CATSA2025 BOOK OF ABSTRACTS

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CATALYSIS SOCIETY OF SOUTH AFRICA

Catalysis Society of South Africa (CATSA)
c/o Department of Chemical Engineering
University of Cape Town
Private Bag
Rondebosch 7701
South Africa
Email: catsaconference@catsa.org.za

Website: https://catsaconference2025.catsa.org.za/

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Preface

Welcoming Remarks:

It is with great pleasure that we welcome you to the 2025 Conference of the Catalysis Society of South Africa (CATSA), a gathering of minds committed to advancing the frontiers of catalysis in service of a more sustainable world.

This year's theme, *using Catalysis to solve the United Nations' Sustainable Development Goal (SDGs)*, reflects our collective ambition to align catalytic science with the United Nations' SDGs. From clean energy transitions and green chemical processes to circular economy innovations and climate resilience, catalysis stands at the heart of transformative solutions.

CATSA 2025 brings together researchers and industry leaders; to explore how catalytic technologies can address pressing global challenges. Through interdisciplinary dialogue and collaborative exchange, we aim to foster breakthroughs that are not only scientifically rigorous but socially and environmentally responsive.

As you engage with the abstracts and presentations showcased in this volume, we invite you to reflect on the catalytic potential of your own work, not just in reaction mechanisms, but in shaping a future that is inclusive, equitable, and sustainable.

Welcome to CATSA 2025. Let the reactions begin!!!!!

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LOCAL ORGANIZING COMMITTEE, 2025:

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Plenary Speaker Introduction

The CATSA 2025 plenary program showcases three distinguished voices in catalysis whose pioneering research addresses the urgent challenges of sustainability, energy transition, and chemical innovation. Their lectures span molecular insight, industrial transformation, and strategic foresight—offering delegates a compelling cross-section of catalytic science in action.

- **Prof Angeliki A. Lemonidou** (Aristotle University of Thessaloniki) opens the programme with a lecture on *Catalysis in a pivotal role for sustainability: The olefins paradigm*. Her work reimagines the production of light olefins—cornerstones of the petrochemical industry—through alternative pathways such as oxidative dehydrogenation and CO_2-assisted catalysis. By leveraging NiO and FeO_x-based catalysts and biomass-derived feedstocks, she demonstrates how tailored catalyst design can reduce energy intensity and enable greener process schemes.
- **Dr Theo Mudzunga** (Sasol Research and Technology) reflect on *75 Years of Fischer-Tropsch Innovation at Sasol*, tracing the evolution of FT technology from coal-to-liquids to gas-to-liquids and now toward renewable integration. Their lecture highlights Sasol's strategic pivot toward Sustainable Aviation Fuel (SAF), including the ZAFFRA joint venture and the CARE-O-SENE catalyst development programme—underscoring the role of feedstock flexibility and catalyst innovation in decarbonizing hard-to-abate sectors.

Together, these plenary lectures illuminate the catalytic frontier—from molecular mechanisms to industrial deployment—reinforcing CATSA's commitment to advancing sustainable science through collaboration, innovation, and critical dialogue.

Plenary speaker: PL1

Catalysis in a pivotal role for sustainability: The olefins paradigm

Angeliki A. Lemonidou

School of Chemical Engineering, Faculty of Engineering, Aristotle University of Thessaloniki, University Campus, 54124 Thessaloniki, Greece
e-mail: alemonidou@auth.gr

Keywords: light olefins, oxidative dehydrogenation, hydrodeoxygenation, CO_2-assisted dehydrogenation.

Abstract

Sustainability is hardly a new discovery in the chemical industry. However, as the chemical industry plays nowadays a vital role in tackling major societal challenges such as climate change, the need for improving the sustainability of the chemical processes has become imperative. Catalysis can play a major role on this target as the use of catalysts in a process can reduce energy consumption, minimize waste, enhance resource efficiency and enable the use of greener feedstocks and reaction media. The cornerstone of the petrochemical industry is the production of light olefins (ethylene and propylene) with volumes more than 370 MMtons/year. The utilization of C_2-C_3 alkanes of shale gas or biomass derivatives, the use of oxidants O_2 or CO_2 and tailor-made catalysts has emerged in the last years as an alternative to the mature and high energy intensive steam cracking technology which is currently commercially employed. The lecture will focus on the research activities for the development of catalysts and process schemes to produce ethylene via oxidative dehydrogenation of ethane in the presence of NiO-based catalysts, the use of CO_2 as alternative oxidant for the same reaction in the presence of FeO_x-based catalysts and the production of propylene via hydrodeoxygenation of biomass derived polyols. The efforts to synthesize active and selective catalysts, their advanced characterization, and the evaluation of catalytic performance combined with mechanistic and kinetic studies will be presented and discussed.

Notes

Plenary speaker: PL2

From Energy Security to Sustainability: 75 Years of Fischer-Tropsch Innovation at Sasol

Theo Mudzunga[a], Denzil Moodley[a], Thirusha Naicker[a] and Thys Botha[a]

[a] *Sasol Research and Technology, 1 Klasie Havenga Rd, Sasolburg, South Africa*
E-mail: theo.mudzunga@sasol.com

Keywords: Fischer-Tropsch, Coal-to-Liquids, Gas-to-Liquids, Sustainable Aviation Fuel

Abstract

Since its first commercial application, Fischer-Tropsch (FT) technology at Sasol has undergone significant evolution through three distinct phases. The initial phase, beginning with the Sasolburg plant in the 1950's, harnessed South Africa's abundant and affordable coal resources to produce liquid fuels, aiming to reduce reliance on imported crude oil [1]. Advances in large-scale commercialization, especially at the Secunda facility, leveraged cost-effective iron catalysts to lower production costs and enabled the extraction of valuable chemicals from high temperature coal-to-liquids (CTL) processes [2].

The second phase marked a transition to natural gas as a feedstock, due to its availability in certain regions and the significantly lower environmental footprint. The Sasolburg site converted completely from coal to a natural gas feedstock in 2004, and Sasol pioneered the development and commercialization of new slurry-phase cobalt catalysts optimized for producing ultra-low sulphur diesel with high paraffinic content [3]. Today, Sasol's low temperature Cobalt FT technology operates across three large-scale gas-to-liquid (GTL) plants with a combined nominal capacity exceeding 100,000 barrels per day. During this phase, product diversification expanded to include waxes, lubricants, and chemicals, strengthening Sasol's market competitiveness.

The ongoing third phase leverages the feedstock flexibility of FT technology to drive sustainability by integrating renewable sources such green hydrogen, unavoidable CO2, biomass and waste-derived syngas. This integration supports emissions reduction and decarbonization efforts, particularly in challenging sectors like aviation [4]. There are various challenges when utilizing these expensive renewable feedstocks and one of them involves developing Fischer-Tropsch catalysts with high conversion efficiencies and improved selectivity to the desired products. In recent times, Sasol has been focussing on the Sustainable Aviation Fuel (SAF) space, with a joint venture (ZAFFRA) established together with Topsoe to accelerate the decarbonisation of the aviation sector. Since 2022, we also co-led a German Government funded project (CARE-O-SENE), that develops and scales-up new FT catalysts for SAF.

Throughout all phases, Sasol Research and Technology has been instrumental in advancing, refining, and innovating in the FT process—a journey that continues to shape the future of sustainable fuels and chemicals.

[1] Verhoef, G.. Rivista di Politica Economica, 2015.
[2] Steynberg, A.P., Espinoza, R.L., Jager, B. and Vosloo, A.C., 1999. Applied Catalysis A: General, 1999, 186, .41-54
[3] Vogel, A.P., Van Dyk, B. and Saib, A.M., Catalysis Today, 2016, 259, 323-330.
[4] Moodley, D., Botha, T., Crous, R., Potgieter, J., Visagie, J., Walmsley, R. and Dwyer, C., 2024. Catalysis for a Sustainable Environment: Reactions, Processes and Applied Technologies, 2024, 1, 73-116.

