek.

Morfologia cząstek hierarchicznych nie odgrywa wiodącej roli w utlenianiu propanu, ale wprowadzenie domieszki Gd różnicuje aktywność katalityczną. Architektura cząstek może służyć jako modyfikator aktywności katalitycznej poprzez inżynierię granic ziaren hierarchicznych katalizatorów cerowo-gadolinowych.



Rys. 1. Obrazy SEM i modele geometryczne hierarchicznych cząstek CeO_2: A) dwunastościan, B) stellowany trzydziestościan rombowy, C) dwunastościan gwiaździsty wielki, D) fraktalnie rozgałęziony dwunastościan gwiaździsty wielki, E) wielościan foremny (W'=102), F) wklęsły dwunastościan.

References

1. P. Woźniak, Acta Materialia 281 (2024) 12037

Flash oral presentations

FO-1

Regioselective Hydrocyanation of Internal Alkynes: Transition-Metal-Free Approach

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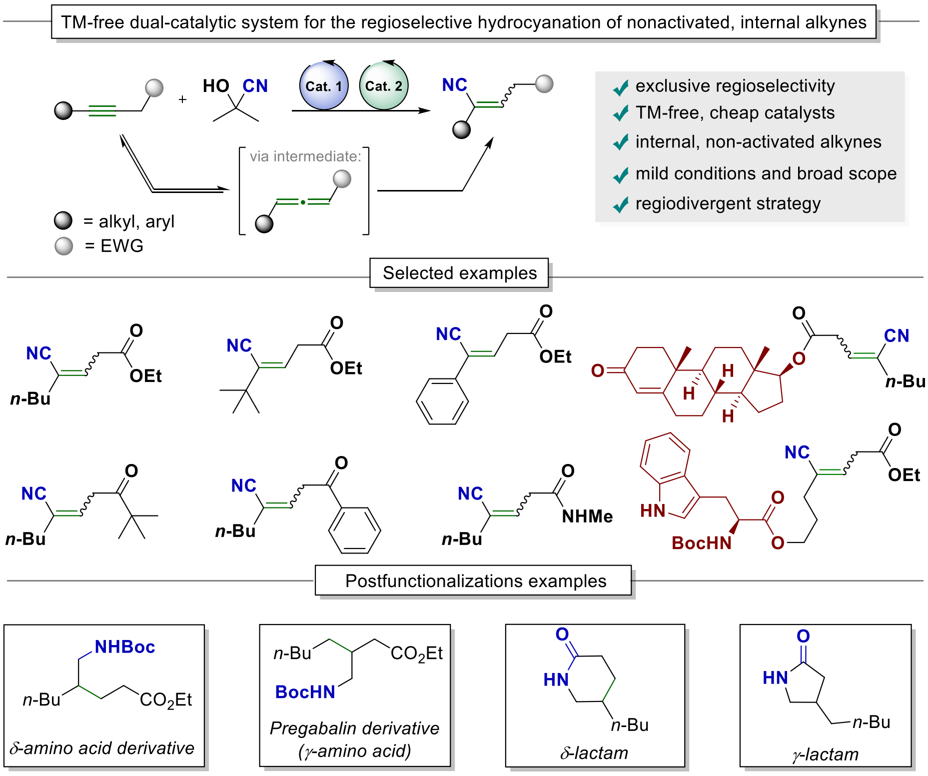
Hydrocyanation of multiple carbon–carbon bonds represents a powerful strategy for the synthesis of nitriles, compounds of high importance in pharmaceuticals, natural products, and synthetic intermediates.[1] However, this transformation suffers from a lack of selectivity control and typically relies on expensive and toxic transition metal (TM)-based catalysts.[2] To address these challenges, we have designed and implemented an exclusively regioselective hydrocyanation of unbiased alkynes, driven by base-catalyzed reversible alkyne–allene isomerization and phosphine-catalyzed HCN transfer to the allene.[3] This dual organocatalytic approach introduces an unprecedented mode of selectivity control via regioselective hydrocyanation of the allene intermediate. Moreover, by altering one catalyst in the dual-catalytic system, we demonstrated a regioselectivity switch, thereby facilitating regiodivergent hydrocyanation. Overall, our approach enables the synthesis of a broad range of vinyl nitriles (>40 examples) with yields of up to 97% and Z/E stereoselectivity exceeding 20:1, including complex natural product derivatives. A comparison with TM-based systems highlighted a 2500-fold cost reduction, along with the elimination of the troublesome separation of regioisomers. Mechanistic studies elucidated the reaction pathway, unraveling the origin of regioselectivity. In a broader context, the disclosed approach provides a foundation for developing the next generation of TM-free strategies for regioselective hydrofunctionalizations of unbiased alkynes.



References

1. (a) S. Li, *Nat. Prod. Rep.* **2024**. (b) W. Barlow, *Nat. Prod. Commun.* **2022**. (c) C. A. Montanari, *RSC Med. Chem.* **2023**.
2. K. Dong, *Org. Biomol. Chem.* **2020**.
3. A. Zasada, D. Lichosyt, *ChemRxiv*; **2025**.

Acknowledgements: This study was financially supported by the National Science Center, Poland, project number: 2020/39/D/ST4/01152.

FO-2

Mixed Nb-Mn oxides for efficient degradation of tetracycline in water via catalytic ozonation: Insight into the origin of synergistic interaction between Nb and Mn

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Ozone is a highly reactive molecule capable of quickly oxidizing organic contaminants in water, but it exhibits a relatively low efficiency in their mineralization [1]. To fully exploit its potential application for water purification, catalysts are required to convert ozone into other oxidizing species known for their stronger ability to mineralize organic substances (e.g., hydroxyl radicals, $HO^\bullet$) [2]. The present study is devoted to the development of novel Nb-Mn mixed oxides as promising heterogeneous catalysts for efficient activation of ozone and degradation/mineralization of tetracycline (TC) as a model antibiotic pollutant.

All catalysts used in this work were synthesized using the sol-gel method and characterized by means of XRD, SEM-EDS, ICP-OES, FT-IR, DR UV-vis, XPS, TEM/EDS/EELS, N_2 physisorption, and zeta potential measurements. The efficiency of TC degradation was determined on the basis of UV-vis and TOC analyses. The contribution of selected reactive oxygen species (ROS) to the degradation of TC was assessed using various ROS scavengers. The degradation pathways and products were identified based on LC-MS measurements.

The results obtained in this study revealed that all mixed Nb-Mn oxides exhibited higher activity in the degradation of TC than the pristine metal oxides (Fig. 1A). In terms of tetracycline mineralization, no significant increase in TOC removal was reported for Nb_2O_5 (Fig. 1B). On the contrary, the ozonation processes carried out in the presence of MnO_2 enabled ca. 2.5 times higher TOC removal than that established for ozone itself (Fig. 1B). Interestingly, the highest TOC removal efficiency was observed for $Mn_{0.2}Nb_{0.8}O_x$ which contained the lowest Mn loading from among all materials prepared in this study. This observation led us to conclude that the manganese species in $Mn_{0.2}Nb_{0.8}O_x$ must exhibit more desirable properties for efficient activation of ozone and degradation of TC than the manganese species in bulk MnO_2. More details on the origin of the improved activity of mixed Nb-Mn oxides and the nature of synergistic interactions between Nb and Mn species in the degradation of TC via catalytic ozonation will be provided during the presentation.

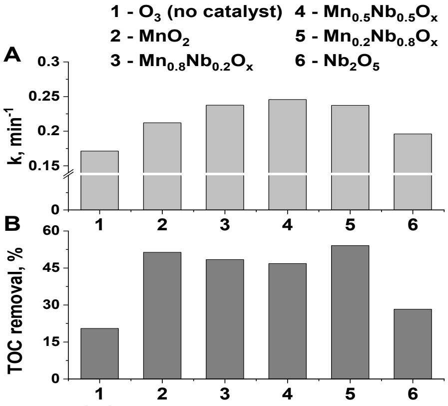

Fig. 1. (A) Reaction rate established for the degradation of TC in the presence of catalysts used in this study. (B) The efficiency of TC mineralization after 2 h of the ozonation process.

References

1. L. Fu, et al., Chemosphere 233 (2019) 34
2. I. J. De La Cruz, et al., J. Environ. Chem. Eng. 11 (2023) 110753

Acknowledgements: We thank the National Science Center, Poland (NCN), grant Sonata (no. 2023/51/D/ST5/00216), for financial support of this work.

FO-3

Studies on Alkali Thermal Desorption of Oxide Catalysts

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Alkali metal additives are widely used in heterogeneous catalysis, playing a crucial role in processes such as ammonia synthesis, ethylbenzene dehydrogenation, soot combustion and N_2O decomposition [1]. They are also essential in the steam reforming of ethanol - a process in which ethanol reacts with steam at high temperatures, leading to the production of hydrogen [2]. The presence of alkali metals on the catalyst surface significantly enhances the efficiency of ethanol steam reforming by increasing ethanol conversion, improving selectivity towards hydrogen, and enhancing catalyst stability, allowing it to maintain high activity over an extended period. However, at the high temperatures required for this process, alkali metals become mobile - they undergo segregation and may desorb from the catalyst surface, gradually deteriorating its properties [3].

Understanding the dynamics of alkali on the catalyst is a key area of research. A unique experimental setup for thermal alkali desorption measurements, developed at Jagiellonian University, provides insight into this phenomenon. The SR-TAD (*Species Resolved Thermal Alkali Desorption*) system enables the detection of desorbing streams of atoms, ions, and Rydberg atoms/clusters, as well as the determination of desorption activation energy. Measurements are conducted under high vacuum conditions, reaching 10^{-8} mbar. The apparatus is equipped with a reactor where samples can be reduced and transferred without exposure to air.

The desorption of alkali from oxide materials such as Co_3O_4, α-Al_2O_3, CeO_2, and Co/CeO_2 was studied. The influence of the type of alkali promoter and the concentration (0.5, 1, and 2wt.%) was examined, including double-alkali doped systems. The study results indicate that the desorption begins at approximately 450°C for all materials, and its progression strongly depends on the type of support material used. The activation energies of potassium desorption from Co_3O_4, α-Al_2O_3, and CeO_2 oxides, for both the heating and cooling stages, are presented in Figure 1. The values range from 1.3 to 2.3 eV, reflecting differences in the strength of potassium interactions with the studied supports.

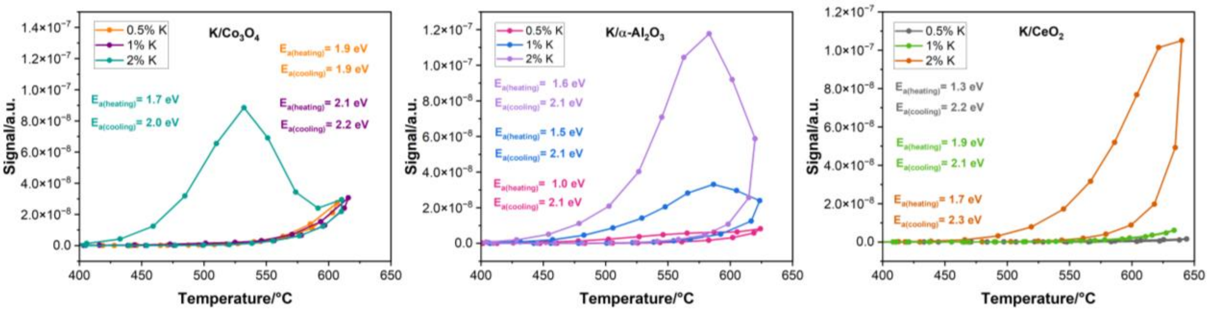

Fig. 1. Signal of potassium desorption from Co_3O_4, α-Al_2O_3, and CeO_2 oxides.

References

1. G. Grzybek et. al., App. Cat. A., 2021, 614, 118051.
2. G. Grzybek, et. al., Int. J. Hydrogen Energy 2020, 45, 22658-22673.
3. L. Holmlid, P. Govind Menon, App. Cat. A. 2001, 212, 247-255.

Acknowledgements: We thank National Science Centre, Poland for funding this research (grant no. 2021/43/D/ST4/03016).

FO-4

The decomposition of industrial organic pollutants via wet peroxidation, and the activity of composite copper catalysts in this process

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In view of escalating water contamination by industrial organic compounds, including pesticides, dyes, and antibiotics, advanced oxidation processes (AOPs) have emerged as a compelling solution. These processes rely on the generation of reactive oxygen species, such as highly reactive hydroxyl radicals ($^{\bullet}OH$) and singlet oxygen ($^1O_2$). The Fenton reaction is one such mechanism that generates these species. However, it is limited in its practical applications due to several factors. To overcome these limitations, numerous modifications of the Fenton reaction have been proposed, including replacing of iron ions with other transition metal ions, which allows optimization of the reaction under different conditions. Other modifications include the development of heterogeneous Fenton catalysts, which allow the reaction to be carried out in a more controlled manner and with a lower risk of unwanted side effects. In addition, heterogeneous catalysts are solid materials, so they can be easily separated from solution after the reaction is complete, which is important for industrial-scale applications. Another method of generating reactive oxygen species is the electroprotic mechanism, in which, in contrast to redox catalysts, there is no electron transfer between the catalyst surface and the solution, and it is only possible within the solution.

A catalyst capable of combining these two mechanisms would be a promising system for use in advanced oxidation processes and could play an important role in the context of environmental protection. Therefore, the main motivation of the conducted research was to obtain such a copper-based catalyst capable of generating reactive oxygen species for the degradation of pollutants found in wastewater (dyes, phenol and its derivatives, pharmaceuticals and pesticides), using hydrogen peroxide as a precursor of the reactive oxygen species. For this purpose, a series of copper-based catalysts for H_2O_2 decomposition were synthesised. The synthesis was carried out using solvothermal and precipitation methods. A number of techniques were used for physicochemical characterization of the obtained materials, including methods for identifying structures and determining elemental composition (XRD, SEM, EDX, XPS), detecting the generated reactive oxygen species (EPR spectroscopy) and investigating the activity in the decomposition of a model water pollutant, such as Direct Blue 15 dye (UV-Vis spectrophotometry).

The obtained results indicate that catalysts comprising two distinct metals with redox properties exhibit the highest activity in the dye degradation process. It was shown that the concurrent presence of copper in multiple oxidation states has a substantial effect on the activity of the active phase. Moreover, the incorporation of a minimal amount of the redox active phase into the support material significantly increases its catalytic efficiency.

Acknowledgements: We thank National Science Centre (NCN), Poland, grant Opus 27 2024/53/B/ST4/03929 for financial support of this work.

FO-5

Katalizatory heterogeniczne na bazie tlenków alkalicznych i tlenków metali ziem rzadkich przeznaczone do transestryfikacji olejów roślinnych w celu produkcji biodiesla

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Transestryfikacja, będąca kluczowym procesem wytwarzania biopaliw, polega na reakcji trójglicerydów z alkoholem, najczęściej metanolem, co prowadzi do powstania estrów metylowych kwasów tłuszczowych (biodiesla) oraz glicerolu jako produktu ubocznego. Głównym aspektem badań było zastosowanie katalizatorów wykazujących zjawisko superzasadowości, które może znacząco poprawić efektywność reakcji oraz stabilność procesu. Wykorzystanie katalizatorów heterogenicznych, w przeciwieństwie do tradycyjnych homogenicznych katalizatorów takich jak NaOH czy KOH, jest korzystne ze względu na łatwiejszą separację produktów oraz minimalizację powstawania odpadów. [1]

Celem badań było określenie wpływu superzasadowości katalizatorów heterogenicznych opartych na tlenkach alkalicznych oraz tlenkach metali ziem rzadkich na produkty procesu transestryfikacji oraz opracowanie wydajnych i stabilnych katalizatorów o wysokiej aktywności, które mogłyby znaleźć zastosowanie w przemyśle biopaliwowym. Hipoteza badawcza zakładała, że katalizatory wykazujące superzasadowość, w zależności od ich składu chemicznego i struktury, będą miały istotny wpływ na konwersję surowców oraz właściwości końcowego produktu, w tym liczbę cetanową, która determinuje jakość paliwa. [2]

W ramach badań zastosowano katalizatory oparte na tlenkach metali, takich jak tlenek wapnia (CaO), tlenek glinu (Al_2O_3) oraz tlenek lantanu (La_2O_3).[3] Przeprowadzono szczegółowe analizy strukturalne i powierzchniowe, obejmujące pomiar superzasadowości metodą desorpcji programowanej temperaturowo (TPD-CO_2), co umożliwiło identyfikację miejsc aktywnych o wysokiej zasadowości, analizę krystalograficzną (XRD) w celu określenia faz krystalicznych katalizatorów oraz chromatografię HPLC do oceny konwersji olejów roślinnych i tłuszczów odpadowych w procesie transestryfikacji.

Badania różnych proporcji katalizatorów wykazały, że ich skład chemiczny wpływa na aktywność. Najwyższą efektywność osiągnięto dla katalizatorów z lantanem i glinem, zapewniających wysoką konwersję i dobrą jakość biodiesla. Nie wszystkie struktury superzasadowe były katalitycznie aktywne, co udowodniono na przykładzie katalizatora CaO/Al_2O_3.

Na podstawie wyników określono optymalne proporcje katalizatora, maksymalizujące konwersję i stabilność procesu. Zasadowość katalizatora okazała się kluczowa dla jego aktywności, a uzyskane wyniki mogą wspierać rozwój ekologicznych i efektywnych technologii biopaliw.

References

1. Meher, L.C.; Vidya Sagar, D.; Naik, S.N. Technical Aspects of Biodiesel Production by Transesterification—A Review. Renew.
2. Lee, H.V.; Juan, J.C.; Taufiq-Yap, Y.H. Preparation and Application of Binary Acid–Base CaO–La2O3 Catalyst for Biodiesel Production. Renew. Energy 2015, 74, 124–132.
3. Park, J.-Y.; Oh, S.-G.; Paik, U.; Moon, S.-K. Preparation of Aluminum Oxide Particles Using Ammonium Acetate as Precipitating Agent. Mater. Lett. 2002, 56, 429–434.

FO-6

Pd on bacterial nanocellulose as a catalyst for cinnamaldehyde hydrogenation

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The bacterial nanocellulose (BNC) was synthesized through the cultivation of the *Komagataeibacter medellinensis* strain in a Hestrin Schramm medium under static conditions. The palladium nanoparticles were supported on BNC using an easy-to-handle method. BNC was cut and impregnated by Pd(II) acetate in acetone (40°C), followed by the reduction of Pd ions using $NaBH_4$ in methanol. The 2%Pd/BNC catalyst (Fig.1f) was washed (acetone, water) and dried in air (22°C). The liquid-phase hydrogenation of cinnamaldehyde (0.03–0.06M CAL, 6 bars H_2, 50°C, batch reactor) in isopropanol or toluene solvent over 2wt%Pd/BNC catalyst was performed (Fig.1c). The liquid products were analyzed by GC-FID chromatography.