Notes

Keynote Speaker Introduction

The CATSA 2025 conference convenes at a pivotal moment for catalysis research, where sustainability, precision, and innovation intersect across disciplines. This year's keynote speakers exemplify the transformative potential of catalytic science—from reimagining legacy processes to pioneering biotechnological frontiers.

We begin with a bold reconfiguration of Sulfur's role in Fischer-Tropsch synthesis. **Dr Esna du Plessis** and colleagues (KN1) challenge conventional wisdom by demonstrating how mechano-chemical sulfur incorporation can selectively enhance olefin production while preserving the robust physical properties of fused iron catalysts. Their work reframes sulfur not as a poison, but as a promoter—unlocking new pathways for industrial relevance.

Prof Dean Brady and the Wits-UP team (KN2) take us into the realm of oxidative biocatalysis, where plant-derived enzymes enable the sustainable synthesis of high-value aroma compounds like nootkatone and carvone. Their lipoxygenase-mediated transformations, boosted by iron salts, offer scalable alternatives to seasonal extraction—bridging green chemistry and commercial viability.

Dr Jairus Lamola and collaborators (KN3) present a state-of-the-art exploration of manganese promotion in cobalt FT catalysis. Through operando characterization and theoretical modeling, they illuminate Mn's dual role in structural and chemical enhancement, reshaping design principles for next-generation catalysts under the CARE-O-SENE program.

Dr Ryan Walmsley and the Sasol-UCT team (KN4) revisit the century-old, fused iron catalyst with fresh eyes. Their work on precarbiding strategies under fluidized-bed conditions demonstrates how phase control can elevate performance in both HTFT and CO_2 hydrogenation, reaffirming the catalyst's versatility in modern energy contexts.

Finally**, Prof L Van Zyl** and the IMBM team (KN5) push the boundaries of microbial biotechnology. By engineering aminolipid biosynthesis through metagenomic discovery and combinatorial gene expression, they unlock a diverse catalogue of custom biosurfactants with applications ranging from wastewater treatment to therapeutics—heralding a new era of tailored lipid innovation.

Together, these keynote contributions reflect the dynamic spirit of CATSA: rigorous, imaginative, and deeply attuned to the challenges and opportunities of a changing world. We invite you to engage with these abstracts not only as scientific milestones, but as catalysts for dialogue, collaboration, and transformation.

Keynote speaker: KN1

Transforming Sulphur's Role: Mechano-chemical pathways to fused iron catalyst enhancement.

Esna du Plessis, Ryan Walmsley, Thirusha Naicker, Tony Lombard and Thys Botha[a]

Sasol Research and Technology, Klasie Havenga Road 1, Sasolburg, South Africa, E-mail: esna.duplessist@sasol.com.

Keywords: Fischer-Tropsch Synthesis, sulphur, catalyst, promotion, selectivity.

Abstract

Light olefins (C_2–C_4) and oxygenates are vital precursors in the chemical industry, forming the basis of numerous consumer and industrial products. Within High-Temperature Fischer–Tropsch (HTFT) synthesis, sulphur poisoning of fused iron catalysts typically results in diminished conversion and a shift toward lighter, hydrogenated hydrocarbons. However, selective sulphur addition to a precipitated iron catalyst (470 mgS/kg) promoted C_2–C_4 olefin production, exceeding Anderson–Schulz–Flory distribution expectations while reducing CH_4 selectivity [1].

Catalyst activity and selectivity are not, however, the only crucial criteria to be considered for a commercial process. Physical properties such as strength and density are just as critical for fluidized bed applications such as the Sasol Advanced Synthol (SAS) process.

This study investigates multiple sulphur incorporation strategies for fused iron catalysts—namely mechanical mixing, high-temperature fusion, and mechano-synthesis—with the objective of modulating sulphur's traditionally deactivating influence to achieve selective promotional effects. These different approaches would allow for the bulk of the fused catalysts' physical properties to be retained potentially simplifying and speeding up commercialization.

The Fischer–Tropsch synthesis (FTS) performance of the modified catalysts was assessed using micro fixed-bed reactor testing, focusing on conversion and olefin selectivity. Through comparative analysis of promotion methods and sulphur species, the study seeks to identify the most effective approach for enhancing light olefin production while minimizing deactivation pathways in high-temperature FTS applications.

[1] Botes, G.F., Bromfield, T.C., Coetzer, R.L.J., Crous, R., Gibson, P., Ferreira, A.C., Development of a chemical selective iron Fischer Tropsch catalyst, *Catalysis Today*, 2016, **275**, 40-48.

Notes

Keynote speaker: KN2

Plant Power: Synthesis of Nootkatone and Carvone by Oxidative Biocatalysis.

D Brady,[a] K Ngwiraa D Pienaara,[b], O Govender[a], C Raboya[a] and Ida Mamolemo Makhubela[a]

[a]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, PO Wits 2050, South Africa; dean.brady@wits.ac.za

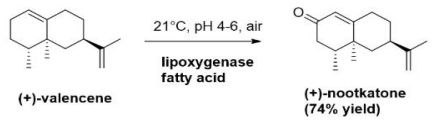
[b]Department of Chemistry, Faculty of Natural and Agricultural Sciences, University of Pretoria, South Africa;

Keywords: biocatalysis, flavours and fragrances, synthesis

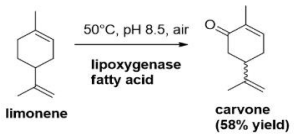
Abstract

Nootkatone (NK), a sesquiterpenoid that contributes to the distinct aroma of grapefruit, is valuable in the flavor and fragrance industry. Likewise, R-(-)-carvone, an oxygen-containing monoterpene, provides the characteristic odor found in spearmint, and is commercially used in the baking, cosmetic and pharmaceutical industries. However, as these compounds are extracted from plant species, supplies are both limited and seasonal and are therefore not able to meet the demand.

Biocatalysis enables the synthesis of nature-identical products acceptable to the flavor and fragrance industry. Both nootkatone and carvone can be prepared by oxidation of inexpensive compounds that can be readily extracted from plants. Thus, we applied crude preparation of lipoxygenase (LOX), an oxidative enzyme that is plentiful in soyabeans, using fatty acids from vegetable oils as a reaction mediator. Valenene from citrus was converted to nootkatone, as has been demonstrated previously (Scheme 1).[1] However, the same enzyme preparation was also able to convert limonene to carvone (Scheme 2).[2] Interestingly, both products were obtained in higher yields after addition of iron salts. These reactions represent highly sustainable chemistry.



Scheme 1: Biocatalytic synthesis of nootkatone.



Scheme 2: Biocatalytic synthesis of carvone.

[1] Makhubela I. M. Zawaira A., Brady D., and Pienaar D. P. (2024) Multifactorial optimization enables the identification of a greener method to produce (+)-nootkatone. Journal of Biotechnology 393: 41-48.

[2] Initially observed by colleagues at Applied Protein Technologies

Notes

Keynote speaker: KN3

Mn Promotion in Cobalt Fischer–Tropsch Catalysis: State-of-the-Art, Theory and Operando Characterization

Jairus Lamola[a], Jana Potgieter[a], Denzil Moodley[a,c], Thys Botha[a], Anna Zimina[b], Felix Studt[b], Enrico Sireci[b], Catalina Jimenez[c], Michael Claeys[d], Eric van Steen[d],

[a]*Sasol Research & Technology, 1 Klasie Havenga Rd, Sasolburg, 1947, South Africa,*
[b]*Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Germany*
[c]*Helmholtz Zentrum Berlin für Materialien und Energie, Department Interface Design, Berlin, Germany*
[d]*Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch 7701, South Africa*
E-mail: jerry.lamola@sasol.com

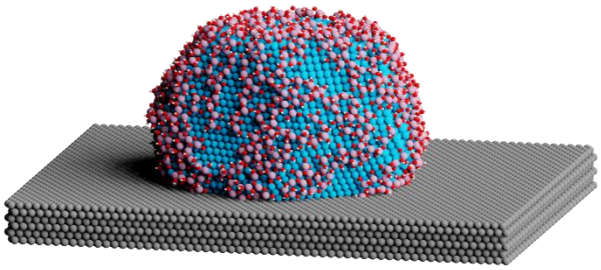
Keywords: catalyst, cobalt, manganese, promotion

Abstract

The promotion of cobalt-based Fischer–Tropsch (FT) catalysts with manganese (Mn) has a long-standing history, dating back to the 1940s, where early empirical studies showed its ability to modulate wax selectivity [1]. However, the molecular-level understanding of the promotional role of Mn has only matured in recent decades, driven by advances in spectroscopy, microscopy, and theoretical modeling [2]. In this presentation, we provide an overview of Mn as a multifaceted promoter in Co-based FT catalysis, encompassing both historical developments and cutting-edge insights.

We discuss the dual role of Mn as a **structural promoter**, affecting cobalt dispersion, reducibility, and phase stability, and as a **chemical promoter**, enhancing the formation of higher hydrocarbons, light olefins and oxygenates. Through state-of-the-art *operando* characterization techniques—such as *in situ* X-ray absorption spectroscopy (XAS), and *in-situ* Magnetometry, we reveal how Mn dynamically influences the cobalt surface under activation and/or reaction conditions.

Special emphasis is given to recent findings from the **CARE-O-SENE** program, where integrated experimental and theoretical approaches (including DFT modeling) provide a detailed understanding of Mn-Co interactions and their potential impact on the FT reaction network. This presentation offers a state-of-the-art perspective on Mn promotion, demonstrating how modern characterization and theory are reshaping the design principles for next-generation FT catalysts.



.

Figure 1: Visualization of a supported Mn-promoted cobalt nanoparticle for FTS (Sireci, KIT)

[1] H. H. Storch, R. B. Anderson, L. J. E. Hofer, C. O. Hawk, H. C. Anderson, and N. Golumbic, "Synthetic liquid fuels from hydrogenation of carbon monoxide. I. Review of literature; Bur. of Mines research on effect of catalyst preparation, reduction, and properties of the catalysts with their activity," vol. 709, 1948.

[2] Vermaak et al, Manganese-enhanced Cobalt Catalysts for FischerTropsch Synthesis: A review of structural and electronic promotion effects: in preparation

Notes

Keynote speaker: KN4

The Sasol Fused Iron Catalyst: Teaching an old dog new tricks

Ryan Walmsley,[a] Thirusha Naicker,[a] Gavin Deas,[a] Toine Cents,[a] Thys Botha,[a] Mohamed Fadlalla,[b] Eric van Steen,[b] Michael Claeys,[b]

[a]Sasol Research & Technology, Klasie Havenga Road, Sasolburg, 1947, South Africa,
E-mail: ryan.walmsley2@sasol.com.
[b]Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch 7701, South Africa

Keywords: Fischer-Tropsch, iron, precarbiding, CO2 hydrogenation

Abstract

Sasol's proprietary High-Temperature Fischer-Tropsch (HTFT) technology remains a cornerstone of its coal- and gas-to-liquids operations. The Secunda facility in South Africa produces around 160,000 bbl/day of synthetic fuels and chemicals using cost-effective fused iron catalysts. Despite its longstanding commercial success, this century-old catalyst technology still holds potential for performance enhancement through modern activation strategies.

Under Fischer-Tropsch conditions, bulk iron catalysts evolve from the pre-reduced phase into a mixture of iron carbide (Fe_5C_3) and magnetite (Fe_3O_4), depending on the gas environment. On a simplistic level, carburization is driven by carbon monoxide, while water results in oxidation. Since iron carbides are recognised as the primary active phase, increasing their relative phase abundance and limiting oxidation can enhance activity, productivity, and energy efficiency.

Most studies in this field rely on fixed-bed reactors, where gas composition gradients are present by default. In contrast, Sasol's Advanced Synthol™ reactors operate under fluidised-bed conditions with a more uniform gas-phase composition and continuous catalyst mixing, fundamentally impacting the performance relative to a fixed bed.

This study investigates the scale-up performance of a commercially relevant precarbided fused iron catalyst under fluidised-bed conditions. Through online monitoring during catalyst activation and synthesis, we track phase evolution over time and link it to catalytic performance.

In addition to HTFT, the benefits of precarbiding were extended to CO_2 hydrogenation—where the process environment is more oxidising and phase stability is critical. Here, the standard fused iron catalyst was tested in its reduced and precarbided form. The latter was also benchmarked against a best-in-class material. Compared to the reduced version, the precarbided catalyst demonstrated superior CO_2 conversion, competing strongly with the best-in-class material. These findings highlight the versatility of the fused iron catalyst, especially in a precarbided form.

Notes

Keynote speaker: KN5

Diversifying aminolipid production through genetic engineering to deliver biotechnological solutions.

L Van Zyl, P Makhubu, P Venter, A Burger, M Trindade

Institute for Microbial Biotechnology and Metagenomics, Department of Biotechnology, University of the Western Cape, 7535, South Africa,
E-mail: ituffin@uwc.ac.za

Keywords: biosurfactant, metagenomics, N-acyl amino acid synthases, ornithine lipids

Abstract

Aminolipids, with different hydrophilic head groups, have been discovered from bacteria exclusively and in addition to being promising biosurfactants, they have therapeutic potential as potent G-protein-coupled receptor agonists, anti-microbials and anti-cancer compounds. Long-chain N-acyl amino acids are produced by N-acyl amino acid synthases. We identified an ornithine acyl-ACP N-acyltransferase (olsB) from a lake sediment metagenome, the overexpression of which in E. coli leads to the production of lyso-ornithine lipid (LOL) and ornithine lipid (OL) in P. putida. By using combinatorial gene expression and modification of fermentation conditions in E. coli as a platform for LOL synthesis, we obtained an overall improvement of 3.5-fold of the four dominant LOL species (C14:0, C16:1, C16:0, C18:0) compared with the starting conditions. Modification of the culturing conditions and mutation of the co-expressed P. putida acyl carrier protein (Pp-acpP) resulted in a shift to shorter chain fatty acids being incorporated (C10:0-C16:1), providing novel ways to control the profile of LOLs produced. For improved OL production we identified and co-expressed a bi-functional N-acyltransferase gene (olsF) from Lacinutrix sp. M09b143 in E. coli and P. putida. We hypothesise that this OlsF is responsible for the production of iso-branched LOLs with anti-bacterial and anti-cancer properties described from Lacinutrix sp. M09b143. Since iso-branched fatty acids are not part of E. coli and P. putida metabolisms, we are currently designing a genetic toolkit to develop Lacinutrix sp. as a platform strain for iso-branched LOL/OL production. To diversify the LOL/OL compounds even further we identified and co-expressed additional genes (olsC, D and E) with olsB or olsF to modify the ornithine and/or to hydroxylate ornithine or either of the acyl chains to produce compounds with more hydrophilic properties. With numerous possible combinations of head group and fatty acid tail modifications we envisage developing a diverse range of ornithine lipids with tailored physico-chemical properties for various applications. The recombinantly produced LOLs have been assessed as anti-biofilm agents for application in wastewater treatment strategies, as agricultural adjuvants, in cosmetic formulations, as anti-fungal agents for the treatment of leather and as anti-inflammatories for irritable bowel syndrome. Their broad potential drives our effort to expand the catalogue of custom aminolipids.