The 2%Pd/BNC was highly active in CAL hydrogenation, reaching 100% conversion (Fig.1a) and high HCAL selectivity (91–96%) towards C=C bond saturation. HCOL product with selectivity <10% and traces of COL (<0.5%) were also detected. HCAL/HCOL selectivities were almost independent of the solvent used (Fig.1b). There was a high recyclability (Fig.1d,e), with similar initial activity and a slight increase in selectivity towards HCOL formation. The results proved the great performance of BNC as a catalytic support.

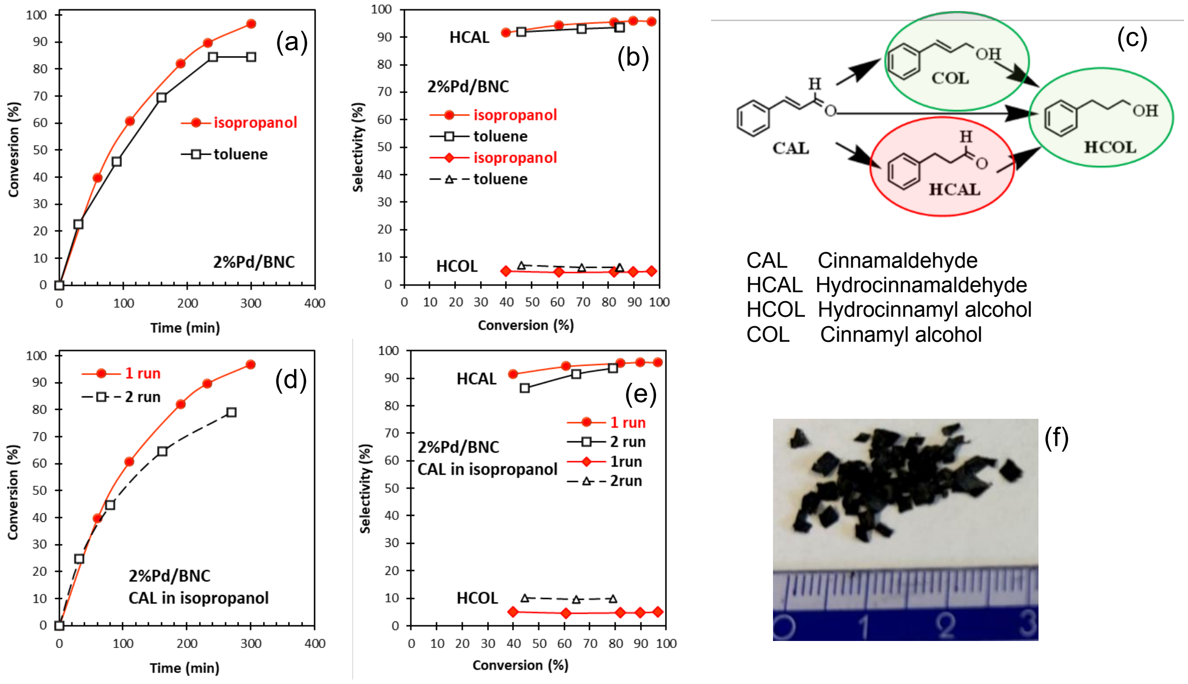

Fig. 1. The conversion (a) and selectivities (b) in CAL hydrogenation over 2%Pd/BNC catalyst (f) in isopropanol or toluene; CAL hydrogenation reactions (c); 2%Pd/BNC recycling in isopropanol (d, e).

Acknowledgements: The research was supported by the statutory research found of Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences and by Ministry of Science, Technological Development and Innovations of the Republic of Serbia, Grant No 451-03-136/2025-3/200042.

FO-7

Ultrasonic preparation of CuPd-HKUST-1 as catalysts for cyclohexene oxidation

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In the undertaken research, we developed the ultrasonic-assisted synthesis of monometallic Cu-HKUST-1 and bimetallic CuPd-HKUST-1 metal-organic framework catalysts with a specified ratio of Cu/Pd ions in the MOF structure, replacing the conventional solvothermal synthesis method. The prepared systems were tested as active catalysts for cyclohexene oxidation, producing surfactants, polymers, agrochemicals, and drugs. All prepared catalysts underwent profound physicochemical characterization mainly by low-temperature nitrogen adsorption, transmission electron microscopy, thermogravimetric analysis, Fourier-transform infrared and µRaman spectroscopies. Furthermore, the Density-Functional Theory modelling was performed.

The spectroscopic characterization of prepared materials employing Raman spectroscopy supported by DFT indicated higher stability of the systems with homonuclear dimers than those with isostoichiometric heteronuclear dimers. Based on the in situ FTIR spectroscopic analyses, the great impact of copper divalent and palladium monovalent ions on the catalytic activity and selectivity of prepared samples was evidenced. The catalysts prepared in the presence of ultrasound were characterized by easier accessibility to Cu^{2+} species, favoring the formation of 2-cyclohexenone. In turn, in the case of the bimetallic catalysts, containing both copper and palladium in the MOF structure, it was indicated the profound impact of the monovalent cation species (Pd^{+} or Cu^{+}) on the growth of the cyclohexene conversion (reaching 96%) and higher selectivity to 2-cyclohexenol (43%) than 2-cyclohexenone (30%).

Based on the microscopic studies, it was concluded that in all prepared samples, metal ions building the MOF structure were uniformly dispersed within the MOF structure. Furthermore, the application of orthophosphoric acid during the sonochemical synthesis of the bimetallic sample resulted in the production of composite material containing palladium nanoparticles.

Acknowledgements: The research was financed with computational grant no. PLG/2024/017158, the Polish State Ministry of Education and Science subvention for AGH University of Krakow under project 16.16.160.557, the Czech Science Foundation through the ExPro project (19-27551X) and from the OP VVV "Excellent Research Teams", project no. CZ.02.1.01/0.0/0.0/15_003/0000417 – CUCAM.

FO-8

Catalytic Properties of Co-MOF derived carbonaceous materials in Chemoselective Hydrogenation Reactions

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A significant aspect of catalytic hydrogenation is its capacity for selective reduction of unsaturated aldehydes to saturated aldehydes or unsaturated alcohols. These compounds are pivotal intermediates in the synthesis of fragrances, flavors, and pharmaceuticals [1].

The present study investigated the continuous-flow chemoselective hydrogenation of unsaturated aldehydes using a new cobalt-base carbon catalyst derived from the thermal transformation of Co-MOF.

The unique properties of MOFs and their composites, such as large surface area, tunable porosity, controllable composition and diverse active sites, can facilitate reactant adsorption and diffusion, enhancing catalytic efficiency and selectivity [2]. This renders them optimal catalysts for the hydrogenation reaction.

The research involved the Co-MOF precursor and the material obtained after thermal transformation at 700 °C in a nitrogen atmosphere. Cobalt was selected as the active metal due to its excellent catalytic properties and potential as a cost-effective alternative to expensive noble metals, making it an attractive choice for sustainable and economically viable catalytic processes.

The catalysts were characterized using advanced techniques, including high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), X-ray powder diffraction (XRD) and Raman spectroscopy. These analyses provided insights into the structural and chemical properties of the materials, as well as the influence of synthesis conditions on their catalytic performance. Hydrogenation reactions were carried out in a continuous-flow reactor under varying pressures and temperatures, allowing for a comprehensive evaluation of catalytic activity under different conditions. These experiments allowed for a more in-depth understanding of the catalytic properties and provided information on the influence of synthesis conditions on the final performance and structure of the catalyst.

References

(1) Lan, X.; Wang, T. Highly Selective Catalysts for the Hydrogenation of Unsaturated Aldehydes: A Review. *ACS Catal.* **2020**, *10* (4), 2764–2790.
(2) Chen, Z.; Chen, J.; Li, Y. Metal-Organic-Framework-Based Catalysts for Hydrogenation Reactions. *Cuihua Xuebao/Chinese J. Catal.* **2017**, *38* (7), 1108–1126.

Acknowledgements: We thank the National Science Centre for financial support within OPUS 25 Project No. 2023/49/B/ST8/00872.

FO-9

Rare-earth doped barium cerate as support for cobalt catalysts in ammonia synthesis

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Ammonia is a raw material used primarily in the production of fertilisers. Its production has been about 150 million tons annually, leading to a consumption of about 2% of the global energy [1]. The constant need for ammonia has led to an intensive search for new catalysts that are more active than iron ones and more affordable than ruthenium ones. Recently, cobalt catalysts have been considered promising. Pure cobalt exhibits low activity due to the weak adsorption energy of N_2 on its surface; thus, to enhance its performance, strategies such as dispersing cobalt on the supports and introducing promoters have been employed [2]. Research attracts attention to the perovskite-type supports such as $BaCeO_3$ and $BaZrO_3$. They offer high thermal stability, abundant oxygen vacancies, and strong basicity, but also easy tunability by doping [3].

This study investigates the ammonia synthesis process over the cobalt-based catalysts supported on rare earth-doped barium cerate, with a particular emphasis on the effects of rare-earth doping. The neodymium, samarium and gadolinium were used as the dopants. The aim was to elucidate the role of doping on the physicochemical properties of the supports and catalysts. The activity of all catalysts was tested in ammonia synthesis at 470 °C and 6.3 MPa. Detailed characterisation studies were conducted using N_2 physisorption, XRD, XRF, STEM-EDX and temperature-programmed methods (*e.g.,* CO_2-TPD and H_2-TPD).

Incorporating rare-earth dopant into barium cerate oxide lattice improved ammonia synthesis reaction rates compared to the catalyst supported on non-doped barium cerate oxide. The rare-earth dopant concentration of 10 mol% was found to be optimal. Samarium was identified as the most effective dopant. The superior performance of the doped catalysts was due to the enhanced electron density on Co, facilitating the N_2 dissociative adsorption, recognised as the rate-determining step of ammonia synthesis.

References

1. J. Humphreys, R. Lan, S. Tao, Adv. Energy Sustainability Res., 2, 2021, 2000043.
2. W. Raróg-Pilecka, M. Karolewska, E. Truszkiewicz. E. Iwanek, B. Mierzwa, Catal. Lett., 141, 2011, 678–684
3. N. Jeon, S. Kim, A. Tayal, J. Oh, W. Yoon, W.B. Kim, Y. Yun, ACS Sustainable Chem. Eng., 10, 2022, 15564.

Acknowledgements: Research was funded by Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme.

FO-10

Investigation of the Ni-MOF-derived carbonaceous material during prenal continuous-flow hydrogenation

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Prenal (3-methylcrotonaldehyde) is known as α,β-unsaturated aldehyde, in which selective hydrogenation of specific double bonds is a challenging reaction. However, it is a key pathway to modern and sustainable fine chemical synthesis. Depending on which unsaturated bond C=C or C=O is hydrogenated, the desired products of 3-methylcrotonaldehyde conversion are:

- 3-methyl-2-buten-1-ol - unsaturated alcohol, an intermediate to pharmaceuticals and fragrances synthesis,

or

- 3-methylbutanal – saturated aldehyde used as a flavour compound and a reagent for producing pharmaceuticals and pesticides [2].

Among the noble metals, platinum is the most often used as a catalyst for prenal hydrogenation [3,4]. However, the high price of this metal significantly reduces its application potential. Therefore, searching for new, readily available and effective substitutes for Pt is ongoing. Our work is part of this search.

Our research focuses on the application of Ni-MOF-derived carbonised catalysts in the continuous flow selective hydrogenation of prenal towards desired products. For this purpose, Ni pyrazolate MOF, with a high nitrogen content, was carbonised under N_2 at a high temperature (700 °C). These synthesis conditions resulted in the formation of Ni nanoparticles anchored on N-doped carbon. The following physicochemical methods were used to characterise the resulting catalyst: high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), X-ray powder diffraction (XRD) and Raman spectroscopy.

References

1. S. Bai, L. Bu, Q. Shao, X. Zhu, X. Huang, Multicomponent Pt-based zigzag nanowires as selectivity controllers for selective hydrogenation reactions, J. Am. Chem. Soc. 140, 8384–8387 (2018)
2. McGinty D., Jones L., Fragrance material review on 3-methyl-2-buten-1-ol, Food and Chemical Toxicology (2010)
3. Kliewer C.; Bieri M.; Hydrogenation of the α,β -Unsaturated Aldehydes Acrolein, Crotonaldehyde, and Prenal over Pt Single Crystals: A Kinetic and Sum-Frequency Generation Vibrational Spectroscopy Study; Journal of the American Chemical Society; 131, 9958-9966 (2009)
4. Arai M.; Obata A.; Activity for liquid-phase hydrogenation of α,β - unsaturated aldehydes of supported platinum catalysts prepared through low-temperature reduction; Applied Catalysis A: General 146; 381-389, (1996)

Acknowledgements: We thank National Science Centre for financial support within OPUS 25 Project No. UMO-2023/49/B/ST8/00872.

FO-11

Single-Atom Quantum-Driven Energy Conversion: Photochemical and Industrial Approaches to Value-Added Products"

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Recently single-atom photocatalysts are emerging as a new research frontline, featuring minimum particle sizes and maximum utilization of co-ordinately unsaturated metal sites. Atoms of a catalytic site arrange into a configuration that essentially offers a specific electronic structure for the catalytic cycle. However; SAC synthesis lacks stability issues; Herein we have optimized microwave irradiation process – Which provides an even distribution of the metal, as well as it maintains the backbone of the carbon nanosheets.

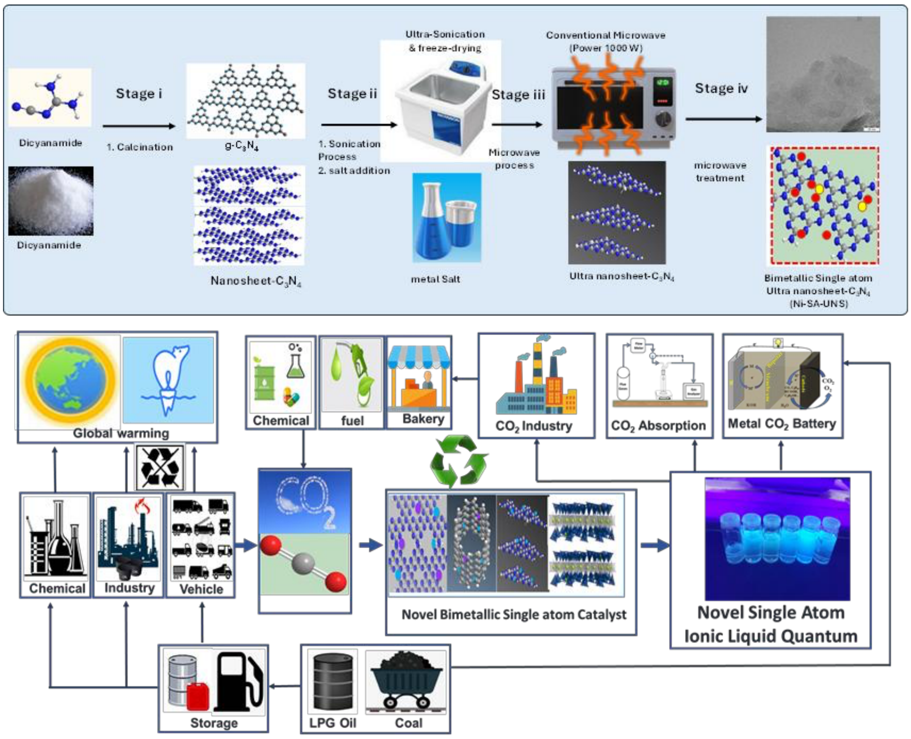

Fig. 1. Single Atom Quantum Industrial Formulation and Application in Various Fields.

Via using microwave process – strictly no calcined protocol - seeking high yield with highly even distribution as single atom, with no loss of material, high yields, no loss of metal (as nanoparticles), no harsh conditions, acid wash (for nanoparticle removal) and no use of costly ligands. Microwave synthesis procedures have a clear path for industrial-scale manufacturing methods which demand stable and high metal loading SACs at low cost[1 2]. Overall, these findings underscore the potential of developed SACs to drive advancements in science with the possible broad applicability in pharmacy, polymer, and agrochemical industries.

References.

1 G. Vilé, P. Sharma, M. Nachtegaal, F. Tollini, D. Moscatelli, A. Sroka-Bartnicka, O. Tomanec, M. Petr, J. Filip, I. S. Pieta, R. Zbořil and M. B. Gawande, *Sol. RRL*, 2021, **5**, 2100176.
2 P. Sharma, S. Kumar, O. Tomanec, M. Petr, J. Zhu Chen, J. T. Miller, R. S. Varma, M. B. Gawande and R. Zbořil, *Small*, 2021, **17**, 2006478.

Acknowledgements: P.S. thanks National Science Foundation for UMO-2022/47/P/ST4/03412 to the research project No. 2022/47/P/ST4/03412.

FO-12

Polypyrrole dye – assisted synthesis – morphology and surface active area determination

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Electroactive polypyrrole is widely used in diverse directions with application ability strongly dependent on the morphology of the material [1,2]. In the current work we studied such materials derived by chemical oxidative polymerisation based on the template methodology with methyl orange (MO) as a structure guiding agent. We focused on the concentration of the dye to trace its templating ability. Surface morphology of material dependent firmly on the amount of the supplied dye (Fig. 1 a,b) – increasing content of the dye provoked a decrease in the diameter of the forming tubes accompanied by a mutual increase in their number. The organization induced by the presence of MO was also reflected in surface active area of powders as determined by BET analysis (Fig. 1 c). The value of surface active area increased markedly (5.8 times) from 12.58 m^2/g for unmodified polymer to 74.00 m^2/g for polymer synthesised in the highest concentration of modifier.

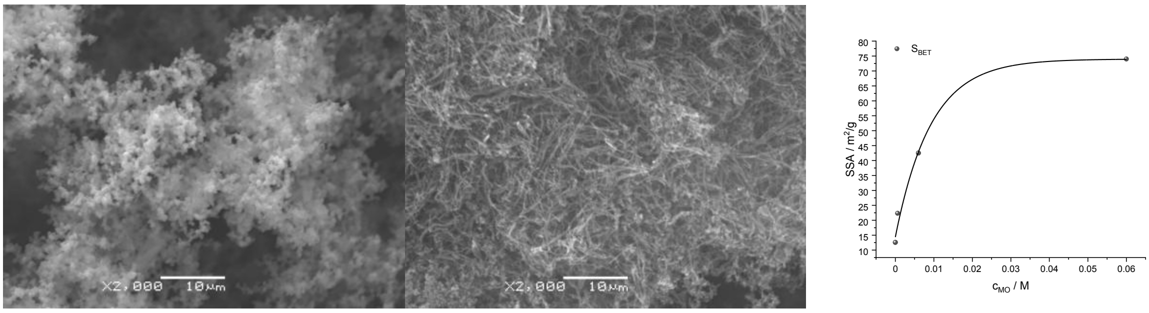

Fig. 1. SEM images of pPy synthesised in a) the absence b) the presence of organic modificator, c) dependence of surface active area of nanostructured polypyrrole with concentration of added dye

References

1. K. Namsheer, Ch. Sekhar Rout, RSC Adv. 11 (2021), 5659
2. Z. Huang, X. Li, Ch. Pan, P. Si, P. Huang, J. Zhou, Materials Chemistry and Physics 279 (2022) 125775

Acknowledgements: The work was founded by Institute of Materials Engineering founds.

FO-13

Efficient Removal of Polystyrene Nanoplastics from Water Using Zeolite Adsorbents: A Case of Carboxylate-modified Polystyrene

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Various analytical methods are employed to identify nanoplastics in aquatic environments. In recent years, UV-Vis spectroscopy has gained increasing attention for detecting and even quantifying microplastics (MPs) and nanoplastics (NPs) [1]. This growing popularity is attributed to its advantages over traditional methods, including rapid analysis, low cost, non-destructive nature, and high accuracy. A key benefit of UV-Vis spectroscopy is its ability to perform real-time assessments with minimal to no sample pre-treatment, avoiding labor-intensive extraction processes such as filtration or sedimentation [2].

Polystyrene (PS) is a widely used plastic in everyday life [3], but its nanoplastic derivatives (PS-COOHs) pose a significant environmental concern. Microplastics and nanoplastics are persistent, nonbiodegradable pollutants with potential toxic effects on aquatic ecosystems and human health. Their effective removal requires innovative technologies, with adsorption emerging as a promising method for water purification [4].

This study focuses on developing a potential zeolite-based adsorbent with high adsorption capacity to remove 0.2 μm polystyrene nanoplastics (PS-COOHs) from aqueous solutions. Only commercially available zeolites with various micro- and mesoporous characteristics and different acidic properties were selected, including H-USY, H-β, X, and clinoptilolite. To analyze the adsorption and desorption process, ultraviolet-visible spectroscopy (UV-Vis), infrared (FT-IR) spectroscopy, X-ray diffraction (XRD), and low-temperature N_2 sorption (BET) were employed. Notably, this study introduced, for the first time, the use of quantitative UV-Vis spectroscopy in both transmission and diffuse reflectance (DR UV-Vis) modes, ensuring precise, repeatable, and reliable quantification of polystyrene concentrations in both the solution and the adsorbent, thereby enabling accurate assessments of sorption efficiency. With minimal sample preparation and real-time monitoring, this method serves as an effective tool for evaluating sorbents in nanoplastic removal.

Experimental results demonstrated that H-USY and clinoptilolite exhibited high adsorption performance at 100 and 200 $mg\cdot L^{-1}$, with a sorption time of 20 minutes. The adsorption capacity of H-USY ranged from 80–91 $mg\cdot L^{-1}$ (100 $mg\cdot L^{-1}$) and 160–166 $mg\cdot L^{-1}$ (200 $mg\cdot L^{-1}$), while clinoptilolite achieved 80–92 $mg\cdot L^{-1}$ and 170–190 $mg\cdot L^{-1}$, respectively, depending on the sorbent dose. These findings highlight the potential of zeolites as efficient, regenerable adsorbents for nanoplastic removal, offering a sustainable approach to mitigating environmental pollution.

References

1. L.S. Pieniazek, M. L. McKinney, J. A. Shein, J. Micropl. 3 (2024) 339
2. L. Wander, L. Lommel, A. Paul, J. Meas Sci Technol. 33 (2022) 075801
3. V. Siipola, H. Romar, U. Lassi, J. Sustain. Biochar for Water and Wastewater Treat. (2022) 393
4. M. Munz, C. Loui, D. Postler, M. Pittroff, S. E. Oswald, J. Micropl, and Nanopl. 4 (2024) 2

Acknowledgments: The work was supported by the National Science Centre, Poland, under research project No. 2021/43/B/ST4/00307.

FO-14

Modulating Actinomycin D Release from Bacterial Nanocellulose Films for a Potential Drug Delivery System

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Efficient drug delivery systems are essential for optimizing therapeutic transport and improving treatment outcomes. This study explores bacterial nanocellulose (BNC) as a natural, biocompatible matrix for the controlled release of actinomycin D (ActD), a potent antibiotic with established anticancer properties.

Bacterial nanocellulose, produced in biocatalytic processes, through microbial fermentation, is a highly sustainable material derived from diverse sources, including degraded biopolymers, petrochemical-biopolymer blends, and lignocellulosic residues [1]. Its high purity, absence of lignin and hemicellulose, and unique physicochemical properties - such as high crystallinity, porosity, mechanical stability, nontoxicity and excellent biocompatibility - make it an ideal candidate for biomedical applications. BNC is widely used in tissue engineering, artificial skin, wound healing, and drug delivery [2].

Actinomycin D, a polypeptide antibiotic derived from *Streptomyces* species, functions as a transcription inhibitor by blocking RNA polymerase progression [3]. It has been FDA - approved for treating various cancers, including testicular, ovarian, and pediatric tumors [4].

To enhance drug loading and control release kinetics, TEMPO oxidation was applied to BNC, introducing functional groups that improved ActD retention. Structural and chemical analyses confirmed successful modification. In vitro release studies demonstrated that oxidized BNC enabled a slower, sustained release compared to unmodified BNC, following a diffusion-controlled mechanism. Antimicrobial testing against *Staphylococcus aureus* confirmed the efficiency of ActD-loaded BNC films. Presented study shows that functionalization of BNC facilitates the drug release control in drug delivery system [5].

References

1. J. A. Araujo, G. Taxeidis, E. Pereira, M. Azeem, B. Pantelic, S. Jeremic, M. Ponjavic, Y. Chen, M. Mojicevic, J. Nikodinovic-Runic, J. Clean. Prod. 443 (2024) 141025
2. N.H.C.S. Silva, J. P. Mota, T. Santos de Almeida, J. P. F. Carvalho, A. J. D. Silvestre, C. Vilela, C. Rosado, C.S.R. Freire, Int. J. Mol. Sci. 21 (2020) 1262
3. G. Finocchiaro, Neuro-Oncol. 22 (2020) 1235–1236
4. D.F. Lu, Y. S. Wang, C. Li, G. J. Wei, R. Chen, D.M. Dong, M. Yao, Int. J. Clin. Exp. Med. 8 (2015) 1904–1911
5. K. Zimowska, Vuk Filipovic, J. Nikodinovic-Runic, J. Simic, T. Ilic-Tomic, M. Zimowska, J. Gurgul, M. Ponjavic, Bioengineering, 11 (2024) 847

Acknowledgements: This research was funded by the Science Fund of the Republic of Serbia, IDEJE, under the agreement number 7730810, BioECOLogics, and the Ministry of Science, Technological Development and Innovations of the Republic of Serbia, Project No. 451-03-66/2024-03/200042. K. Z. mobility was funded by Erasmus+ Programme (Student Mobility for Traineeship).

Plakaty
Posters

P-1

Catalytic performance of copper catalysts in the continuous flow hydrogenation of unsaturated aldehydes

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Heterogeneous catalysis is a crucial field in fine chemical synthesis. In this challenging area, the chemoselective hydrogenation of α,β-unsaturated aldehydes to unsaturated alcohols and saturated aldehydes is vital for the production of fragrances, flavors, and pharmaceuticals [1-4]. Different types of catalysts are used in this reaction such as transition metal catalysts, which offer significant advantages over noble metals. They are more cost-effective and abundant, making them economically viable for large-scale applications. In this work, we investigated the catalytic activity of Cu-catalysts with different metal loadings in the continuous flow hydrogenation of 2-methyl-2-pentenal (MPEA) under a broad range of temperatures (25–100°C) and pressures (10-60 bar). Catalytic performance was correlated with physicochemical properties using ICP-OES, TPR, *in situ* XRD, XPS, NH_3-TPD, CO_2-TPD, and TEM analyses. The Cu^0/Cu^+ ratio played a crucial role in activity and selectivity, with all catalysts achieving 100% selectivity to 2-methylpentanal (MPAA) at ≤65 °C. At higher temperatures and pressures, selectivity toward the fragrance intermediate 2-methyl-2-penten-1-ol (MPEO). The findings highlight the role of Cu^+ species, hydrogen spillover, and acid-base interactions in tuning product distribution, offering valuable insights for industrial applications in fine chemical synthesis.

References

1. Tian, Z.; Xiang, X.; Xie, L.; Li, F. Liquid-Phase Hydrogenation of Cinnamaldehyde: Enhancing Selectivity of Supported Gold Catalysts by Incorporation of Cerium into the Support. *Ind. Eng. Chem. Res.* 2013, *52*, 288–296
2. Zhao, M.; Yuan, K.; Wang, Y.; Li, G.; Guo, J.; Gu, L.; Hu, W.; Zhao, H.; Tang, Z. Metal–Organic Frameworks as Selectivity Regulators for Hydrogenation Reactions. Nature 2016, 539, 76–80
3. Hao, C.-H.; Guo, X.-N.; Pan, Y.-T.; Chen, S.; Jiao, Z.-F.; Yang, H.; Guo, X.-Y. Visible-Light-Driven Selective Photocatalytic Hydrogenation of Cinnamaldehyde over Au/SiC Catalysts. J. Am. Chem. Soc. 2016, 138, 9361–9364
4. He, L.; Yu, F.-J.; Lou, X.-B.; Cao, Y.; He, H.-Y.; Fan, K.-N. A Novel Gold-Catalyzed Chemoselective Reduction of α, β-Unsaturated Aldehydes Using CO and H_2O as the Hydrogen Source. Chem. Commun. 2010, 46, 1553–1555

Acknowledgments: We thank the National Science Centre for financial support within OPUS 25 Project No.2023/49/B/ST8/00872.

P-2

Układy nośnikowe zawierające miedź i/lub cynk - wpływ stężenia fazy aktywej i natury nośnika na właściwości katalitycznie istotne

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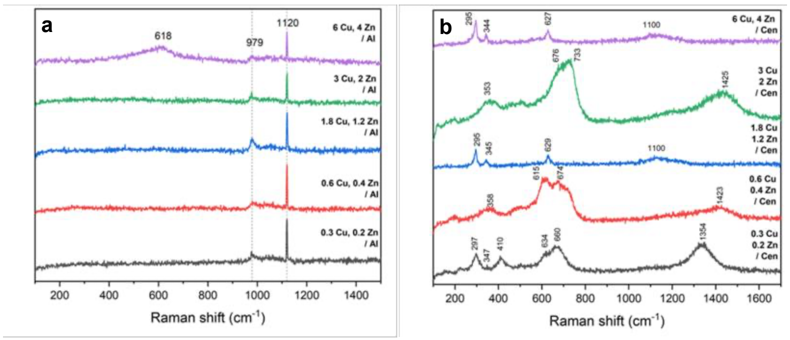
Efektywne kształtowanie architektury powierzchni tlenkowych katalizatorów nośnikowych wymaga wskazania kluczowych parametrów preparatywnych, które w istotnej mierze wpływają na właściwości katalityczne syntezowanych układów, takie, jak: aktywność, selektywność i stabilność. Do takich parametrów należą: wybór ścieżki syntezy, rodzaj użytego nośnika, stężenie fazy naniesionej oraz warunki obróbki termicznej nośników i finalnych katalizatorów. Wymienione parametry mogą w znacznym stopniu determinować porowatość, specjację form powierzchniowych, ich stopień aglomeracji a także stabilność katalizatorów w warunkach reakcyjnych, ze szczególnym uwzględnieniem ewolucji termicznej i zmian zachodzących pod wpływem reagentów. Z poznawczego punktu widzenia niezwykle istotne jest zrozumienie relacji pomiędzy naturą danego parametru i sposobem, w jaki wpływa on na właściwości strukturalne, teksturalne i funkcjonalne finalnego układu. Dobrze jest także określić, czy na etapie syntezy wpływ wybranego parametru ma charakter inwariantny, czy też jego efekt może być niwelowany przez inne zmienne preparatywne. W niniejszej pracy uwaga skupia się na dwóch fundamentalnych parametrach: rodzaju nośnika i stężeniu fazy naniesionej.

W przedmiotowych badaniach korzystano z komercyjnych nośników: γ-Al_2O_3 oraz cenosfer impregnowanych jonami miedzi(II) i/lub cynku. Wszystkie próbki kalcynowano w temperaturze 400°C przez 4h. Układy zawierające 0.5-10.0 $\%_{mol.}$ miedzi/cynku lub kombinację 0.3-6.0 $\%_{mol.}$ miedzi i 0.2-4.0 $\%_{mol.}$ cynku poddano wnikliwej charakterystyce metodami: XRF, XRD, RS, SEM/EDS, BET, DRIFT i UV/Vis-DR.

Przeprowadzone badania potwierdziły kluczową dla architektury powierzchniowych form oksometalicznych rolę doboru nośnika oraz stężenia fazy naniesionej. Charakterystyczne było przy tym wyraźne sprzyjanie przez cenosfery stabilizacji form silnie zaglomerowanych (typu CuO i/lub ZnO), nawet przy tak niskich stężeniach, jak 0.2 $\%_{mol.}$. Z kolei, γ-Al_2O_3 faworyzował stabilizację form o dużej heterogeniczności, silnie zależną od stężeń składników naniesionych.



Rys. Wyniki badań strukturalnych wykonanych techniką RS
dla γ-Al_2O_3 a) i cenosfer b) funkcjonalizowanych jonami cynku i miedzi.

Podziękowania: Realizowane badania zostały dofinansowane ze środków *POB Anthropocene (PF Man-Mind-Environment Hub) w ramach Programu Strategicznego Inicjatywa Doskonałości w Uniwersytecie Jagiellońskim.*

P-3

Centra funkcjonalne na powierzchni niemodyfikowanych i funkcjonalizowanych cenosfer pozyskiwanych z popiołów lotnych

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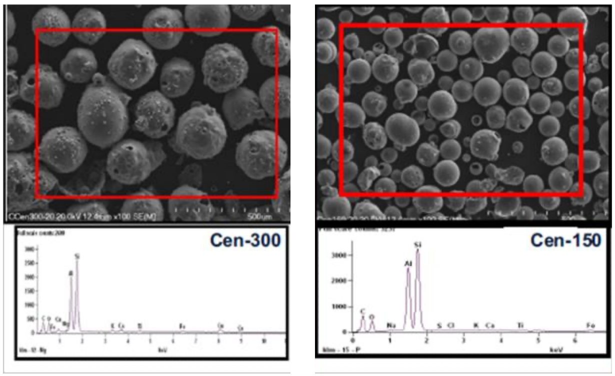
Cenosfery występują powszechnie w popiołach lotnych generowanych masowo w trakcie przemysłowego spalania paliw stałych dla celów energetycznych. Ich udział w stałych produktach spalania jest zmienny i zawiera się w dość szerokim zakresie: od 0,01 do 35,6 $\%_{wag.}$ [1]. Pierwiastkami najczęściej identyfikowanymi w składzie cenosfer są krzem, glin i żelazo, których tlenki stanowią do 89$\%_{wag.}$ materiału. Głównymi frakcjami mineralnymi, które wchodzą w skład cenosfer są: mullit, kwarc i kalcyt. Średnice cenosfer mogą się zawierać w przedziale od 5 do 500 μm, przy czym najczęściej w popiołach lotnych występują cenosfery o wymiarach 20-300 μm. Cenosfery charakteryzują się niską gęstością objętościową (0,2 - 0,8 g/cm^3) i można je stosunkowo łatwo wyodrębnić z popiołów metodami grawitacyjnymi [1]. Sferyczny kształt oraz wysoka trwałość mechaniczna i stabilność termiczna predestynują cenosfery do zastosowań katalitycznych, zwłaszcza wysokotemperaturowych. Materiały te mogą być wykorzystywane jako nośniki lub, po odpowiedniej funkcjonalizacji, jako katalizatory [2]. Funkcjonalizacja może obejmować wprowadzenie na ich powierzchnię np. tlenków metali przejściowych, wykazujących wysoką aktywność w reakcjach redoks o znaczeniu środowiskowym, takich, jak np. deNO$_x$, deSoot, deVOC, czy też reakcje waloryzacji CO_2.

Zarówno nanoszenie stabilnych faz oksometalicznych na powierzchnię cenosfer, używanych jako nośników, jak i efektywna funkcjonalizacja tych materiałów wymaga wnikliwej charakterystyki centrów powierzchniowych, pozwalających na molekularne zakotwiczenie nanoszonych składników. W trakcie niniejszych badań skorzystano z komercyjnych cenosfer o średnicach 150 μm i 300 μm. Cenosfery funkcjonalizowano 0.5-10.0 $\%_{mol.}$ miedzi/cynku lub 0.3-6.0 $\%_{mol.}$ miedzi i 0.2-4.0 $\%_{mol.}$ cynku. Charakterystykę centrów powierzchniowych przeprowadzono metodami: RS, DRIFT i UV/Vis-DR.

Przeprowadzone badania potwierdziły złożoną strukturę centrów powierzchniowych tak w przypadku cenosfer niemodyfikowanych, jak i funkcjonalizowanych jonami miedzi i/lub cynku. Na podkreślenie zasługuje fakt, iż zarówno heterogeniczność zidentyfikowanych grup hydroksylowych, jak i centrów chromoforowych odzwierciadlała z jednej strony kompozytowy charakter powierzchni cenosfer, z drugiej zaś efekty wynikające z ich funkcjonalizacji.

Literatura
1. E. Haustein, B. Quant,
Gosp. Sur. Min., 27 (2011) 95
2. B. Samojeden et al.,
Catalysts 9 (2019) 1066

Podziękowania: Realizowane badania zostały dofinansowane ze środków POB Anthropocene (PF Man-Mind-Environment Hub) w ramach Programu Strategicznego Inicjatywa Doskonałości w Uniwersytecie Jagiellońskim.



Rys. Obrazy SEM/EDS niemodyfikowanych cenosfer.

P-4

Investigation of support effects during ethanol steam reforming over nickel-based catalysts

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The political and social sustainability awareness stimulates interest in researching and developing new technologies for more environmentally friendly fuel production. In this context, H_2 is becoming increasingly important as it is seen as a promising energy vector and its fundamental role as a traditional raw material for many products (including its combination with CO as synthesis gas [syngas]). One alternative for the sustainable production of H_2 or syngas is to take advantage of the existing steam reforming technologies and to make adaptations to replace the natural gas (methane) feedstock with biomass-derived feedstock (such as bioethanol or bio-oil). Specifically, bioethanol steam reforming (ESR) stands out as one of the promising technologies for hydrogen production, contributing to the advancement of clean and sustainable energy systems. However, this process implicates many reaction intermediates and unstable products, especially at low temperatures. The metal active sites are essential in activating and breaking C-C and C-H bonds in the ethanol molecule. So far, a wide range of catalytic systems has been investigated, including metallic catalysts such as Pt, Pd, Ru, Rh, Co or Ni deposited on oxide supports. The high activity strengthened by the cost-effectiveness of nickel-based catalysts makes these systems attractive candidates for the ESR process. Moreover, the ESR performance of the nickel-based catalysts is strongly affected by the characteristics of the support, which is proposed to play a role in determining overall reactivity, including acid–base properties, redox properties and the strength of the metal–support interaction [1-4].