Notes

Oral Presentations Introduction

Oral Presentations at CATSA 2025, features 56 cutting-edge contributions (OP1–OP56) from researchers across South Africa and international collaborators. This collection reflects the vibrant and interdisciplinary nature of catalysis research in the region, with strong representation from leading institutions including the University of Cape Town's Catalysis Institute (e.g., OP1, OP3, OP9, OP11–OP13, OP16, OP19, OP21, OP23, OP27, OP30–OP31, OP44, OP48–OP51), the Institute for Catalysis and Energy Solutions (ICES) and Institute for Nanotechnology and Water Sustainability (iNanoWS) at the University of South Africa (e.g., OP3, OP7–OP8, OP15, OP17, OP25, OP29, OP32–OP33, OP35–OP36, OP39, OP46–OP47, OP52–OP53, OP55–OP56), Durban University of Technology (OP1, OP14), North-West University (OP4, OP42), the University of the Witwatersrand (OP6, OP10, OP45, OP50), and others such as Rhodes University (OP22, OP41), Stellenbosch University (OP50–OP51), and CSIR (OP20, OP55).

The presentations span core catalysis themes with a clear emphasis on sustainability, green energy, and resource valorization. Fischer-Tropsch Synthesis (FTS) remains a cornerstone, addressed in depth through iron- and cobalt-based catalysts (OP1, OP5, OP7, OP9, OP21), tail gas utilization in fuel cells (OP3), and poison effects via molecular modeling (OP5). CO_2 hydrogenation emerges as a prominent focus for carbon utilization and methanol production (OP36, OP38, OP40, OP42, OP44, OP56), complemented by methane activation (OP27, OP48) and ammonia decomposition for H_2 generation (OP31). Hydrogen-related technologies are well-represented, including photocatalytic water splitting (OP25, OP29), PEM electrolysis (OP24, OP30), electrocatalytic production (OP26, OP28), and biomass-derived H_2 via pyrolysis (OP37). Biocatalysis and enzymatic processes feature in selective oxyfunctionalization (OP2), industrial scaling (OP20), xylanase immobilization (OP22), and nitrilase mechanisms (OP43), alongside chemoenzymatic synthesis (OP45). Environmental applications highlight pollutant degradation (OP15, OP17, OP32, OP54) and water treatment catalysts (OP55), while polymer upcycling addresses plastic waste through dehydrogenation/metathesis (OP4), hydrogenolysis (OP14), and microwave-assisted decomposition (OP49). Additional topics include biofuel production (OP8, OP18), high-entropy alloys with machine learning design (OP36, OP53), perovskite catalysts (OP8, OP13, OP56), and advanced characterization techniques (OP9, OP19).

This year’s program showcases a rich tapestry of expertise—from early-career researchers to seasoned pioneers spanning universities, research institutes, and industry partners. Each talk invites us to engage critically with science, challenge assumptions, and explore new frontiers in catalysis. Whether probing the atomic intricacies of catalyst design or scaling up green technologies for real-world impact, these speakers exemplify the ingenuity and resilience driving our field forward.

We encourage attendees to participate actively, ask bold questions, and forge connections that transcend disciplines and borders. May these sessions spark dialogue, inspire innovation, and catalyze lasting collaborations.

Oral presentation: OP1

Spray-dried and attrition resistant iron catalysts for promoting Fischer-Tropsch Synthesis

Amanda S. Buthelezi[a],*Chelsea. L. Tucker[b] Hero J. Herees[c], Henk de van Bovenkamp[b] and Pinkie Ntola[a]

[a]*Department of Chemistry, Durban University of Technology, P.O Box 1334, Durban, 4001, South Africa*
[b]*Department of Chemical Engineering, University of Groningen, Nijenborg 4, 9747 AG Groningen, Netherlands bDow Benelux, Herbert H. Dowweg, 5, 4542 NM Hoek, Netherlands*
Email:21707285@dut4life.ac.za

Keywords: Spray-drying; Fischer-Tropsch; selectivity; hydrocarbons; attrition resistance

Abstract

Iron is used as catalyst in the industrial process Fischer-Tropsch Synthesis (F-TS), which is a catalytic chemical reaction that transforms synthesis gas (CO + H2) to create paraffins and olefins for fuels and chemicals [1]. Attrition is the process by which fragments of fine particles are created from solid pieces as they strike the reactor walls after being under pressure [2]. The attrition causes high surface catalytic loss, hardships in wax/catalyst separation, and less performance of the catalyst in the F-TS reaction [3]. This study aimed to design iron catalysts with a high surface area and attrition resistance for F-TS. α-Fe2O3, K/Cu/Fe and 0.367 M K/Cu/Fe spray-dried at 200 °C catalysts were prepared using the co-precipitation, impregnation and spray-drying methods. The catalysts were then characterized using various characterization techniques including thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET) analysis, scanning electron microscopy (SEM), X-ray diffraction (XRD), and X-ray fluorescence (XRF). Attrition resistance comprised physical tests with the accredited standard method of testing materials (ASTM). The results showed that the 0.367 M K/Cu/Fe spray-dried at 200 °C catalyst has a large surface area of 39 m2/g. The α-Fe2O3 catalyst was found to have more physical and chemical attrition resistance. All the catalysts including α-Fe2O3, K/Cu/Fe and 0.367 M K/Cu/Fe spray-dried at 200 °C demonstrated good selectivity characteristics (low methane and high C5+) hydrocarbons. The α-Fe2O3 catalyst showed high activity and stability, as there was minimal loss of catalytic activity as compared to other catalysts. The activity and selectivity of the catalysts need to be improved before the industrial application.

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[1] Gholami, Z., Tisler, Z. and Rubas, V. 2021. Recent advances in Fischer-Tropsch synthesis using cobalt-based catalysts: a review on supports, promoters, and reactors. Catalysis Review, 63: 45 48.
[2] Amblard, B., Bertholin, S., Bobin, C. and Gauthier, T. 2015. Development of an attrition evaluation method using a Jet Cup rig. Powder Technology, 274: 455–465.
[3] Lin, Q., Cheng, M., Zhang, K., Li, W., Wu, P., Chang, H. and Men, Z. 2021. Development of an iron-based Fischer-Tropsch catalyst with high attrition resistance and stability for industrial application. Catalysts, 11(8), 908.

Notes

Oral presentation: OP2

Selective biocatalytic oxyfunctionalization using unspecific peroxygenases.

Dirk Opperman

[a]*Department of Microbiology and Biochemistry University of the Free State, Bloemfontein, 9300, South Africa,*
E-mail: opperdj@ufs.ac.za.

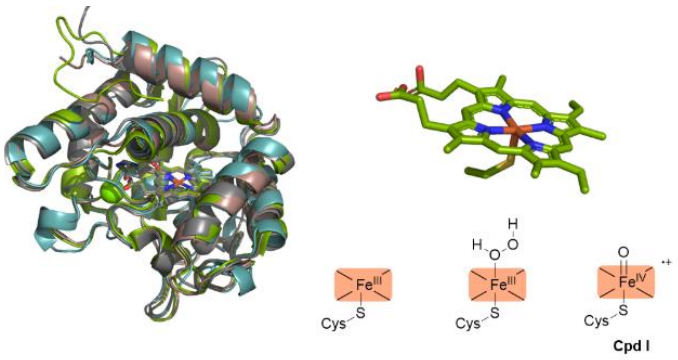
Keywords: oxyfunctionalization, unspecific peroxygenases, hydrogen peroxide.

Abstract

Unspecific peroxygenases (UPOs) are a class of heme-thiolate biocatalysts from fungi that can catalyze oxyfunctionalization reactions of non-activated C-H bonds under mild-conditions. In addition to C(sp3)–H hydroxylation, they also catalyze C(sp2)–C(sp2) epoxidation, aromatic hydroxylation and heteroatom oxidation. These reactions often occur with high regio- and stereoselective. UPOs contain a heme (iron porphyrin ring) prosthetic group able to activate hydrogen peroxide for oxyfunctionalization reactions. Catalysis is generally mediated via a ferryl (FeIV)-oxo porphyrin-pi-cation radical (Cpd I). For hydroxylation, Cpd I abstracts a hydrogen from the target C–H bond to form a ferryl-hydroxy species (Cpd II) and a substrate radical, which, via radical rebound, hydroxylates the substrate. The protein scaffold surrounding the iron porphyrin ring provides the steric constrains and the basis for selectivity. The simplicity and available biocatalytic, or electro(chemical) methods for in situ hydrogen peroxide production makes UPOs ideal for sustainable and scalable reactions.

We have determined the X-ray crystal structures of 4 UPOs, displaying conserved heme binding whereby the proximal face of the heme is coordinated by a cysteine thiolate ligand. This thiolate ligand donates electron density to the Fe centre which stabilizes high-valent iron-oxo intermediates (e.g. Cpd I and II). A conserved acid-base pair at the distal side of the heme (active site) is responsible for H2O2 activation (sixth ligand) through heterolytic cleavage. Here we will give an overview of the structural determinants for H2O2 activation and the potential of a Fe(III)-H2O2 complex for sulfoxidation reactions by removing the acid-base pair and exploring additional oxidants such as tert-butyl hydroperoxide. Additionally, the selectivity and specificity of the UPOs will be explained through structural insights into the binding pocket (active site) and access channels of the UPOs.

Figure 1: Superimposed ribbon diagram of UPO crystal structures (left) with structure of the iron porphyrin ring (right) with reactive species shown below.



Notes

Oral presentation: OP3

Feasibility analysis of Fischer-Tropsch synthesis tail gas as a fuel for solid oxide fuel cells

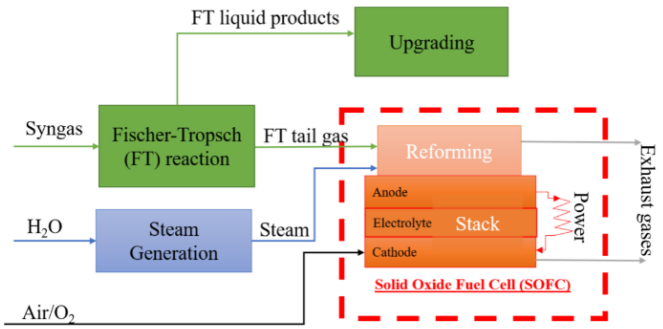
Keyan Wei,[a] Cairong Jiang[b] and Yali Yao[a]

[a]*Institute for Catalysis and Energy Solutions, University of South Africa, Florida, South Africa, E-mail: 19650167@mylife.unisa.ac.za.*
[b]*School of Materials Science and Engineering, Sichuan University of Science and Engineering, Zigong, Sichuan, PR China*

Keywords: carbon deposition, electricity, FTS tail gas, H2/CO ratio, solid oxide fuel cells

Abstract

The tail gas of Fischer-Tropsch synthesis (FTS) contains unconverted syngas and gaseous hydrocarbons. It is usually treated at a high-cost and low efficiency method, whereas it is a feasible fuel for solid oxide fuel cells (SOFCs). Herein, we evaluated the carbon deposition temperature of the FTS tail gas obtained at various reactor pressures. Thermodynamic calculation showed that the FTS tail gas could be used in SOFCs without the risk of car bon deposition. By adding 5% water, the initial non-carbon deposition temper ature was dropped from 830°C (without water co-feeding) to 720°C. Under reforming, the syngas (H2/CO) ratio is about 2 when it reaches equilibrium states, which can be recycled back into the FTS process. Theoretically, a current of 6.5-7.1 A per 100 mL FTS tail gas could be generated by the SOFC. This study demonstrates that it is promising to use the FTS tail gas as a carbon containing fuel for SOFCs.



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Notes

Oral presentation: OP4

Selective degradation of polyethylene via heterogeneously catalysed dehydrogenation and metathesis

Jaco D. J. Becker,[a] John R. Bunt,[a] Hein W. J. P. Neomagus,[a] Naldo J. A. Meyer,[a] and Christien A. Strydom[a]

[a]*Centre of Excellence in Carbon-based fuels, North-West University, Potchefstroom, 2531, South Africa,*

E-mail: jacobecker85@gmail.com

Keywords: polyethylene, chemical recycling, dehydrogenation, metathesis, tandem heterogeneous catalysis

Abstract

In light of the mounting environmental pressures posed by polyethylene (PE) waste [1], a viable recycling pathway is required that not only preserves resource value but also overcomes the shortfalls of conventional mechanical [2] and pyrolytic recycling routes. [3] Tandem dehydrogenation and olefin cross-metathesis (TDOCM) has emerged as a promising chemical recycling method for PE, offering selective conversion to linear alkane products under mild conditions. [4], [5] This work evaluates a novel fully heterogeneous catalyst pairing, Pd/γ-Al_2O_3 for dehydrogenation and WO_x/SiO_2 for metathesis which is capable of degrading virgin and commercial-grade PE feedstocks using n-decane or inexpensive light alkanes as co-reagent at 300 °C and moderate pressure.

Initial experiments confirmed the degradation of high-density polyethylene (HDPE), yielding exclusively alkane products without detectable formation of aromatics or alkenes. Comparative control studies revealed the necessity of both catalysts in facilitating TDOCM, with single-catalyst configurations failing to achieve significant polymer breakdown or cross-incorporation of n-decane. Catalyst efficiency was further demonstrated in reactions using commercial recycled PE containing additives, where comparable conversions and product distributions were observed. Detailed product analysis via GC-MS, FTIR, and GPC revealed that reaction parameters including polymer structure (HDPE vs. LDPE), light alkane concentration, pressure, and catalyst loading substantially influenced yield and product composition. Branched PE (LDPE) exhibited marginally improved conversion and favoured iso-alkane formation, while higher reaction pressures enhanced n-decane incorporation and suppressed light gas formation. Increasing the catalyst-to-polymer ratio accelerated polymer breakdown but skewed distribution towards gaseous products due to redundant metathesis reactions.

Finally, petroleum ether was evaluated as an alternative, economically attractive co-reactant. Despite its branched alkane profile, it too facilitated TDOCM with HDPE under similar operating conditions, further validating the robustness of the catalyst system.

This study demonstrates that TDOCM using WO_x/SiO_2 and Pd/γ-Al_2O_3 is a practical, and plausible chemical recycling route for polyethylene waste, capable of producing well-defined alkane mixtures under relatively mild conditions. Its sensitivity to reaction conditions also provides avenues for tuning product profiles depending on downstream valorisation needs.

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Notes

Oral presentation: OP5

Molecular modelling study into the effects of poisons on manganese-promoted cobalt-based Fischer Tropsch catalysts

Julie-Ann Hoffman[a], Thobani Gambu[a] and Eric van Steen[a]

[a]Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch, 7700, South Africa
*E-mail: hffjul001@myuct.ac.za. **
This work is supported by the German Federal Ministry of Research, Technology and Space (BMFTR) within the CARE-O-SENE project (03SF0673).

Keywords: Fischer Tropsch, cobalt catalysts, manganese promotor, genetic algorithm.