The chemical composition and textural properties of the support and synthesis method play essential roles in preparing highly active steam reforming catalysts since they can improve the dispersion of the metal. Thus, in this work, CeO_2, MnO_x, and CeXMn (where X(%mol)=nCe/(nCe+nMn)·100%) supports have been prepared to develop nickel-based catalyst for ESR reaction. The textural properties, phase compositions, microscopic morphologies, and reducibility of catalysts are characterised by N_2 adsorption/desorption, X-ray diffraction (XRD), transmission electron microscopy (TEM), and H_2-TPR methods, respectively. The reduction temperature of NiO gradually shifted to a higher value with the increase in the MnO_x amount, indicating that the presence of MnO_x made the reduction process of NiO phase more difficult. The highest ethanol conversion among the tested catalysts showed the Ni/CeO_2. However, the highest selectivity to hydrogen and C1 products (CO, CO_2, CH_4) and the lowest production of highly undesired C2 (acetaldehyde) and C3 (acetone) products exhibits the Ni/MnO_x sample.

References

1. J. Valecillos, S. Iglesias-Vázquez, A. Remiro, J. Bilbao, A.G. Gayubo, Fuel 385 (2025) 134082.
2. G. Grzybek, O. Wasiłek, M. Rudzińska, P. Stelmachowski, P. Legutko, M. Greluk, G. Słowik, M. Rotko, A. Kotarba, Catal. Today 439 (2024) 114808.
3. N. Ferreira, L. Coronel, M.S. Moreno, L.M. Cornaglia, J.F. Múnera, Fuel Process. Technol. 217 (2021) 106814.
4. E. Martono, J. M. Vohs, J. Catal. 291 (2012) 79-86.

P-5

CeO_2-supported Cobalt Catalysts for Steam Reforming of Ethanol: The Role of the Preparation Method and Alkali Promotion

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Sharply increasing global energy demand, climate changes due to massive CO_2 emissions, as well as limited fossil fuel resources have led to an extensive search for new renewable and eco-friendly fuels. Hydrogen can be considered a promising solution due to its high energy density and zero CO_2 emissions during combustion [1]. Steam reforming of ethanol (ESR) arises as a potentially efficient way of hydrogen production by biomass utilization [2]. In our research, we have developed efficient alkali-doped ceria-supported cobalt catalysts for the ESR process. Ceria was chosen as a support due to its activity towards the combustion of carbon species [3] formed on the catalyst surface during the ESR reaction.

Initially, cerium oxide was prepared – from $Ce(NO_3)_3{\cdot}6H_2O$ as a precursor – using hydrothermal – CeO_2(HT) and sonochemical – CeO_2(SC) synthesis methods. The ceria materials, as well as ceria commercially purchased from Sigma-Aldrich – CeO_2(COM), were tested in the model experiment of soot combustion (using Printex U soot, purchased commercially) in the flow of 5% oxygen in helium in tight and loose contact mode [4]. Next, CeO_2 supports were doped with potassium by the impregnation technique. CeO_2(HT) exhibited the highest shift of 50% soot conversion temperature (from 654℃ to 520℃ in loose contact mode) upon doping with potassium. Thus, it was chosen as a support for cobalt catalysts for the ESR reaction. Subsequently, the role of the cobalt deposition procedure was investigated, comparing hydrothermal – Co(HT)/CeO_2(HT), sonochemical – Co(SC)/CeO_2(HT), and impregnation – Co(IWI)/CeO_2(HT) methods. The catalysts were thoroughly characterized using XRD, RS, XPS, DR-UV/Vis, and H_2-TPR techniques, as well as SEM and TEM microscopy, and tested in both the ESR process and the soot combustion. The differences in their catalytic activity were attributed to variations of ceria morphology, the ratio between Ce^{3+} and Ce^{4+} concentration on the surface, and the dispersion of the cobalt active phase.

References

1. R. Kumar, R. Singh, S. Dutta, Energy Fuels 38 (2024) 2601−2629.
2. X. Feng, Y. Zhao, Y. Zhao, H. Wang, H. Liu, Q. Zhang, RSC Advances 13 (2023) 23991.
3. S. B. Putla, M. Kamali, B. Swapna, B. M. Reddy, P. Sudarsanam, ACS Appl. Nano Mater. 7 (2024) 6749−6771.
4. G. Grzybek, A. Wojtowicz, P. Legutko, M. Greluk, G. Słowik, A. Sienkiewicz, A. Adamski, A. Kotarba, Molecules 30 (2025) 358.

Acknowledgements: We thank National Science Centre, Poland for funding this research (grant no. 2021/43/D/ST4/03016).

P-6

Incorporation of rare-earth elements to Pt nanoparticles over MFI zeolites for modulating the selective hydrogenation of cinnamaldehyde

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Cinnamaldehyde (CAL) contains two distinct unsaturated functional groups (C=O and C=C), making the selective hydrogenation of a specific functional group particularly challenging. The partially hydrogenated products, cinnamyl alcohol (COL) and hydrocinnamaldehyde (HCAL), serve as valuable platform chemicals in the pharmaceutical, perfumery, cosmetics, and chemical industries [1].

Pt-based catalysts, characterized by a wide d-bandwidth, preferentially hydrogenate the C=O bond, exhibiting high selectivity toward COL. The incorporation of secondary transition metals (e.g., Fe, Co, Ni, Sn) enhances COL selectivity through geometric and electronic modifications of Pt nanoparticles [2].

MFI zeolites containing silanol nests facilitate the stabilization of rare-earth elements (REEs) at the atomic scale, enabling the formation of Pt-REE alloy nanoparticles with nanoscale dimensions (<2 nm) within the zeolite micropores [3]. The high REE content effectively minimizes Pt ensembles and modulates the selective hydrogenation of cinnamaldehyde.

This study investigates the impact of incorporating REEs (Ce, La, and Y) into Pt nanoparticles on the catalytic performance of cinnamaldehyde selective hydrogenation. We demonstrate how these modifications influence the physicochemical properties of the catalyst and elucidate their role in tuning hydrogenation selectivity.

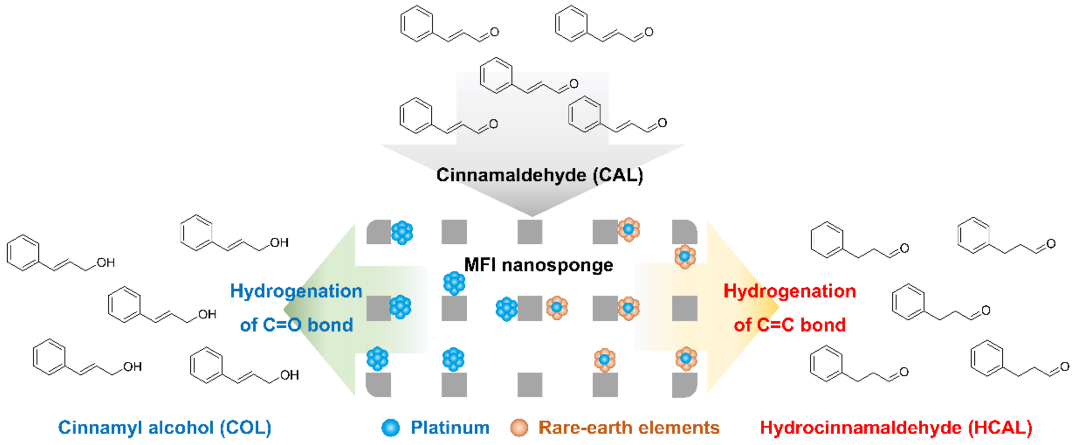

Fig. 1. Reaction pathways for selective hydrogenation of cinnamaldehyde over Pt-REE nanoparticles

References

1. Xiaofeng Wang, ACS Catal. 10 (2020) 2395-2412
2. Komal N. Patil, J. Environ. Chem. Eng. 11 (2023) 109168
3. Ryoo R., Nature 585 (2020) 221-224

Acknowledgments: We acknowledge the support of the Czech Science Foundation for the project no. 25-14521L.

P-7

Ammonia as a hydrogen storage medium – LDH origin catalysts with Co, Ni, Fe for ammonia decomposition

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Hydrogen is a clear energy carrier, but for the most purposes its low volumetric energy density in a compressed gas makes its storage and transportation a serious problem. Compared with other potential hydrogen storage materials, ammonia has a high hydrogen storage capacity (17.6 wt%), energy density (3000 Wh/kg) and can be easily liquefied at 20°C and 0.8 MPa. These advantageous of ammonia make it promising for the hydrogen storage and transportation. It has been reported that transition metals such as Co and Ni are effective catalysts of ammonia decomposition [1-2]. Acidity and basicity of support used for metal catalysts deposition have an important role in tailoring efficient catalytic systems for ammonia decomposition [3]. The layered double hydroxides (LDH), offer great opportunities for synthesis catalysts with the desired properties.

The series of LDH materials with Co, Ni, and Fe and bimetallic Co-Ni, Fe-Ni, and Co-Ni – were synthesised. The prepared catalysts were characterised by various methods, including low-temperature N_2 adsorption-desorption, XRD, H_2-TPR, NH_3-TPD, N_2-TPD, TGA/DSC. The samples obtained were tested as catalysts for ammonia decomposition (dcNH3) in the temperature range of 250 - 800°C, with a space velocity of 300 cm3/g_{cath} NH_3. All samples prior to the catalytic tests were calcined at 600°C for 12 h and then reduced to 800°C for 12 h in a flow of pure hydrogen.

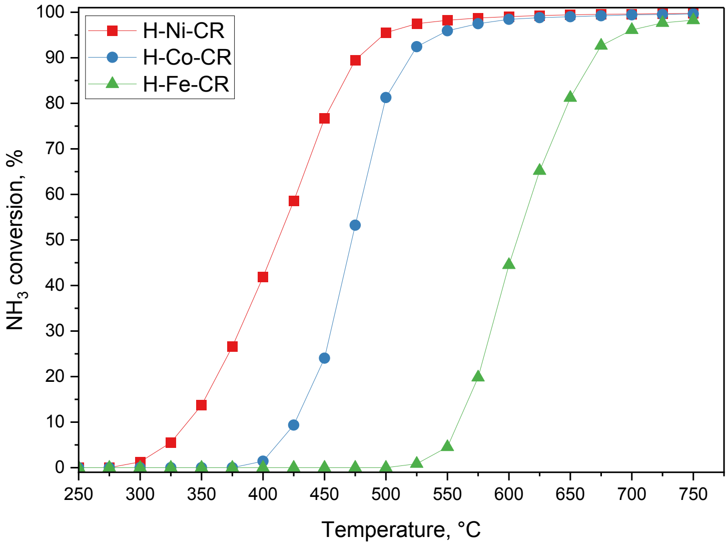

Fig. 1. Results of catalytic tests for Ni-, Co-, Fe-LDH-origine catalyst calcined at 600°C and reduced at 800°C.

References

1. *Ying-Qiu Gu, Zhao Jin, et al., J. Mater. Chem. A, 2015, 3, 17172.*
2. *E. Medina, C. Fernández , A. Karelovic , R.I Jiménez, Int. J. Hydrog. Energy, 2024, 90, 1435.*
3. *J. Zhang, H. Xu, X. Jin, Q. Ge, W. Li, Appl. Catal. A, 2005 290, 87.*

Acknowledgements: The research has been supported by a grant from the Faculty of Chemistry under the Strategic Programme Excellence Initiative at Jagiellonian University.

P-8

Effect of modification of CMK-3 carbons with nitrogen and oxygen functionalities on their activity in redox processes

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In recent years nitrogen-modified carbon catalysts have gained increasing interest from researchers in various applications, including catalysis and electrochemistry, due to their favorable physicochemical properties, environmental friendliness and relatively easy regeneration. Modification of carbon materials with nitrogen and oxygen functional groups significantly affects their acid-base and electronic properties, enhancing their activity in various chemical processes. The effectiveness of these modifications depends on many factors such as the type of generated groups, their concentration, distribution, as well as polarity. Understanding the real role of nitrogen-containing functionalities present on the surface of carbon materials is essential for their application in advanced chemical technologies. In this study, the effect of surface modification of CMK-3 carbon nanoreplicas with N and O groups on the catalytic and electrochemical performance was investigated.

Ordered mesoporous CMK-3 carbons modified with N and O functionalities were obtained by structural nanoreplication of a SBA-15 silica matrix. A solution of carbon and nitrogen precursor, in the form of the mixture of sucrose or sucrose and urea with defined N/C molar ratio (0, 0.14 and 0.51) was introduced into the pores of template by the incipient wetness method. The obtained materials were carbonized in an inert atmosphere in the temperature range of 600-1000°C. The CMK-3 carbons were characterized in terms of textural parameters (low-temperature adsorption of nitrogen), structure and morphology (XRD, Raman spectroscopy, SEM), surface and bulk composition (XPS, CHNO analysis), electrochemical properties (CV), and were tested as catalysts in the oxidation of sulfuric acid in the aqueous phase (OSA). The materials were also subjected to post-synthetic modifications in order to change the distribution of functional groups on the surface and to check their influence on activity in the OSA reaction. The obtained carbons were oxidized in concentrated aqueous solution of nitric acid, reduced in gaseous ammonia, and modified by combination of these both processes. The catalytic activity in the OSA process increased significantly with higher carbonization temperatures, demonstrating the key role of graphite-like structures in enhancing electron transport and activating molecular oxygen. Furthermore, these effects were notably strengthened by the presence of surface nitrogen groups.

References

1. S. Jarczewski, M. Drozdek, P. Michorczyk, C. Cuadrado-Collados, J. Gandara-Loe, J. Silvestre-Albero, P. Kuśtrowski, Microporous Mesoporous Mater. 271 (2018) 262.
2. S. Utgenannt, F. Hansen, O. Klepel, S. Jarczewski, A. Wach, P. Kuśtrowski, Catal. Today 249 (2015) 38.

Acknowledgements: The authors thank the Deutsche Forschungsgemeinschaft (DFG) for funding.

P-9

Ceramic monolithic structures decorated with Cu and Co oxides for total oxidation of volatile organic compounds

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Volatile organic compound (VOCs), released into the atmosphere due to human activity, contribute to the formation of photochemical smog, the degradation of the ozone layer, and atmospheric haze. Given the ongoing tightening of emission demands, several technologies for VOCs removal have been developed, including their catalytic combustion, which occurs at much lower temperatures compared to thermal oxidation. Noble metal-based catalysts (such as Pt, Pd, Rh) demonstrate high efficiency in the low-temperature total oxidation of VOCs. However, their use is often constrained by high production costs and a tendency to deactivation in the presence of sulfur- and halogen-containing compounds. As a more cost-effective and chemically stable alternative, transition metal oxides, like CuO, MnO_2, Fe_2O_3, and Co_3O_4, have been increasingly employed [1]. Their catalytic performance can be further improved by using a properly selected support. For this purpose, the application of a ceramic monolith structure with a controlled shape and size should drastically reduce the cost of catalyst synthesis, limit the required amount of active phase, and exhibit lower pressure drop and exceptional resistance to clogging. Furthermore, it is possible to quickly dissipate excess heat generated during the exoenergic combustion process preventing catalyst deactivation [2].

In this work, a new approach to designing monolithic structures doped with copper and cobalt oxides was proposed. A particularly important part of the research was the production of ceramic monoliths, which were obtained by nanoreplication of 3D printed resin templates with specific dimensions and shapes. The process of deposition of the active phase layer on the surface of a non-porous ceramic monolith turned out to be highly complex. To increase adhesion, an additional two-step functionalization approach was implemented, consisting in anchoring of an aminosilane coupling agent and subsequent polymerization in solution. The CuO and Co_3O_4 phases were incorporated by adsorption with a forced flow of the modifying solution through the monolith channels. A physicochemical characterization of the produced catalysts was performed, including analysis of morphology (SEM-EDX), elemental composition (XRF), structure (XRD), and chemical environment (UV-Vis-DR). A critical aspect of the study was the evaluation of the catalytic activity of the obtained materials in the total oxidation of toluene. Various combinations of the catalyst bed were tested, including those containing a varying number of monolith pieces with different oxide phases arranged in a different order in relation to the input of the reaction gases into the catalyst bed.

References

1. P. Kuśtrowski, A. Rokicińska, T. Kondratowicz, Adv. Inorg. Chem. 72 (2018) 385.
2. S. Mo, Q. Zhang, Q. Ren, J. Xiong, M. Zhang, Z. Feng, D. Yan, M. Fu, J. Wu, L. Chen, D. Ye, J. Hazard. Mater. 364 (2019) 571.

P-10

Influence of hollow @SiO_2 and @TiO_2 support on catalytic activity of CuO and Co_3O_4 phases in toluene combustion

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VOCs are environmental pollutants recognized as substances causing photochemical smog, as well as carcinogenic and/or mutagenic effects in humans. Therefore, limiting the amount of VOCs released into the atmosphere is crucial for the protection of the environment and human health. A very promising method of controlling VOCs emissions is their catalytic combustion, but it requires the development of appropriately effective catalysts [1]. Particularly important in this context is a deeper understanding of the role of interactions between an active phase and a support, which can lead to improved catalytic properties [2]. The dispersion and type of the active phase, as well as physicochemical properties of the support must be selected appropriately when designing catalysts, including novel core-shell materials. The advantage of the latter materials is not only the unique properties related to their nanometric structures, but also the arrangement of the individual components of the system that provides a well-controlled contact between the core and the shell [1,3].

The TiO_2 and SiO_2 supports of similar morphology and porosity were synthesized in order to exclude the influence of these parameters on the catalytic activity of CuO and Co_3O_4 phases in the total oxidation of toluene. The supports of uniform spherical shape with comparable BET surface area of 38 m^2/g and 29 m^2/g for @SiO_2 and @TiO_2, respectively, were obtained. The active phase was introduced by wet impregnation in amount of 5, 10 and 15 wt% of transition metal, respectively. XRD measurements for the catalysts containing Cu showed the formation of the CuO phase. In the case of the Co-containing materials, the Co_3O_4 phase was formed only for the @SiO_2 support, while for the @TiO_2_Co catalysts, the $CoTiO_3$ phase additionally appeared beside the spinel phase. Similar observations were made based on the results of UV-Vis-DR measurements. The synthesized materials were characterized by high catalytic activity in the process of total oxidation of toluene. Depending on the active phase - support system used, the catalytic properties of the studied materials change. The best activity was achieved over the @TiO_2_Cu and @SiO_2_Co catalysts. A stronger interaction of the cobalt oxide precursor with the @TiO_2 support resulted in the formation of the surface $CoTiO_3$ phase, which is more resistant to reduction than Co_3O_4. In turn, separate particles of Co_3O_4 phase were formed on the @SiO_2 support, which more effectively participate in the reaction according to the Mars–van Krevelen mechanism.

References

1. A. Rokicińska, P. Łątka, B. Olszański, M. Żurowska, M. Dębosz, M. Michalik, P. Kuśtrowski, Chem. Eng. J. 480 (2024) 148173.
2. R. Riva, H. Miessner, R. Vitali, G. Del Piero, Appl. Catal. A Gen. 196 (2000) 111.
3. Z. Li, J. Hou, X. Gu, L. Gao, G. Su, F. Li, J. Mater. Sci. 57 (2022) 4990.

Acknowledgements: We thank the National Science Centre of Poland for financial support in the implementation of research (grant no. 2020/39/D/ST5/02703).

P-11

Wpływ domieszkowania miedzią na właściwości katalityczne szkła potasowego

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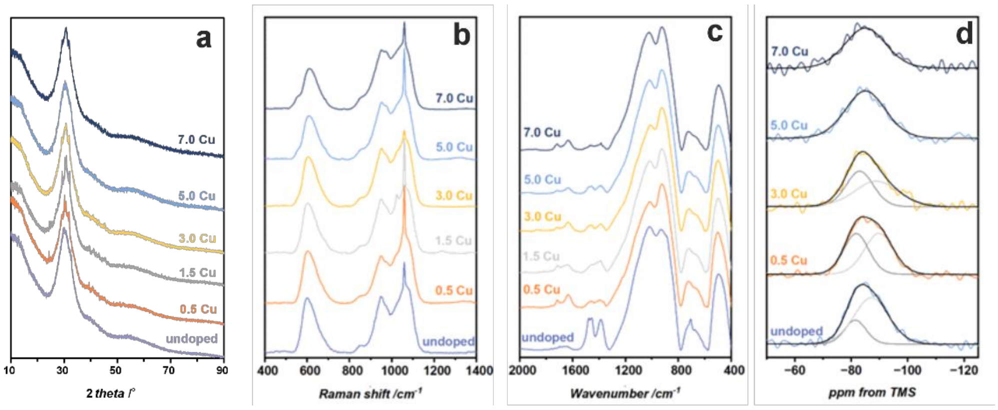
Układy katalityczne oparte na szkłach wykazują szereg pozytywnych cech, takich jak wysoka stabilność termiczna, wytrzymałość mechaniczna, czy obecność centrów katalitycznie aktywnych. Celem niniejszych badań było zbadanie wpływu stężenia miedzi na właściwości strukturalne, powierzchniowe i aktywność katalityczną szkła potasowego.



Rys.1. Dyfraktogramy (a), widma ramanowskie (b), FTIR (c) oraz ^{29}Si MAS-NMR (d) domieszkowanych miedzią szkieł potasowych.

Synteza podstawowego szkła potasowego obejmowała topienie odpowiednich prekursorów (SiO_2, K_2CO_3, $CaCO_3$) w temp. 1345°C przez 1 godzinę. Szkło o składzie molowym 25%K_2O-59%SiO_2-16%CaO było następnie domieszkowane miedzią na poziomie 0-7% *mol.* poprzez przetapianie szkła z CuO. Uzyskane preparaty zostały następnie dogłębnie scharakteryzowane pod kątem strukturalnym i funkcjonalnym. Aktywność katalityczna uzyskanych układów została zbadana w reakcji dopalania sadzy (kontakty ścisły i luźny, w atmosferze 10% O_2 i 0-500ppm NO).

Analiza strukturalna (XRD, RS, FTIR, NMR) potwierdziła amorficzny charakter uzyskanych preparatów (Rys.1). Porównanie składu objętościowego (XRF) i powierzchniowego (XPS) sugeruje, że domieszka miedziowa lokuje się wewnątrz struktury. Techniki takie jak XAS, XPS oraz UV/Vis-DR pozwoliły stwierdzić, że miedź występuje zarówno na +1, jak i +2 stopniu utlenienia, udziały obu form zmieniają się wraz ze stężeniem domieszki, przy czym nie jest to zmiana monotoniczna. Obserwowana aktywność w dopalaniu sadzy była wysoka (T_{50} w przedziale 350-380°C w przypadku kontaktu ścisłego i 440-500°C w przypadku luźnego) i również wykazywała niemonotoniczne zmiany w funkcji stężenia miedzi, co sugeruje, że udział form miedzi jest jednym z czynników warunkujących aktywność.

Podziękowania: Niniejsza praca została sfinansowana ze środków Priorytetowego Obszaru Badawczego Anthropocene w ramach programu „Inicjatywa Doskonałości – Uczelnia Badawcza" w Uniwersytecie Jagiellońskim.

P-12

Charakterystyka strukturalna i teksturalna układów modelowych zawierających ZnO osadzony na Al_2O_3 i cenosferach z popiołów lotnych jako nośnikach

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Lity, osadzony na nośnikach i modyfikowany tlenek cynku jest wykorzystywany w katalizie heterogenicznej m.in. jako materiał wykazujący aktywność w procesach waloryzacji CO_2 do produktów o szerokim znaczeniu komercyjnym takich jak metanol czy biodiesel, do usuwania zanieczyszczeń wód substancjami organicznymi poprzez ich degradację fotokatalityczną czy też do syntezy istotnych aplikacyjnie związków heterocyklicznych. W niniejszej pracy podjęto badania nad układami modelowymi, zawierającymi ZnO osadzony na dwóch różnych nośnikach: γ-Al_2O_3 oraz cenosferach, będących frakcją popiołów lotnych generowanych podczas spalania konwencjonalnych paliw stałych. Nominalne stężenia fazy naniesionej odpowiadały zawartości 0,5-10%$_{mol}$ ZnO względem γ-Al_2O_3. Badane próbki zostały otrzymane metodą mokrej impregnacji a następnie kalcynowane w temp. 400°C przez 1h. Uzyskane próbki poddano charakterystyce metodami takimi jak XRD, RS, UV/Vis-DR, SEM, BET.

Wyniki dyfrakcyjne potwierdziły stabilizację krystalitów ZnO (3D) na cenosferach w szerokim zakresie stężeń. Przy tym intensywność maksimów charakterystycznych dla nanokrystalitów ZnO widocznych w dyfraktogramach proporcjonalnie wzrastała ze wzrostem stężenia nominalnego fazy naniesionej. Jednocześnie, dla wysokich stężeń powyżej 3%$_{mol}$ spektroskopia Ramana wykazała wyraźną heterogeniczność geometryczną ZnO na powierzchni cenosfer. Z kolei, na powierzchni γ-Al_2O_3 obecność krystalitów ZnO (3D) została potwierdzona wyłącznie dla próbki o najwyższej zawartości ZnO, co świadczy o lepszej zwilżalności powierzchni tlenku glinu przez fazę naniesioną w porównaniu z powierzchnią cenosfer. Podobne zróżnicowanie zależne od rodzaju użytego nośnika potwierdzono w odniesieniu do właściwości teksturalnych badanych próbek.

Opisane różnice w strukturze próbek ZnO_x/nośnik i specjacji fazy naniesionej manifestują się także w ich właściwościach funkcjonalnych, decydujących o parametrach katalitycznych. Uzyskane wyniki pozwoliły lepiej zrozumieć rolę nośnika i stężenia fazy naniesionej dla architektury powierzchniowej ZnO na powierzchni γ-Al_2O_3 i cenosfer.

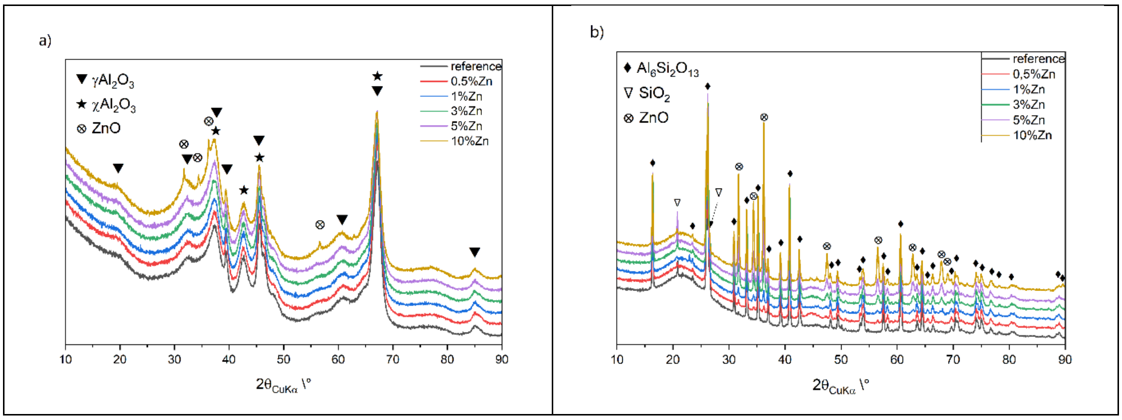

Fig. Dyfraktogramy serii ZnO na nośnikach Al_2O_3 a) oraz cenosferach b).

Podziękowania: Realizowane badania zostały dofinansowane ze środków *POB Anthropocene (PF Man-Mind-Environment Hub) w ramach Programu Strategicznego Inicjatywa Doskonałości w Uniwersytecie Jagiellońskim.*

P-13

Utleniające odwodornienie propanu na katalizatorach na osnowie zeolitów

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Enzymy są naturalnymi katalizatorami ważnych procesów biochemicznych w organizmach żywych. Zazwyczaj zawierają one pojedyncze centra metaliczne, ale znane są również takie, w których znajdują się dwa jony metali położone blisko siebie. Enzymy posiadające dwuatomowe miejsca aktywne są odpowiedzialne za różnorodne procesy chemiczne, takie jak m.in. utlenianie metanu. Przykładem jest np. monooksygenaza metanowa, która w postaci cząstek zawiera dwa jony miedzi w centrum aktywnym lub w przypadku rozpuszczalnej monooksygenazy metanowej zawierającej dwa jony żelaza w centrum aktywnym.

Naszym celem było zbadanie reaktywności dwuatomowych centrów metalicznych wprowadzonych do matryc zeolitowych jako nieorganicznych analogów miejsc aktywnych występujących w enzymach. Równolegle do badań na układach zeolitowych skonstruowano modele teoretyczne centrów dwuatomowych ($[TMI(Por)]_2$, gdzie TMI = Fe, Mn, Co, Ni; Por = ligand porfirynowy), które posłużyły za modele do badania takich czynników jak rodzaj metalu, stopień utlenienia, odległość TMI-TMI i ich wzajemne ułożenie.

Wykazaliśmy, że dwuatomowe centra metali przejściowych wprowadzone do matryc zeolitowych mogą nie tylko aktywować małe cząsteczki (O_2, N_2O) i generować z nich tzw. ugrupowania tlenu α, ale i utleniać lekkie węglowodory [1]. Nasze badania pokazują przewagę układów zeolitowych z wprowadzonymi centrami dwuatomowymi nad tymi, gdzie jony metali są izolowane (nie tworzą par), w procesach utleniania propanu: w niskiej temperaturze te pierwsze wykazują znacznie większą aktywność. Wykazaliśmy również, że dwuatomowe centra żelazowe posiadają zdolność do aktywacji i rozszczepienia cząsteczki O_2 niezależnie od charakteru „matrycy” (zeolit, porfiryna) [2].

References

1. A. Kornas, E. Tabor, D. K. Wierzbicki, J. E. Olszowka, R. Pilar, J. Dedecek, M. Sliwa, H. Jirglova, S. Sklenak, D. Rutkowska-Zbik, K. Mlekodaj, Applied Catalysis B: Environmental 336 (2023) 122915
2. A. Drzewiecka-Matuszek, J. Dedecek, D. Rutkowska-Zbik, Catal. Today, submitted.

Podziękowania: Badania zostały wykonane w ramach projektu OPUS-LAP finansowanego przez Narodowe Centrum Nauki nr 2020/39/I/St4/02559.

P-14

Właściwości spektroskopowe wybranych pochodnych MIL-68 w kontekście zastosowań w fotokatalizie: obliczenia DFT

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Sieci metalo-organiczne (ang. metal-organic framework, MOF) to klasa materiałów, których strukturę stanowi sieć kationów lub klastrów metali połączonych cząsteczkami organicznymi. Dzięki dobrze rozwiniętej powierzchni oraz wewnętrznej strukturze porów są często badane pod kątem zastosowań jako sorbenty, nośniki substancji aktywnych (np. leków), lub też katalizatory. Wykorzystanie MOFów w katalizie obejmuje zarówno procesy katalizy „termicznej", jak również elektro- i fotokatalizy.

Celem niniejszych badań jest określenie właściwości spektroskopowych wybranych pochodnych MOFu MIL-68 w kontekście możliwości ich użycia jako fotokatalizatorów do konwersji CO_2. MIL-68 jest układem, w którym nano-wstęgi indowo-tlenowe połączone są cząsteczkami anionami kwasu tereftalowego (patrz Rysunek 1). Badane modyfikacje obejmują pochodne kwasu tereftalowego, w których do pierścienia fenolowego wprowadzono następujące podstawniki: NH_2, NO_2, Br, OH.

Dla badanych układów wykonano obliczenia w formalizmie DFT i TD-DFT, wykorzystując funkcjonał B3LYP, stosując dla lekkich atomów bazy funkcyjne 6-31g(d,p), dla In zaś pseudopotencjały LanLDZ. Do obliczeń użyto program Gaussian 09.

Wyznaczono geometrię badanych układów i porównano z dostępnymi danymi z dyfrakcji promieni x. Scharakteryzowano ich strukturę elektronową – obliczono rozkład ładunków na poszczególnych atomach oraz wykreślono kontury orbitali granicznych. Obliczenia teoretyczne TD-DFT pozwoliły na porównanie z doświadczalnymi widmami UV-VIS i umożliwiły charakterystykę obserwowanych przejść elektronowych. Wysunięte wnioski pozwoliły na wyjaśnienie aktywności pochodnych MIL-68 w procesie aktywacji CO_2 pod wpływem absorpcji promieniowania.

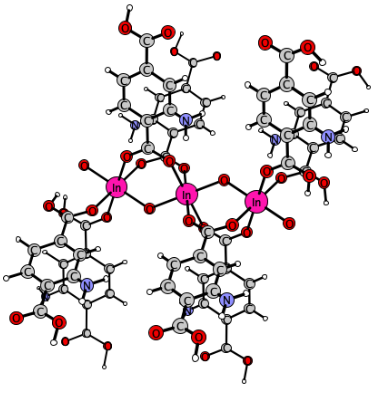

Fig. 1. Struktura MIL-68.

Podziękowania: Badania zostały wykonane w ramach projektu OPUS finansowanego przez Narodowe Centrum Nauki nr UMO-2021/43/B/ST4/02969.

P-15

Single-Site Pd Innovation: Redefining Hydrogen Generation Efficiency Compared to Pt

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Photocatalytic hydrogen production has emerged as an appealing subject for delivering clean alternative energy, which will alleviate the future energy demands. However, rapid photogenerated charge recombination substantially reduces hydrogen efficiency. The use of single atoms as co-catalysts has emerged as an efficient method to improve photocatalytic performance by introducing active sites and boosting charge separation.

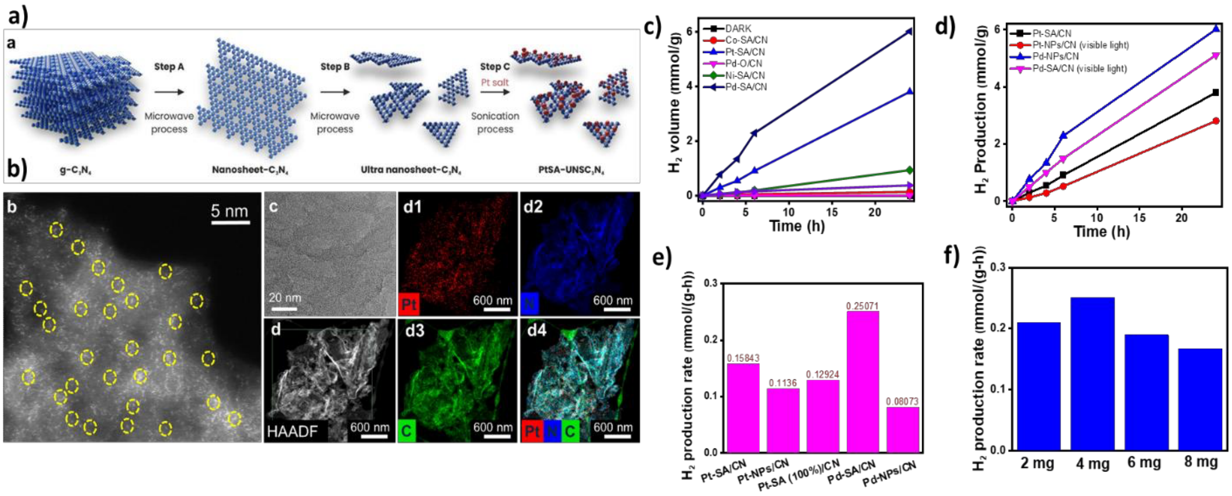

Fig. 1. Photocatalytic H_2 production performance of different Single atoms decorated g-C_3N_4 nanosheets under simulated sun light illumination.

Classic experimental volcano plots support theoretical assumptions that Pt is the most efficient co-catalyst for H_2 evolution, both in electrocatalysis and in photocatalysis. In the present study, we study the ability of four distinct metal co-catalysts (Pd, Pt, Co, and Ni) decorated as single atoms on traditional graphitic carbon nitride[1]. We assess the photocatalytic H_2 production rate and compare it to the conventional nanoparticle co-catalysts on the nanosheets after anchoring identical loadings of single Pd, Pt, Co and Ni atoms[2]. The decorated **Pd single atoms on g-C_3N_4 (6.01 mmol g^{-1})** showed excellent photocatalytic H_2 production, which is 1.58, 6.44 and 43.88 times higher than that of Pt-SA/CN (3.8 mmol g^{-1}), Ni-SA/CN (0.93 mmol g^{-1}) and Co-SA/CN (0.137 mmol g^{-1}) photocatalysts respectively. While nanoparticles yield the well-established hydrogen evolution reaction activity sequence (Pt > Pd), for the single atom form, **Pd radically outperforms Pt, Ni and Co. This research sheds new light on the design of single-atom catalysts**.

References.

1 G. Vilé, P. Sharma, M. Nachtegaal, F. Tollini, D. Moscatelli, A. Sroka-Bartnicka, O. Tomanec, M. Petr, J. Filip, I. S. Pieta, R. Zbořil and M. B. Gawande, *Sol. RRL*, 2021, **5**, 2100176.
2 V. Jeyalakshmi, S. Wu, S. Qin, X. Zhou, B. B. Sarma, D. E. Doronkin, J. Kolařík, M. Šoóš and P. Schmuki, *Chem. Sci.*, 2025, **16**, 4788–4795.

Acknowledgements: P.S. thanks National Science Foundation for UMO-2022/47/P/ST4/03412 to the research project No. 2022/47/P/ST4/03412.

P-16

Tailoring Chemical Reactions: Regioselective Catalysis with Platinum SAC Innovation

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Selective diboration and hydroboration of alkenes face significant challenges, including achieving high regioselectivity, functional group tolerance, and catalyst stability under mild conditions. These challenges are nearly exclusively addressed and investigated with the use of homogenous catalysts.