Abstract

The Power-to-Liquids process incorporating the Fischer-Tropsch (FT) synthesis is an efficient approach to produce alternative fuels, which can efficiently reduce CO2 emissions and aligning the transition towards the United Nations Sustainable Development Goals [1,2]. Cobalt-based catalysts are preferred in the industrial FT-process as they exhibit high selectivity for long-chain hydrocarbons, low water-gas shift activity, and resistance to oxidation in the presence of water [3,4]. The design of Co-based FT catalysts has been extensively studied and steered towards producing high selectivity of long-chain hydrocarbons, with low selectivity of by-products such as methane and CO2. The addition of small amounts of manganese to the catalyst system results in a higher activity, and a shift in the product selectivity towards the production of the favourable long chain hydrocarbon products [5], although the mechanism through which this promotional effect occurs is not well understood [6].

More active catalysts typically result in stronger deactivation. Cobalt-based catalysts may deactivate through sintering, carbon formation, oxidation or poisoning.These poisons adsorb onto and block the active sites of the catalyst, preventing the FT reactants from accessing these sites, leading to inhibition and decreased performance towards the reaction [7,8]. Various poisons can be present in the feed for the FT synthesis e.g., compounds containing sulphur (H2S, COS and CS2), and nitrogen (NH3 and HCN) [9]. As such in recent years, molecular modelling has been utilised to investigate this interaction [10,11].

Here, co-adsorption of poisons (e.g. N and S) and Fischer Tropsch species (e.g. H, C & O) on Co(111), Co(100) and Co(644) and Mn-promoted Co-surfaces were investigated to explore effects going beyond the blocking effect. This was investigated using a genetic algorithm (GA) coupled with machine learning (ML) approach to study multiple configurations in a relatively short period of computational time. Previous calculations showed that a string-like MnxOy complex formation was favoured on the cobalt surfaces studied. Henceforth, this manganese oxide complex was considered. One key result was that sulphur on the stepped Co(644) surface led to the ‘restructuring’ of the MnxOy structure from a ‘string’ to a cluster structure. These results illustrate the importance of establishing the effect of poisons on the Mn promotor as may play integral role in the strength of the promotional effect, especially the structural promotion effects, of manganese.

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Notes

Oral presentation: OP6

Ruthenium complexes of pyrazolyl-pyridine ligandsas catalyst precursors for formic acid dehydrogenation/ Carbon Dioxide/(bi)carbonate Hydrogenation

Rotondwa Mphephu,[a] Andrew J. Swarts[a]

[a]*Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa*
Email: 1938482@students.wits.ac.za

Abstract

Hydrogen is a clean and renewable energy source, which provides an attractive alternative to fossil fuels [1]. Significant research efforts have been geared toward developing efficient hydrogen carriers. To this end, formic acid has emerged as the carrier of choice due to its favorable properties, which includes high hydrogen content by weight, ease of transport and handling [2]. The research efforts of the Swarts Research Group focus on the development of catalyst systems derived from earth-abundant metals [3]. Recent efforts in our group has been geared toward the development of new ligand scaffolds with tunable steric and electronic properties which can be exploited in catalysis. Herein, we report on a series of pyridine-pyrazolyl Ru(II) complexes bearing different electronic and steric properties as catalysts in formic acid dehydrogenation (Figure 1). The complexes, upon activation with formate, showed activity towards the dehydrogenation of FA to produce H2 and CO2. Optimisation of the various reaction conditions revealed the influence of temperature, solvent, substrate concentration and the nature and amount of formate additives on the activity of the catalyst. We demonstrated that the catalyst could dehydrogenate formic acid to CO2 and H2 in quantitative yields within 1 hour (5 mmol FA, 0.005 mmol catalyst loading, 3 mmol HCOOK, 100oC, DMSO) with TON's and TOF's of ~1030 and ~1230 h-1 respectively. Preliminary mechanistic studies also revealed the formation of hydride complex in the catalytic cycle. To our delight, the pyrazolyl-pyridine Ru(II) catalyst [C4] also exhibited reversible formate-CO2/(bicarbonate) dehydrogenation−hydrogenation in water.

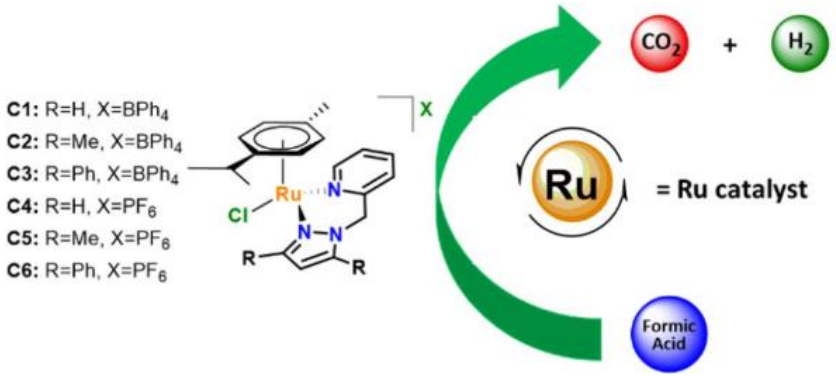

Figure 1: Formic acid dehydrogenation catalysed by Ru(II) pyridine-pyrazolyl complexes

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Notes

Oral presentation: OP7

Catalyst Pore Size Effects on the Fischer-Tropsch Synthesis Product Distribution using Co/SiO2.

Nicholas Jim,[a] Joshua Gorimbo[b] and Linda Jewell[a]

[a]*Department of Chemical and Materials Engineering, University of South Africa, c/o Pioneer Avenue and Christian De Wet, Florida, Private bag X6, 1710, South Africa.*
[b]*Institute of Catalysis and Energy Solutions University of South Africa, c/o Pioneer Avenue and Christian De Wet, Florida, Private bag X6, 1710, South Africa *Corresponding author:*
18211135@mylife.unisa.ac.za.

Keywords: Fischer-Tropsch, synthesis, cobalt, silica, catalyst.

Abstract

Fischer-Tropsch Synthesis (FTS) is suitable for the production of clean, sustainable aviation fuel, provided that the feed is derived from biogas and green hydrogen, reducing reliance on conventional petroleum resources. The development of better catalysts with increased activity, selectivity, and stability leads to more productive and profitable FTS processes, which in turn offer a sustainable and competitive technology to supply fuels and chemicals to international energy suppliers [1]. Cobalt supported on silica, which can be promoted by various metals [2] is one of the most common catalysts used in the FT process and was the catalyst type used in this study. This work explores how the size of the pores in the catalyst affects the product selectivity during Fischer–Tropsch Synthesis (FTS). Four cobalt-based catalysts, all supported on silica with different pore sizes, synthesised using the Stöber process, were implemented in the study while keeping the reaction conditions and catalyst loading constant. Techniques such as BET, XRD, SEM, TPR, and hydrogen chemisorption were used to characterize the catalysts. Mesoporous catalysts of a pore size range of 14 – 30 nm were then tested for 150 hours, at 220℃ and 2 bar in a fixed-bed reactor, where the CO conversion was found to be between 2% and 23%.

The results showed a clear link between pore size and the product distribution. The catalyst with the largest pore size produced the most long-chain hydrocarbons (C_5^+), with selectivity up to 88%. Smaller pores tended to generally produce more methane and short-chain hydrocarbons (C_2–C_4), likely due to restricted diffusion and more side reactions. The variation of carbon monoxide conversion and product selectivity over time was also deduced, which showed that the pore structure plays a key role in maintaining active sites and controlling the product mix.

This study highlights how tailoring the pore size in cobalt catalysts is crucial for maximizing the production of valuable long-chain hydrocarbons in FTS using Co/SiO2 catalysts. It also sheds light on how the catalyst's structure and properties interact to affect its performance throughout the reaction.

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Notes

Oral presentation: OP8

Sustainable BioFuel Production via One-Pot C-C Coupling and Hydrodeoxygenation of Biobased Compound over Versatile LaNi1-xCuxO3±δ Inorganic Perovskites.