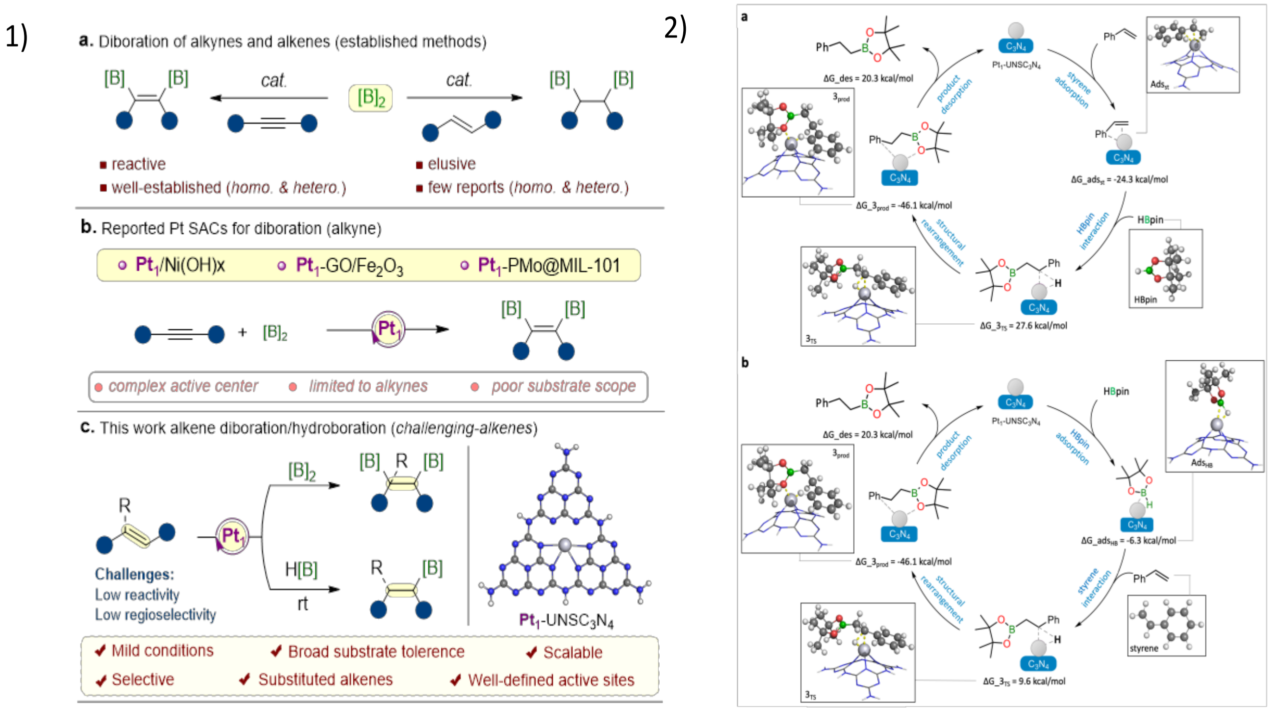

Fig. 1. a) Schematic representation of diboration of alkynes and alkenes, (b) previously utilized Pt SACs for alkyne diboration, and (c) our innovative approach for the diboration of substituted olefins and the hydroboration of olefins using Pt SACs.

At the same time, Pt-SAC was highly efficient in the hydroboration of alkenes using pinacolborane as the hydroboration reagent producing mono-borylated alkylboranes and achieving exceptional selectivity towards anti-Markovnikov products (99%). Similarly, the catalyst enables selective hydroboration of alkynes, successfully synthesizing vinylboranes, essential building blocks in organic synthesis, even at room temperature.

References.

1 G. Vilé, P. Sharma, M. Nachtegaal, F. Tollini, D. Moscatelli, A. Sroka-Bartnicka, O. Tomanec, M. Petr, J. Filip, I. S. Pieta, R. Zbořil and M. B. Gawande, *Sol. RRL*, 2021, **5**, 2100176.

2 V. Jeyalakshmi, S. Wu, S. Qin, X. Zhou, B. B. Sarma, D. E. Doronkin, J. Kolařík, M. Šoóš and P. Schmuki, *Chem. Sci.*, 2025, **16**, 4788–4795.

Acknowledgements: P.S. thanks National Science Foundation for UMO-2022/47/P/ST4/03412 to the research project No. 2022/47/P/ST4/03412.

P-17

Pre-testing of candidates for work in CO_2 methanation reactor

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The CO_2 methanation process, also known as the Sabatier reaction, has been known since the early 20th century as a catalyst-driven conversion of CO_2 to CH_4. The process has applications including the purification of the gas stream used for ammonia synthesis and the purification of hydrogen for fuel cells. Currently, the process is gaining importance for converting larger amounts of CO_2 to synthetic natural gas in power–to–gas plants [1]. In industry, nickel catalysts deposited on alumina are typically used for CO_2 methanation due to their high selectivity to methane and relatively low cost.

The goal of the project conducted at the Warsaw University of Technology is to integrate two key innovations: carbonate fuel cells for CO_2 separation and a Sabatier reactor for obtaining methane. Preliminary work includes preparation and wide characterization of nickel contacts supported on oxide materials. The commercial catalyst RANG 19 (INS Puławy) was also tested. The research aim is to select the best candidate to efficiently convert captured CO_2 into methane.

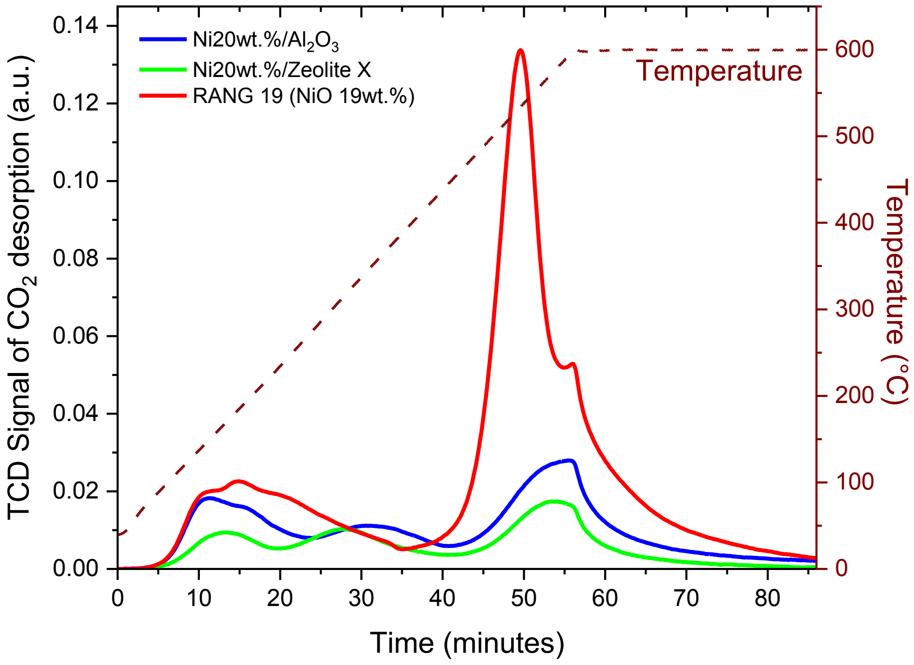

Fig. 1. CO_2-TPD profiles of Ni catalysts

References:

[1] J. Gorre, F. Ortloff, C. van Leeuwen, Appl Energy 253 (2019) 113594

Acknowledgements: Research was funded by POB Energy of Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme.

P-18

Acetic acid and methanol from CO_2 and CH_4: the case of Cu-FER catalyst

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The effective catalytic transformation of greenhouse gases such as carbon dioxide and methane into valuable products is one of the urgent needs to be processed over the past few decades. Active copper sites in zeolites are essential for the catalytic conversion of CH_4 and CO_2; nevertheless, the influence of the active site characteristics on the transformation pathways is not yet fully understood.

The presented study highlights the efficiency of Cu-FER catalysts with varying copper loadings in CO_2 and CH_4 transformation into value-added products, namely methanol or acetic acid.

The Cu-FER samples (Cu-FER-L of Cu/Al 0.06 and Cu-FER-H of Cu/Al 0.24) were prepared by a Cu-ion-exchange reaction from parent NH_4-FER, then calcined. Comprehensive analyses using XAS, UV-Vis spectroscopy, FTIR, and combined *in-situ* FTIR/Mass spectrometry measurements were performed to investigate the nature of copper sites and their role in CH_4 and CO_2 reaction.

In both Cu-FER-L and Cu-FER-H zeolites, copper is observed as Cu(II). Depending on copper content, the presence of a high fraction of isolated Cu^{2+} cations or a significant presence of Cu oxo-species in Cu-FER catalysts takes place. In the case of Cu-FER-H sample, the low population of Brønsted acid sites was observed due to the extensive ion exchange for copper. The copresence of copper(II) species and protonic acidity appears to be crucial for catalytic performance.

Low-loaded Cu-FER-L sample containing bare Cu(II) cations, in synergy with Brønsted acid sites, promotes the conversion of CO_2 and CH_4 into CH_3COOH. On the other hand, the absence of Brønsted acid sites and the dominance of Cu oxo-species in Cu-FER-H sample leads to the CO_2 and CH_4 transformation into CH_3OH. It is important to note that such production of methanol or acetic acid can be effectively provided at temperatures below 300°C opens up an opportunity to tailor proposed Cu-FER zeolite-based catalysts for the efficient utilization of CO_2 and CH_4 in an environmentally friendly mode.

Acknowledgements: The authors acknowledge the financial support provided by the National Science Centre, Poland (2022/47/I/ST4/00607).

P-19

Catalytic properties of Keggin type heteropolyacid supported on the modified boron nitride

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Boron nitride was used for the first time as a support of active phase in the Ba–Ru/BN catalyst for ammonia synthesis in 2001 [1], whereas as a support for $H_3PW_{12}O_{40}$ (HPW) heteropolyacid in methanol conversion in 2017 [2]. In this study we focus on the modification of hexagonal BN support by low temperature oxygen plasma to enhance the catalytic properties of HPW/BN materials. After the thorough physicochemical analysis (XRD, SEM, NMR, FTIR) of HPW/BN samples all catalysts were tested in gas-phase n-butanol conversion at the temperature range 90 – 230°C (Fig.1).

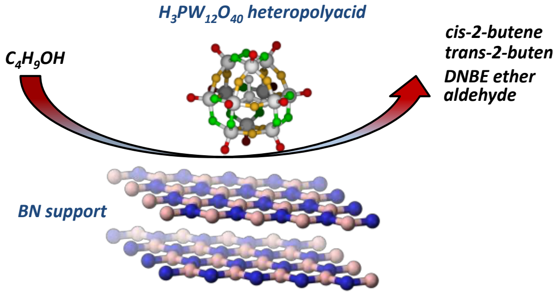

Fig. 1. Graphical scheme of the investigated catalytic system

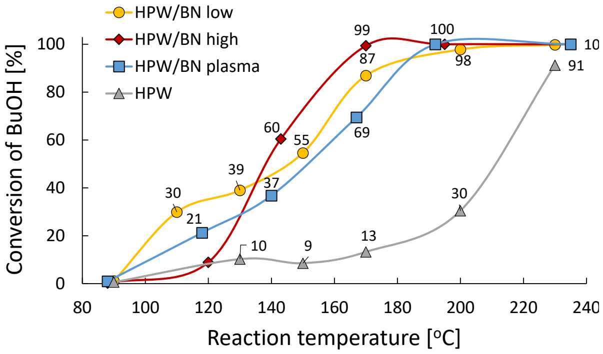

Fig. 2. Conversion of n-butanol vs. reaction temperature over unsupported HPW and supported HPW/BN

A series of HPW/BN obtained by the impregnation of BN supports by 10 %wt. HPW heteropolyacid differ in specific surface area (HPW/BN-low, S= 9 m^2/g, HPW/BN-high, S=30 m^2/g, HPW/BN-plasma, S=27 m^2/g), showed significantly higher n-butanol dehydration compare to the unsupported HPW (Fig. 2). The total alcohol decomposition over HPW/BN-high sample was reached about 170 °C whereas for pure HPW at 230 °C. The main product of n-butanol conversion was cis-2-butene. Selectivity to the particular products follows the order: cis-2-butene >> trans-2-butene > DNBE> butylaldehyde.

References

1. C.J.H. Jacobsen, J. Catal. 200 (2001) 1.
2. J. Schnee, A. Eggermont, E.M. Gaigneaux, ACS Catal. 7 (2017) 4011.

P-20

Enzymatic bioassay for detection of reactive aldehydes in blood stream – the application of tungsten aldehyde oxidoreductase

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Reactive aldehydes, such as 4-HNE (4-hydroxynonenal), 4-ONE (4-oxo-2-nonena), 4-HHE (4-hydroxyhexenal), are increasingly recognized as pivotal biomarkers of oxidative stress, particularly in conditions such as diabetic nephropathy [1]. While traditional analytical methods like LC-MS provide excellent sensitivity, their high cost, complexity, and lengthy processing times limit routine clinical application. In response, our research aim is to develop an electrochemical biosensor that leverages the unique properties of tungsten-dependent aldehyde oxidoreductase (AOR) from *Aromatoleum evansii* for rapid and cost-effective detection of reactive aldehydes.

Tungsten-dependent AOR distinguishes itself from conventional NAD-dependent oxidoreductases by operating at lower redox potentials and exhibiting reversible redox behaviour - traits that are ideally suited for efficient electrochemical transduction. Electrochemical sensors harness AOR to oxidize aldehydes to acids. Electrons are transferred via a mediator to the electrode, where the mediator is reoxidized. This efficient process at minimal overpotential enhances both sensor sensitivity and selectivity [2].

In our preliminary investigations, we cultured *Aromatoleum evansii,* genetically modified to express AOR [3], in two 5 L-bioreactors. During cultivation, we monitored nitrate levels, optical density and redox potential. Post-cultivation, the bacterial cultures were cryopreserved and subsequently analysed through activity assays conducted under both aerobic and anaerobic conditions. We compared enzyme activity using NAD^+ with assays using artificial electron acceptors i.e., dichlorophenol indophenol (DCPIP) and methylene blue. The enzyme activity was tested within the physiological range of pH (7.0-8.0) indicating pH 8.0 as the optimal for the activity. As a proof-of-concept, the activity with 9-hydroxynonanal was confirmed with UV-vis-based assay and LC-MS. The enzyme exhibited a linear response of its activity to substrate concentration in the range of 0.050 – 0.5 mM 4-HNE.

Based on previous successful demonstration of the use of AOR in an electrochemical system for the detection of a wide range of aldehydes [2] our preliminary results provide a sound basis for further development of both AOR-based UV-vis assay and electrochemical biosensor for aldehyde biomarkers in blood plasma, thereby offering a transformative approach for clinical screening of reactive aldehydes as markers of diabetic nephropathy and other oxidative stress-related diseases.

References

1. C. Harkin, D. Cobice, J. Watt, M. J. Kurth, S. Brockbank, S. Bolton, F. Johnston, A. Strzelecka, J. V. Lamont, T. Moore, P. Fitzgerald, and M. W. Ruddock, Front. Nutr. 9 (2023) 997015
2 P. Kalimuthu, D. Hege, A. Winiarska, Y. Gemmecker, M. Szaleniec, J. Heider, and P. V. Bernhardt, Chem. Eur. J. 29 (2023) e202203072
3. A. Winiarska, D. Hege, Y. Gemmecker, J. Kryściak-Czerwenka, A. Seubert, J. Heider, and M. Szaleniec, ACS Catal. 12 (2022) 8707−8717

Acknowledgements: We acknowledge the financial support of the National Science Centre Poland grant OPUS 2023/51/B/ST4/01224.

P-21

Metallo-porphyrin electrocatalytic solution for high performance Li-S Batteries

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Lithium-sulfur (Li-S) batteries with a promising and remarkable theoretical energy density of 2600 Wh kg^{-1} are seen as a desirable choice for future energy storage [1]. However, the multiphase sulfur redox reaction is challenging [2]. Herein, the organic framework-based electrocatalytic polymer composite, incorporating zinc-zinc(II) 5,10,15,20-tetrakis-(2,2'-bithien-5-yl)porphyrin (Zn-Por) sites to polybisthiophene (PBTh) linkers on carbon nanotubes (CNTs) surface, significantly enhances the sulfur redox reaction kinetics. The ZnPor-PBTh/CNTs electrocatalyst was characterized by SEM, EDAX, XPS, and FTIR, confirming its composition and structure. In the Li-S coin cell, electrochemical studies (CV,EIS, GCD) of ZnPor-PBTh/CNTs as cathode and Li as anode, demonstrated high capacity (1390.2 mAh/g), low charge transfer resistance (45 Ω), stable cycling performance with reduced polarization and suppressed polysulfide shuttling.

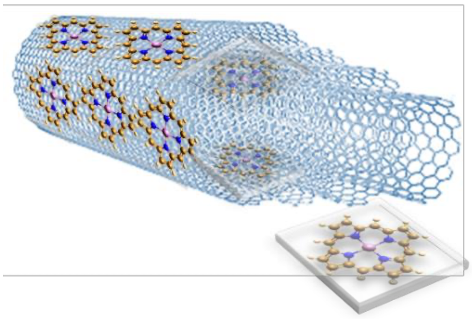

Fig. 1. Carbon nanotubes functionalized with Zn-Por sites linked by PBTh.

References

1. BQ Li, HJ Peng. 1 (2019) 128

2. CX Zhao, XY Li. 143 (2021) 19865

Acknowledgment

The financial support from the National Science Centre, Poland in the form of grant OPUS 24 Project No. 2022/47/B/ST5/03077 is acknowledged.

P-22

Dendrimer-Based Nanocarriers for Delivery of 5-fluorouracil or Doxorubicin

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Nanoparticle-based drug delivery systems offer a promising alternative to conventional cancer treatments. Poly(amidoamine) (PAMAM) dendrimers are characterized by monodispersity and high stability in aqueous solution. Their multifunctional structure allows the binding of active molecules in two ways, by encapsulation in internal spaces as well as immobilization on the surface. The physicochemical characterization of PAMAM dendrimers in their application as nanocarriers for selected anticancer drugs (5-fluorouracil, doxorubicin) is presented.

Analytical and theoretical methods were used to evaluate dendrimer-drug complexes, assessing size, surface charge, accumulation efficiency, and drug localization. Accumulation in PAMAM dendrimers increased with the drug's deprotonation while controlling carrier ionization. Process optimization revealed that alkaline conditions favor efficient binding, achieving loading capacities of 18.0% for G4.0 PAMAM-5FU and 39.2% for G4.0 PAMAM-DOX [1,2]. The drugs exhibited different affinities and localizations due to their chemical properties: doxorubicin interacts via hydrophobic and electrostatic forces, while 5-fluorouracil interacts electrostatically with amine groups present in the dendrimer structure. The way the drugs are immobilized in the PAMAM structure directly impacts the drug release mechanism from the nanocarriers. Additionally, complementary QCM-D and MP-SPR techniques confirmed the successful functionalization of the gold surface with PAMAM dendrimers. The resulting dendrimer monolayer holds potential as a biosensor for detecting and analyzing the kinetics of interactions with doxorubicin [3,4].

In vitro studies demonstrated that G4.0 PAMAM-5FU complex reduced cell viability, with increased selectivity for glioma (SNB-19), while G4.0 PAMAM-DOX complex specifically targeted malignant melanoma (A375) and lung cancer (NCI-H23) [1,3]. The findings have confirmed that optimizing dendrimer-based drug delivery systems enhances efficacy and selectivity against cancer cells.

References

[1] M. Szota, K. Reczyńska-Kolman, E. Pamuła, O. Michel, J. Kulbacka, B. Jachimska, Int. J. Mol. Sci. 2021, 22(20), 11167
[2] M. Szota and B. Jachimska, Pharmaceutics 2023, 15(3), 875
[3] M. Szota, U. Szwedowicz, N. Rembiałkowska, A. Janicka-Kłos, D. Doveiko, Y. Chen, J. Kulbacka, B. Jachimska, Int. J. Mol. Sci. 2024, 25(13), 7201
[4] B. Jachimska, M. Goncerz, P. Wolski, C. Meldrum, Ł. Luśtyk, T. Pańczyk, Mol. Pharmaceutics 2024, 21, 11, 5892–5904

Acknowledgements: This work was supported by project NCN OPUS 2021/41/B/ST5/02233.

P-23

Biological activity of dendrimer nanocarriers with 5-fluorouracil

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The success of novel therapeutic strategies relies strongly on the development of a reliable active agent delivery mechanism. There is a growing interest in drug delivery systems (DDS) because they provide targeted drug delivery, enhance drug efficacy, minimize drug loss, and reduce potential side effects. Despite the constant development of research in biomedicine, there remains a low number of systematic studies on hybrid systems from a molecular perspective. Dendrimers are extensively studied prototypes for biomedical usage, especially as carriers of anticancer drugs. They have highly branched, regular, and well-defined structures that are highly controlled over the synthesis method. PAMAM dendrimers display pH-dependent drug release behavior. At high pH, the dendrimer's tertiary amines are deprotonated, leading to the collapse of the molecule. Conversely, at acidic pH, the tertiary amine groups are protonated, resulting in the molecule swelling. This dendrimer behavior is fundamental for its application as a drug carrier in targeted delivery to tumor tissues with an acidic microenvironment. Since the primary problem with many drugs is their low water solubility, dendrimers were designed to have water-soluble terminal groups and hydrophobic interiors, which facilitates the encapsulation of hydrophobic drugs.

The zeta potential measurement was used to assess the effectiveness of dendrimer interaction with 5FU and to determine the number of drug molecules immobilized within the dendrimer structure. The significant changes to the surface potential of G4 PAMAM dendrimers confirm the presence of 5-fluorouracil molecules attached to the dendrimer surface, which, together with the UV-Vis experiment, suggests that both internal and external drug molecules are bound. The optimal conditions for the formation of the complex were confirmed using fluorescence spectroscopy, NMR, FTIR, and QCM-D methods.

The effectiveness of ligands binding to the dendrimer structure depends strictly on the complex formation conditions, including molar ratio, ionic strength, pH, and dendrimer generation. The fact that drug molecules bind most effectively under alkaline conditions when the dendrimer is close to its isoelectric point indicates a more significant influence of the ligand charge, which occurs in a deprotonated form. Studies have confirmed the system's ability to attach approximately 20 5FU molecules per dendrimer molecule for the fourth-generation dendrimer.

Acknowledgments: This work was supported by project NCN OPUS 2021/41/B/ST5/02233.

P-24

Comparison of conformational stability of lysozyme adsorbed on a hard and soft surface

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The conformational stability of protein layers at the solid-liquid interface is crucial for maintaining the protein's biological activity and understanding the interaction of adsorbed protein with lipid membranes. Changes in protein structure can lead to many diseases, including neurodegenerative diseases. This study investigated lysozyme adsorption on two different surfaces: a rigid gold substrate and a soft layer of POPC/POPS liposomes. A quartz crystal microbalance with dissipation monitoring and multi-parametric surface plasmon resonance were applied to determine the efficiency of lysozyme adsorption, hydration, and thickness of the adsorbed protein layer at different pH conditions. Results from both methods showed that lysozyme adsorption on the gold surface was more efficient at pH 4.0 than 7.4. The effectiveness of lysozyme adsorption on the liposome surface was similar at both pH conditions. The affinity of lysozyme molecules to the liposome surface was higher than to the gold at both pH conditions. The content of lysozyme's secondary structure components was evaluated by FT-IR spectral analysis and deconvolution of the Amide I band. The results showed that lysozyme interacts with a gold and liposome surface differently, even if the charge of protein and substrate is similar under the given pH conditions. We found differences in the lysozyme secondary structure composition, which may suggest that the participation of individual structures in the interaction with the surface is different depending on the surface type.

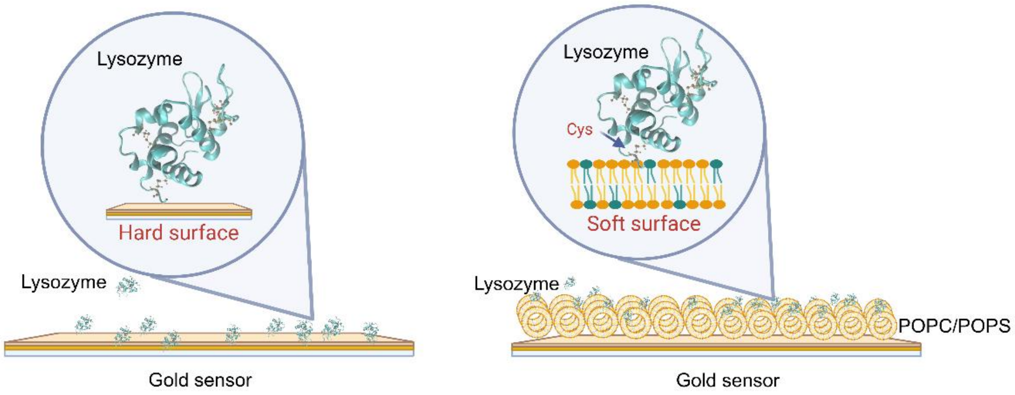

Fig. 1. Scheme of lysozyme's adsorption on the gold surface and lipid membrane.

Acknowledgments: This work was supported by project NCN OPUS 2021/41/B/ST5/02233.

P-25

Metal−Organic Frameworks As Efficient Tools For Future Drug Detox

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The growing number of acute drug abuse overdoses demands the development of novel detoxification strategies for emergency purposes [1]. In the undertaken research, we present the application of porous Zr-based metal−organic frameworks (Zr-MOFs) with NU-1000, MOF-808 and UiO-66 structures as an efficient tool against the acute overdoses of popular drugs, such as amphetamine (AMP), methamphetamine (mAMP), cocaine (COC), and 3,4-methylenedioxymethamphetamine also known as ”ecstasy” (MDMA). The efficacy of drug removal using Zr-MOFs was determined taking into account drug dosage and adsorption time. The selected model Zr-MOFs indicated impressive efficiency in drug removal. In the case of NU-1000, the adsorption of AMP reached 90% and 100% from water and simulated nasal fluid (SNF) solution, respectively. Additionally, the high adsorption efficiency of NU-1000 was evidenced in a multidrug adsorption experiment, where overall MDMA and COC removal was equal to 90% and 100%, respectively. The efficient adsorption of considered drugs of abuse was confirmed by Raman differential spectroscopy (RDS) and by DFT vibrational analysis.
The biological experiments (including cardiotoxicity and neurotoxicity) indicated low cytotoxicity of the prepared Zr-MOFs, showing their potential application for living organisms.
The proposed concept of the application of Zr-MOFs opens new horizons in the development of novel drug removal systems, which could be used on-site by non-specialists in emergencies.

References

1. L.F. Liu, J.X. Li, Acta Pharmacol. Sin. 39 (2018) 1823.

Acknowledgements: The work was supported by the National Science Centre, Poland, under the research project ”MOF-antidote: Novel detoxification materials based on metal−organic frameworks for drugs of abuse removal - synthesis, chemical characterization, toxicity, and efficacy in vivo and in vitro studies”, no. UMO-2021/43/B/NZ7/00827. Graphical TOC was partially created with BioRender.com. We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Center: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2024/017158. The XRF experiments were carried out with the equipment purchased thanks to the financial support of the European Regional Development Fund within the framework of the Polish Innovation Economy Operational Program (contract number POIG.02.01.00-12-023/08.1.).

P-26

The photoreactor ReactoReQ

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The photoreactor from the IPC PAS consists of a glass vessel with threaded neck, placed inside a metal housing that provides isolation from external light and facilitates the removal of any heat that may be released. The design of the set ensures linearity of the light source relative to the reactor and control over the immersion of the optical fiber inside the reaction mixture.

This reactor can be used for chemical reactions in gas, liquid, suspension and on films. The proper connectors ensure tightness even for hydrogen generation.
Photocatalytic test reaction in batch system with possible analysis of gas phase above liquid, suspension or films.

Dedicated holder for solid tile with film can be used. The set is designed for use in scientific laboratories and educational institutions.

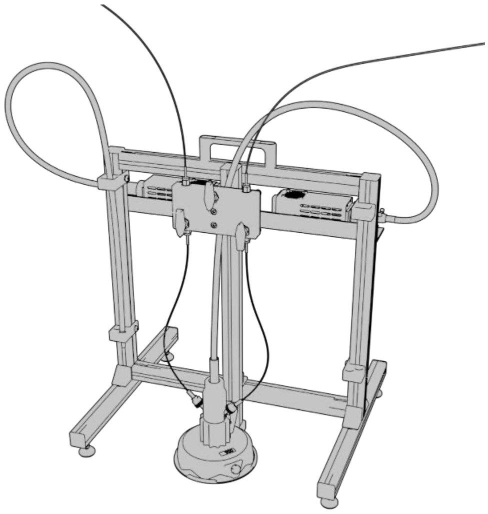

Fig. 1. Photoreactor ReactoReQ

Features:
- aligned light with the reactor,
- controlled light intensity,
- magnetic stirring,
- easier heat dissipation,
- protection against external light,
- tight volume with flowing or static gas,
- ability of using films on solids,
- versatility of use.

www: https://photo-catalysis.org/

P-27

Characteristics of the surface of anode material modified to limit carbon deposition during SOFC cell operation

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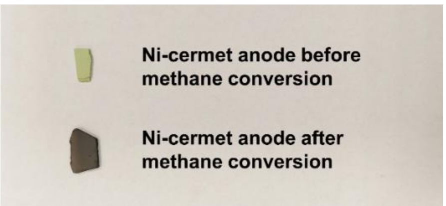
Solid Oxide Fuel Cells (SOFC) are one type of high-temperature fuel cells. These devices are constantly the subject of many scientific studies leading to obtaining the best possible parameters of their operation. It is common knowledge that fuel cells operate with high efficiency, but commonly used materials and technologies constantly require improvement and development. SOFC cells operate at high temperatures (600 - 1000 ^{o}C), which increases the efficiency of these devices, but at the same time limits the availability of materials used for their construction. One of the main advantages of SOFCs is the ability to power them with various fuels, which is why many companies are interested in implementing them in the energy industry. Ni-cermet based anodes are the most widely used anode materials in SOFCs due to their excellent electrochemical catalytic activity in the fuel oxidation reaction, high electrical conductivity, good stability and relatively low cost. In methane-fuelled SOFCs, internal fuel conversion is possible, which significantly simplifies the design of the device, but at the same time, causes the anode material to be exposed to contamination by carbon deposited during the conversion reaction. For SOFC technology, the choice of anode material is crucial. It is necessary to develop new anode materials that ensure efficient and stable operation of the SOFC cell powered by syngas. It is very difficult to develop a suitable anode material. Such an electrode should be active for supplied gases and well conductive for oxide ions and electrons because there where electrochemical reactions take place. In addition, there should be a visible porous microstructure that facilitates rapid gas transport. Anode materials must be stable and resistant to poisoning of their surface by the forming carbon.



The use of a nanocoating made of cathode material and applied to the anode material is an effective way to prevent its degradation. This is one example of the use of thin films applied to the anode as a form of its modification. Thin layers was made of composite materials such as: $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_3$ and $La_{0.6}Sr_{0.4}Co_{0.2-x}Ir_xFe_{0.8}O_3$, as well as $La_{0.6}Sr_{0.4}Co_{0.2-x}Ba_xFe_{0.8}O_3$, $La_{0.6}Sr_{0.4}Co_{0.2-x}Bi_xFe_{0.8}O_3$, $La_{0.6}Sr_{0.4}Co_{0.2-x}Ca_xFe_{0.8}O_3$, $La_{0.6}Sr_{0.4}Co_{0.2-x}Mn_xFe_{0.8}O_3$. The aim of this work is to study the structural properties of modified anode materials using the following techniques: SEM, EDS, BET, XRD, EIS impedance spectroscopy and catalytic tests. The results of these studies will allow for the design of optimal anode materials that meet the requirements for preventing degradation of anode materials during the operation of a SOFC cell powered directly by methane.

P-28

RGBChem: Image-like Representation of Chemical Compounds for Properties Prediction

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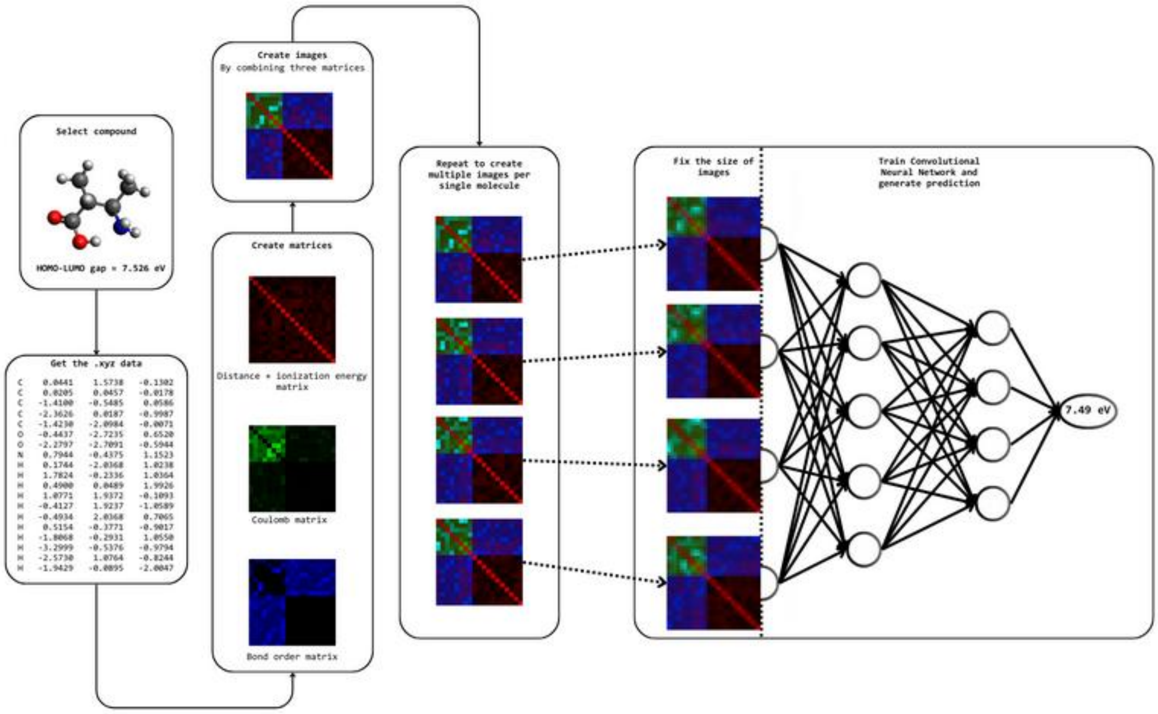
RGBChem is a novel approach for converting chemical compounds into image representations, which are subsequently used to train a convolutional neural network (CNN) to predict the HOMO-LUMO gap for compounds from the QM9 database. By modifying the arbitrary order of atoms present in .xyz files used to generate these images, it has been demonstrated that expanding the initial training set size can be achieved by creating multiple unique images (data points) from a single molecule. This study shows that the presented approach leads to a statistically significant improvement in model accuracy, highlighting RGBChem as a powerful approach for leveraging machine learning (ML) in scenarios where the available dataset is too small to apply ML methods effectively.



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C    0.0441   1.5738  -0.1302
C    0.0205   0.0457  -0.0178
C   -1.4100  -0.5485   0.0586
C   -2.3626   0.0187  -0.9987
C   -1.4230  -2.0984  -0.0071
O   -0.4437  -2.7235   0.6520
O   -2.2797  -2.7091  -0.5944
N    0.7944  -0.4375   1.1523
H    0.1744  -2.0368   1.0238
H    1.7824  -0.2336   1.0364
H    0.4900   0.0489   1.9926
H    1.0771   1.9372  -0.1093
H   -0.4127   1.9237  -1.0589
H   -0.4934   2.0368   0.7065
H    0.5154  -0.3771  -0.9017
H   -1.8068  -0.2931   1.0550
H   -3.2999  -0.5376  -0.9794
H   -2.5730   1.0764  -0.8244
H   -1.9429  -0.0895  -2.0047
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Fig. 1. Overview of RGBChem workflow

Acknowledgements: We thank Academia Profesorum Iuniorum of Wrocław University of Science and Technology for facilitating interdisciplinary collaboration.

P-29

Study on the rheological properties of biodiesel in the form of goose fat methyl ester

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Biodiesel as an alternative fuel is gaining increasing interest in the context of sustainable development and emission reduction. Unlike traditional fossil fuels, it is a renewable energy source derived from vegetable oils and animal fats, including goose fat. Its production, based on the transesterification process, yields a fuel with properties similar to conventional diesel but with lower emissions of sulfur oxides and particulate matter. The physicochemical properties of biodiesel, such as density, viscosity, and surface tension, are crucial for optimizing combustion and injection processes in diesel engines. Moreover, spray parameters influence combustion efficiency and pollutant emissions, making their analysis an essential aspect of assessing biodiesel's suitability as a replacement for fossil fuels.

The aim of this study was to analyze the rheological properties and spray characteristics of biodiesel obtained from goose fat methyl ester in the context of its application as a sustainable alternative fuel for diesel engines. The biodiesel was synthesized via transesterification and subsequently evaluated for physicochemical parameters, including density, viscosity, surface tension, and zeta potential. Density measurements showed compliance with the EN 14214 standard, with values ranging from 860 to 900 kg/m³, decreasing linearly with increasing temperature [1]. Viscosity tests conducted at 20°C, 40°C, and 100°C confirmed its strong dependence on temperature, indicating improved flow properties at higher temperatures [2]. Meanwhile, surface tension measurements provided insights into fuel atomization efficiency, which is critical for the combustion process in diesel engines [3]. Zeta potential analysis revealed limited colloidal stability, suggesting the need for further modifications in fuel formulation [4].

Spray characteristics were examined at injection pressures of 30 MPa and 50 MPa using a high-speed imaging system. A comparison of goose fat biodiesel with conventional diesel fuel showed similar penetration and spray patterns at elevated pressure. However, biodiesel exhibited a slightly smaller spray cone angle and greater fuel jet penetration length [5]. These results confirm that biodiesel derived from goose fat meets fundamental quality standards and exhibits favorable combustion properties. However, to enhance its usability in various climatic conditions, optimizing injection parameters and incorporating additives to improve flow properties at low temperatures are necessary.