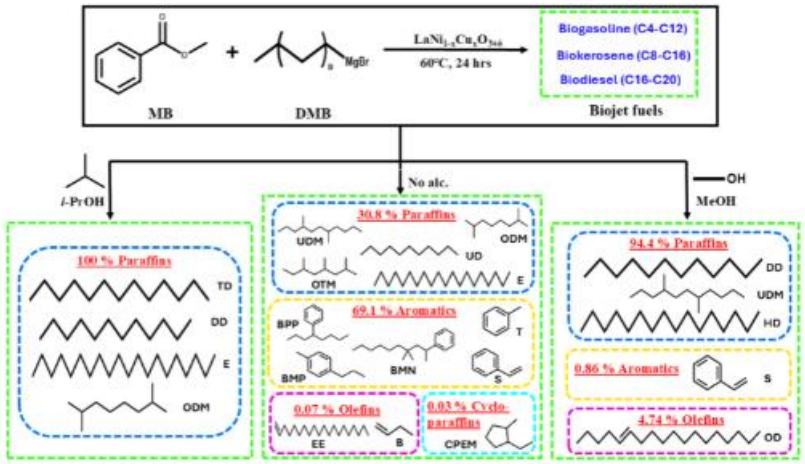
Hlengane Precious Mokwena[a], Sithandile Ngxangxa[b], Isaac N. Beas[c], Nangamso Nathaniel Nyangiwed, Hui Lie, and Ndzondelelo Bingwa[a]

[a]*Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, Roodepoort 1709, E-mail: hlenganemokwena@gmail.com.*
[b]*Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, PO Box 524, Johannesburg, 2001, South Africa.*
[c]*Department of Natural Resources and Materials, Botswana Institute for Technology Research and Innovation, Maranyane House, Plot 50654 Machel Drive, Gaborone, Botswana.*
[d]*Department of Natural Resources and Materials, Botswana Institute for Technology Research and Innovation, Maranyane House, Plot 50654 Machel Drive, Gaborone, Botswana.*
[d]*Tshwane University of Technology, Department of Physics, 175 Nelson Mandela Dr, Arcadia, Pretoria, South Africa. e School of Thermal Engineering, Shandong Jianzhu University, Jinan, 250101, PR China.*

Keywords: perovskites, oxygen vacancies, carbon-carbon coupling, hydrodeoxygenation.

Abstract

Processing of biomass to energy chemicals starts from pyrolysis to oxygenated platform molecules that require hydrodeoxygenation (HDO) to biofuels. Also, the composition and carbon chain lengths from direct pyrolysis make direct utilization in specialized engines difficult due to compatibility issues. Therefore, tailormade carbon-carbon (C-C) coupling and hydrodeoxygenation of bioderived platform molecules become central to attainment of green and sustainable biofuels. In this work, the catalytic activity of LaNi1-xCuxO3±δ ($0 \leq x \leq 1$) perovskites was assessed in the attainment of biofuels, including biogasoline, biokerosene, and biodiesel. The acquired results suggest that the metal ratios of the B-site cations (B and B`) significantly influence the catalytic performance of the perovskites in the conversion of biobased compound to biofuels. Notably, the synthesized LaNi0.5Cu0.5O3±δ perovskites demonstrated efficient one pot C-C coupling and HDO of methyl benzoate and dodecylmagnesium bromide, a Grignard reagent, achieving 58.1% conversion and 100% selectivity towards fuel hydrocarbons at relatively low temperatures (60 to 90 °C). While reactions involving a Grignard reagent normally yield oxygenated products, for the first time the as-synthesized catalysts demonstrated a highly efficient one-pot C-C coupling and dehydration of the biofuel intermediates. Thus, this study provides valuable insights into the design of effective perovskite catalysts for sustainable synthesis of biofuels by looking at the effect of different alcohols as reaction media. Furthermore, this work presents the first use of a Grignard reagent for chain length extension in sustainable synthesis of biofuels.



Scheme 1: Summary of product distribution of biofuel components from one-pot C-C coupling and HDO of MB without alcohol and with the addition of MeOH and i-PrOH over the prepared LaNi1-xCuxO3±δ ($0 \leq x \leq 1$) perovskites.

Notes

Oral presentation: OP9

An *in-situ* RCR study of model cobalt catalysts: exploring the influence of particle size on titania-coated Stöber silica spheres

Shabaaz Abdullah,[a,*] Revana Chanerika,[a] Mohamed I. Fadlalla,[a] Catalina E. Jimenez,[b] Marianne Van der Merwe,[b] Dirk Wallacher,[b] Ivo Zizak,[b] Alexander Dillmann,[b] Marcus Bär,[b] Denzil J. Moodley,[c] and Michael Claeys,[a,*]

[a] *Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch 7700, South Africa. *E-mail: abdsha039@myuct.ac.za and michael.claeys@uct.ac.za.*
[b] *Dept. Interface Design, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str.15, 12489, Berlin, Germany*
[c] *Research and Technology, Sasol, 1 Klasie Havenga Road Sasolburg, 1947, South Africa*

Keywords: cobalt, titania, silica, model, support, size, reduction, carburization.

Abstract

The production of sustainable aviation fuels (SAF) is crucial for recycling carbon within the global energy sector. The Fischer-Tropsch synthesis (FTS) offers an appealing and practical method for producing SAF, making it a focal point for CARE-O-SENE, a German-South African project funded by BMFTR (German Federal Ministry of Research, Technology and Space). In low-temperature (LT) FTS, cobalt (Co)-based catalysts are industrially utilized for the selective production of long-chain hydrocarbons (C_{5+}) from syngas, which can be further processed (*e.g.*, through hydrocracking) to yield the SAF fraction (C_{8-16}) [1].

To improve the activity, selectivity, and stability to C_{5+} hydrocarbons over Co-based FTS catalysts, these metal catalysts are anchored on an oxidic support, namely, alumina, silica, or titania [2]. In this study, a titania-coated silica sphere support material is suggested to mimic the titania dispersions present on an industrial support, as reported elsewhere [3], to assist with the dispersion of cobalt oxide on the support. While carburization is often regarded as a deactivation pathway in FTS, the reduction–carburization–reduction (RCR) approach exploits this transformation to generate the hcp-rich Co phase, which has been reported to exhibit higher intrinsic FTS activity [4]. Given the size-dependence of FTS [5], it is crucial to investigate how the initial Co particle size influences both the propensity for carburization and the regeneration of active-metal through carbide decomposition (see **Fig. 1**.)

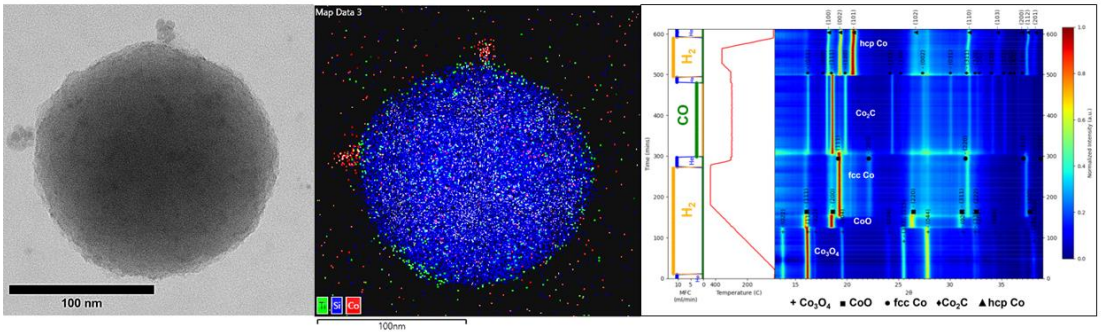


Figure 1. *(left)* TEM and STEM-EDX micrograph of Co_3O_4 nanoparticles dispersed on a model TiO_2-coated SiO_2 sphere support. (*right*) RCR heatmap as studied *via* synchrotron-based *in situ* XRD.