The conducted research contributes to a better understanding of alternative biodiesel sources and their behavior in the combustion process in internal combustion engines.

References

1. S.K. Hoekman, A. Broch, C. Robbins, E. Ceniceros, M. Natarajan, Renewable and Sustainable Energy Reviews, 16(1), (2012) 143–169.
2. G. Knothe, J. Van Gerpen, J. Krahl, The Biodiesel Handbook. Champaign, Illinois: AOCS Press (2005).
3. P.X. Pham, K.T. Nguyen, T.V. Pham, V.H. Nguyen, ACS Omega, 5(33), (2020) 20842–20853.
4. H.K. Suh, C.S. Lee, Renewable and Sustainable Energy Reviews, 58, (2016) 1601–1620.
5. J. Naber, D.L. Siebers, SAE Technical Paper (1996) 960034.

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Oxygen plasma approach in modification of BN structure - structural analysis

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Boron nitride (BN) exists mainly in cubic and hexagonal forms similar to carbon materials. Cubic BN is analogous to diamond with a comparable hardness. Hexagonal boron nitride is isostructural with graphite and is known for its outstanding electrical, thermal, and lubricating properties. Increasing attention is being paid to the use of boron nitride in the emerging front of research as an alternative energy carrier with the potential to replace fossil fuels. It should, however, be borne in mind that the surface properties of materials used as supports play a crucial role not only in the catalytic but also in energy-related processes.

This study concerns the application of plasma treatment as a useful and facile technique for surface modification of boron nitride. In this project, the hexagonal boron nitride nanoparticles (h-BN) were oxygen plasma treated to generate the new functional groups on the surface, to provide the new centers and potentially trigger its catalytic properties.

The series of h-BN materials: with low (BN-low, S= 9 m^2/g) and high (BN-high, S=42 m^2/g) specific surface areas were comparatively investigated with the oxygen plasma-treated one (BN-plasma, S=36 m^2/g) by advance spectroscopic FTIR, ^{1}HNMR and ^{11}BNMR methods. Plasma modification triggered the distinct nanotopology changes of the parent BN (Fig.1). The regular plate-like grains (BN-low) underwent refinement (BN-high) and preservation upon plasma treatment (BN-plasma).

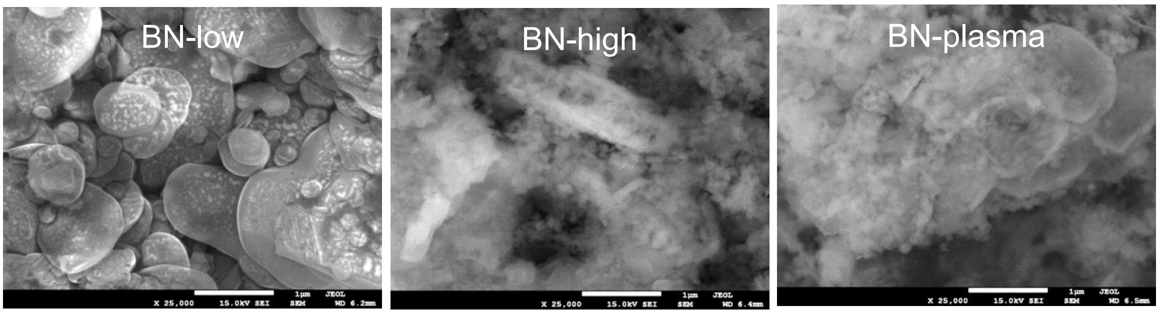

Fig. 1 SEM images of BN before (BN-low, BN-high) and after plasma treatment.

EDS analysis shows that all samples exhibit low content of oxygen, with the highest contribution in BN-plasma sample (3.7% wt.). Simultaneously the appearance of new XRD reflection around $2\theta = 42^o$ was observed.

FTIR spectroscopy in the middle range was used to assess the surface and bulk changes after the plasma modification. FTIR analysis shows intensive B-N vibrations at 1379 cm^{-1} (ν) and 814 cm^{-1} (δ) in all samples, and a shoulder around 768 cm^{-1} (δ) attributed to B-O bonds in BN-high and BN-plasma samples confirming enrichment of parent BN into oxygen species. Additionally, the BN-plasma spectrum exhibits new well-developed vibration at 3214 cm^{-1} corresponding to the generation of OH groups, also supported by ^{1}H NMR results.

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Ocena właściwości zasadowych mineralnych nanokompozytów hybrydowych-badania in-situ

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Kluczowe koncepcje Zielonej Chemii wymuszają redukcję stosowania oraz wytwarzania szkodliwych materiałów i chemikaliów, a także redukcję wytwarzania i emisji gazów cieplarnianych. Dlatego poszukuje się nowych rozwiązań pozwalających na zminimalizowanie poziomu emisji CO_2, a jednym z głównych celów zrównoważonego rozwoju jest dążenie do opracowania nowatorskich metod mających na celu obniżenie poziomu CO_2 w atmosferze poprzez jego wychwytywanie a następnie transformację w bardziej pożądane produkty. Nie bez znaczenia jest też powinowactwo molekuł CO_2 do materiałów wyposażonych w centra o właściwościach zasadowych, a CO_2 reaguje z centrami O^{2-} i OH^- tworząc jony węglanowe (CO_3^{2-}) i wodorowęglanowe (HCO_3^-).

Celem tej pracy była ocena właściwości zasadowych hybrydowych kompozytów mineralnych generowanych na osnowie anionowych minerałów warstwowych, aktywnych w wychwytywaniu i sekwestracji CO_2 z gazów spalinowych. W projekcie skupiliśmy się na otrzymaniu i modyfikacji prekursorów hydrotalkitowych, ich pochodnych otrzymanych w wyniku traktowania termicznego oraz hybryd, anionowo-kationowych szczotek mineralnych.

Stosując metodę współstrącania, otrzymano serię wysokopowierzchniowych, anionowych warstwowych podwójnych wodorotlenków, o strukturze hydrotalkitu (Ht) $[M^{2+}_{1-x}M^{3+}_x(OH)_2][An^-]_{x/n}\cdot mH_2O$ różniących się składem (Mg-Al=2:1, 3:1, 5:1), czasem starzenia (0h, 24h 168h), stopniem krystaliczności oraz wielkością ziaren hydrotalkitu, kontrolowanych warunkami syntezy. Otrzymane materiały zostały scharakteryzowane z wykorzystaniem metod XRD, FTIR, SEM/EDS, oraz adsorpcji/desorpcji N_2, w celu przeprowadzenia korelacji strukturalno-sorpcyjnej. Po raz pierwszy, z wykorzystaniem metod spektroskopowych *in situ* z wykorzystaniem CO_2 jako cząsteczki sondy wykonano badania jakościowo-ilościowe wygenerowanych centrów zasadowych, które zweryfikowano metodą Temperaturowo-Programowanej Desorpcji CO_2. Zbadano wpływ parametrów syntezy na naturę generowanych centrów zasadowych, ich moc, kinetykę procesu adsorpcji/desorpcji CO_2 oraz pojemność sorpcyjną. Otrzymane prekursory posiadały strukturę krystaliczną, charakterystyczną dla węglanowej formy hydrotalkitu o symetrii romboedrycznej R3m. Wielkości krystalitów Ht w zależności od czasu krystalizacji zmieniały się w przedziale 10, 20, 30, 50 nm, a powstałego tlenku MgO miały wielkość 3-6 nm. Badania spektroskopowe FTIR anionowych prekursorów Ht oraz ich mieszanych tlenków, wykazały, że CO_2 reaguje z centrami O^{2-} i OH^- tworząc jony węglanowe (CO_3^{2-}) i wodorowęglanowe (HCO_3^-). Węglany i wodorowęglany powstają przy niskich pokryciach powierzchni i nie ma preferencji, które centra zasadowe O^{2-} czy OH^- reagują z CO_2 w pierwszej kolejności. Czas starzenia i krystaliczność wpływa na dostępność generowanych centrów zasadowych oraz ilość powstających grup OH. Kalcynacja wyraźnie zwiększa zasadowość hydrotalkitu, centra O^{2-} wykazują wyższą moc niż grupy OH^-. Tlenki tworzą więcej węglanów niż ich prekursory, co jest wynikiem większej liczby dostępnych centrów O^{2-}. Dużą rolę w sorpcji molekuł CO_2 odgrywa woda, która wpływa na zwiększenie pojemności sorpcyjnej materiału.

Podziękowania: Badania finansowane w ramach Projektu Rozwojowego IKiFP PAN nr 2/PR-MZ/2024

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S-1

Najnowsze aparaty do pomiarów powierzchni właściwej, rozkładu wielkości porów oraz właściwości katalizatorów.
Aparatura do pomiaru wielkości i kształtu cząstek

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Anton Paar w ostatnich latach pod swoją marką, kontynuuje rozwój produktów amerykańskiej firmy ***Quantachrome Instruments***, założonej w 1968r i znanej jako topowa firma na świecie w dziadzienie charakteryzacji materiałów porowatych, która od 2018r została wcielona do koncernu Anton Paar.

Analizatory adsorpcji i chemisorpcji - nowoczesne, w pełni automatyczne aparaty do precyzyjnych pomiarów adsorpcji fizycznej gazów w niskich i wysokich ciśnieniach, służące także do wyznaczania izoterm adsorpcji pary oraz pomiarów właściwości katalizatorów metodą chemisorpcji statycznej i przepływowej. Urządzenia zapewniają możliwość precyzyjnego ustalenia rozkładu wielkości porów, powierzchni właściwej BET oraz specyficznych interakcji pomiędzy gazami i ciałami stałymi. Wszystkie te parametry są istotne dla optymalizacji produkcji, doboru adsorbentów, charakteryzacji właściwości katalizatorów, farmaceutyków, a także komponentów do produkcji baterii oraz wielu innych materiałów porowatych w nowoczesnych technologiach przyszłości.

W ostatnich latach firma Anton Paar zainstalowała na Polskim rynku już kilkanaście najnowocześniejszych na świecie aparatów sorpcyjnych pod swoim szyldem, bazujących na pewnych sprawdzonych rozwiązaniach Quantachrome Instruments, jednak zaprojektowanych w większej części już zgodnie z nową koncepcją i technologią naszej firmy: *Nova 600/800* oraz nasz najbardziej zaawansowany *Autosorb 6100, 6200 i 6300*. Urządzenia poza innowacyjną technologią i nowym oprogramowaniem, wyróżnia także nawet 2-krotnie krótszy czas uzyskiwania wyników analizy w porównaniu do innej podobnej aparatury oraz ich modułowość i stosunkowo kompaktowa budowa.

Porometry kapilarne i porozymetry rtęciowe - aparaty kapilarno-przepływowe zaprojektowane do dokładnych pomiarów porów otwartych w materiałach filtracyjnych, a także łatwe w obsłudze i bezpieczne podczas użytkowania porozymetry rtęciowe zdolne do pomiaru rozkładu wielkości oraz objętości porów dostępnych na zewnętrznej powierzchni materiału w najszerszym dostępnym zakresie średnicy od 3,6nm aż do 1100µm.

Odnośniki do naszej strony w zakresie aparatury do pomiaru porowatości i katalizatorów:
https://www.anton-paar.com/pl-pl/produkty/grupa/analizatory-adsorpcji/
https://www.anton-paar.com/pl-pl/produkty/grupa/porometers-porosimeters/
https://www.anton-paar.com/pl-pl/produkty/grupa/bulk-density-analyzers/

Aparatura do pomiaru wielkości i kształtu cząstek w skali nano, mikro i mm

S-1

Znajomość rozkładu wielkości cząstek materiału jest niezbędna dla rozwoju produktu i kontroli jakości, ponieważ te dwa parametry mają wpływ na powtarzalność, a także właściwości produktu końcowego.

Analizatory serii Litesizer DLS 100, 500 i 700 służące do charakteryzowania nanocząstek w ciekłych dyspersjach w zakresie **0,3 nm – 12 µm**. Urządzenia pozwalają na pomiar wielkości cząstek, potencjału zeta, masy cząsteczkowej, stężenia oraz możliwość wyznaczenia współczynnika załamania światła dla odpowiedniego rozpuszczalnika, w którym zawieszono nanocząstki i przy odpowiedniej długości fali światła laserowego używanego w pomiarze. Pomiary DLS z użyciem 3 automatycznie dobieranych kątów pomiarowych i ciągłego pomiaru transmitancji światła, w zależności od rodzaju badanych próbek, dla uzyskania lepszej precyzji wyników. 3 letnia bezwarunkowa gwarancja w podstawowej cenie urządzenia.

Aparaty z serii Litesizer DIA 100, 500 i 700 **pozwalają w prosty, w pełni automatyczny i niezawodny sposób** scharakteryzować dokładny kształt i wielkość cząstek poprzez bezpośrednią analizę obrazu każdej poszczególnej cząsteczki. DIA wykorzystuje kamerę o bardzo wysokiej częstotliwości odświeżania, aby w krótkim czasie uchwycić obraz ogromnej liczby pojedynczych cząstek w zakresie od **0,8 µm - 8000 µm**. W rezultacie, w ciągu kilku sekund, uzyskuje się zarówno dokładny wymiar każdej cząsteczki jak i jej kształty, z możliwością pełnej charakteryzacji zgodnie z wyznaczonymi kryteriami użytkownika, dzięki rozwiązaniom jakie zapewnia autorskie oprogramowanie Anton Paar Kalliope. **Szybkie,** jednoetapowe przełączanie między trzema jednostkami dyspersyjnymi - mokrą, suchą i swobodnego spadku - umożliwia uzyskanie doskonałej dyspersji niemal każdego rodzaju próbki.

Analizatory serii Litesizer DIF – pomiar wielkości cząstek metodą dyfrakcji laserowej zarówno w postaci dyspersji ciekłych, jak i suchych proszków w zakresie **10 nm – 3500 µm**. Absolutnie proste w montażu jednoetapowo przyłączane jednostki dyspersyjne, kompatybilne z serią analizatorów DIA.

Aparatura do pomiaru adhezji powłok i nanotwardości powierzchni oraz zużycia pod kontrolą mikroskopową: zaawansowana aparatura pomiarowa, która ze szwajcarską dokładnością i precyzją jest w stanie identyfikować właściwości mechaniczne powierzchni materiałów w skali mikro i nano przy jednoczesnym obrazowaniu powierzchni za pomocą mikroskopu świetlnego i to w sposób wysoce zautomatyzowany.

Odnośniki do naszej strony w zakresie aparatury do pomiaru wielkości i kształtu cząstek:
https://www.anton-paar.com/pl-pl/produkty/grupa/analizatory-wielkosci-czastki/
Odnośniki do naszej strony w zakresie aparatury do pomiarów adhezji powłok i nanotwardości:
https://www.anton-paar.com/pl-pl/produkty/grupa/tester-zarysowania/
https://www.anton-paar.com/pl-pl/produkty/grupa/oprzyrzadowany-twardosciomierz/

S-2

Labsoft – Lider w Zaawansowanych Technologiach Badawczych

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Labsoft od ponad 30 lat dostarcza zaawansowane rozwiązania badawcze i pomiarowe dla jednostek naukowych oraz przemysłu. Portfolio produktów obejmuje aparaturę badawczą dla instytucji naukowych oraz urządzenia pomiarowe i produkcyjne dla przemysłu. Dzięki współpracy ze światowymi liderami technologii dostarczamy kompleksowe rozwiązania wspierające rozwój nauki i innowacji. Oprócz sprzedaży zapewniamy pełne wsparcie techniczne i aplikacyjne, obejmujące instalację, serwis oraz doradztwo w zakresie użytkowania aparatury.

Nasze doświadczenie pozwoliło nam na wprowadzenie do Polski wielu pionierskich technologii, takich jak pierwszy mikroskop TEM z działem polowym, pierwszy mikroskop FIB/SEM czy pierwsze kriogeniczne mikroskopy elektronowe TEM. Nasz zespół liczy ponad 30 wysoko wykwalifikowanych specjalistów, a serwis techniczny Labsoft jest największy w regionie, zdobywając uznanie także poza granicami kraju.

Labsoft jest autoryzowanym dystrybutorem mikroskopów elektronowych Thermo Fisher Scientific – lidera w technologii badawczej, cenionego za swoje flagowe produkty, takie jak:

Skaningowe mikroskopy elektronowe (SEM) – m.in. Apreo i Axia ChemiSEM, zapewniające wysoką rozdzielczość i precyzyjną analizę powierzchni próbek.

Transmisyjne mikroskopy elektronowe (TEM) – takie jak Talos i Spectra, umożliwiające badania strukturalne na poziomie atomowym.

Systemy DualBeam (FIB-SEM) – obejmujące linię mikroskopów Helios, które łączą funkcjonalność SEM z wiązką jonową FIB, umożliwiającą precyzyjną modyfikację próbek.

Spektroskopy fotoelektronów rentgenowskich (XPS) – topowe urządzenia ESCALAB QXi i Nexsa G2 do analizy składu chemicznego powierzchni materiałów.

Mikroskopy elektronowe i spektrometry XPS Thermo Fisher Scientific znajdują zastosowanie w wielu dziedzinach nauki i przemysłu – od badań nad nowoczesnymi materiałami, przez elektronikę i półprzewodniki, po biologię i diagnostykę medyczną. Dzięki innowacyjnym rozwiązaniom, takim jak automatyczna analiza obrazów, korekcja aberracji czy integracja z systemami sztucznej inteligencji, użytkownicy mogą szybko i precyzyjnie uzyskiwać wyniki badań. Współpracując z naukowcami i inżynierami, Thermo Fisher Scientific nieustannie rozwija swoje technologie, wspierając postęp naukowy i technologiczny.

Referencje:
1.www.labsoft.pl

S-3

Advancing Catalysis Research with PREVAC's Standard HPPES Systems

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Understanding catalytic processes under realistic conditions is essential for improving material performance in energy conversion, environmental protection, and chemical synthesis. X-ray Photoelectron Spectroscopy (XPS) and High-Pressure Photoelectron Spectroscopy (HPPES) provide crucial insights into the surface chemistry and electronic structure of catalysts, helping to optimize their efficiency and stability.

Recent research utilizing the EA15 analyser has demonstrated its effectiveness in studying catalytic materials, particularly in identifying oxidation states, reaction intermediates, and surface reconstructions under operational conditions. By enabling measurements at pressures up to 50 mbar, this system bridges the gap between traditional ultra-high vacuum (UHV) conditions and real-world catalytic environments.

This presentation will showcase the design and technical advantages of PREVAC's HPPES Systems and highlight case studies where the EA15 analyser has been successfully applied in catalytic research. These examples will demonstrate how advanced photoemission techniques contribute to a deeper understanding of catalytic mechanisms, ultimately supporting the development of more efficient and durable catalysts for industrial applications.

Fig. 1. PREVAC's HPPES systems

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ISBN 978-83-60514-40-5