Acknowledgement
This work was supported by the German Federal Ministry of Research, Technology and Space (BMFTR) within the CARE-O-SENE project (03SF0673)

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Notes

Oral presentation: OP10

Ethanol-Enabled Pyridyl-pyrazole Manganese (I) Catalysis: Sustainable Transfer Hydrogenation of Nitriles with Amine Boranes

Tshegofatso Molapo[a], Andrew J. Swarts[a]

[a]*Swarts Research Group, School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa.*

Keywords: manganese catalysis, transfer hydrogenation, pyridyl-pyrazole ligands, amine boranes, sustainable chemistry

Abstract

Manganese catalysts offer sustainable alternatives to precious metals for nitrile transfer hydrogenation (TH), yet solvent selection remains critical. While isopropanol dominates TH for its hydrogen-donor capacity and recent Mn catalysis utilised diethyl ether [1], ethanol's potential is unexplored despite superior green metrics. Pyridyl-pyrazole Mn(I) complexes were evaluated for nitrile TH using dimethylamine borane (DMAB). Conversions (19F NMR/GC-MS) and selectivity were assessed at 65–80°C. Kinetic studies probed mechanistic pathways. Under optimised conditions (3 mol% catalyst, 3 equiv. DMAB), ethanol achieved 93.4–94.8% conversion, rivalling isopropanol (96.6 – 97.1 %) while offering enhanced sustainability (low cost, toxicity). Catalyst-free controls confirmed ethanol's negligible background conversion (0% vs. 16.6 % for isopropanol). Ethanol's efficiency, unprecedented in TH catalysis, enables near-quantitative reductions without noble metals. This work establishes pyridyl-pyrazole Mn complexes as efficient catalysts for nitrile hydrogenation in ethanol - a breakthrough solvent for sustainable transformations. The ligand design overcomes limitations of commonly used phosphine systems and challenges of isopropanol/ether dependence.

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Notes

Oral presentation: OP11

Mn and Fe promoted Co3O4/CeO2 catalysts for the preferential oxidation of carbon monoxide.

Wavhudi Nevhutalu,[a] Noluvuyo Ndila,[a] and Patricia J. Kooyman[a]

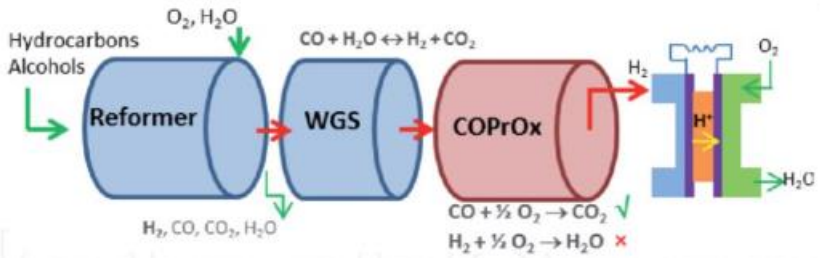
[a]*Catalysis Institute, Department of Chemical Engineering, University of Cape Town, South Ln, Rondebosch, 7700, South Africa.*
Email: nvhwav001@myuct.ac.za

Keywords: Promoters, Co_3O_4, CO-PRO

Abstract

Goal 7 of the Sustainable Development Goals (SDGs): providing affordable and clean energy, propels the continuous development of reliable and environmentally friendly energy generation operations. Considering the dire effects of climate change on the environment due to greenhouse gas emissions, the transition from the use of coal to the use of fuel cells for energy generation decreases the overall impact of global warming [1]. Hydrogen is considered a leading fuel for the use of fuel cells and Figure 1 illustrates the process of the hydrogen production.

Figure 1: Processes of the production of hydrogen for fuel cells (Taken from [2])



The final hydrogen stream of the water-gas shift reaction contains 1% of carbon monoxide which is poisonous to the platinum catalyst in the anode of the fuel cell. The preferential oxidation of carbon monoxide (CO-PROX) is employed due to its high efficiency and low energy consumption to reduce the carbon monoxide content to 10 ppm before the hydrogen is introduced to the fuel cell [3]. A ceria-supported cobalt oxide (Co3O4/CeO2) catalyst that is used during CO-PROX deactivates at 225°C, due to the reduction of the active cobalt ion to metallic cobalt. Consequently, methanation occurs.

This study builds on the work of [4] to determine the effect that manganese and iron promoters have on the catalyst during CO-PROX, by enhancing the catalyst synthesis methods. It is hypothesised that the promoted catalyst will deactivate well above 225°C. Furthermore, the conversion of CO is expected to increase significantly at lower temperatures, deeming manganese and iron suitable promoters to increase the activity and stability of the catalyst.

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Notes

Oral presentation: OP12

In-situ encapsulation of single Pt atoms inside MFI for hydrocracking

Thabiso Ntlebi, and Patricia J. Kooyman*

The Catalysis Institute, Department of Chemical Engineering, University of Cape Town, South Lane, Rondebosch 7700, South Africa,
**E-mail: patricia.kooyman@uct.ac.za.*

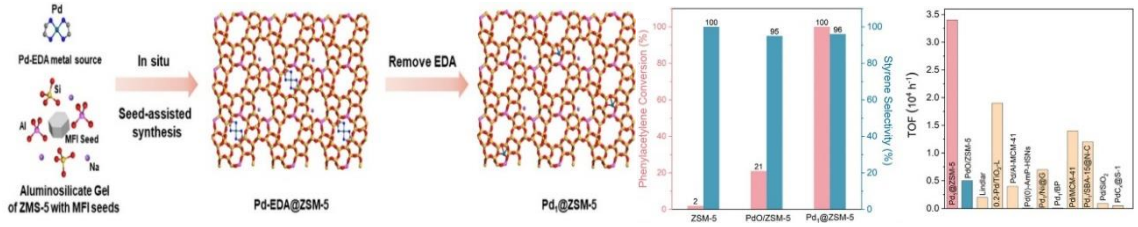
Keywords: single atoms, platinum, hydrocracking, zeolite, Fischer-Tropsch.

Abstract

1. Introduction

Single-atom catalysts offer a promising approach by maximizing efficiency through uniform dispersion [1]. Platinum (Pt) metal supported on zeolites is the preferred catalyst for hydrocracking Fischer-Tropsch wax due to its high activity and selectivity in these reactions [2]. In MFI zeolite, well-dispersed single Pt atoms are hypothesized to enhance catalytic activity in hydrocracking processes significantly.

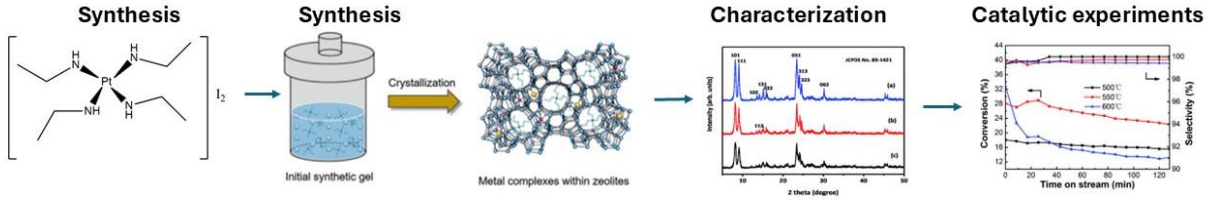
Generally, Pt metal is supported on zeolites through impregnation or ion exchange methods. However, these approaches often result in a non-homogeneous distribution of metal species and inefficient utilization of noble metal [3]. An alternative method involves the *in-situ* incorporation of the metal ion during the synthesis process, which allows the metal precursor to be integrated directly inside the zeolite. Recent work by Liu et al. [4] demonstrated the encapsulation of palladium (Pd) single-atom sites within ZSM-5 zeolite using ethylenediamine as a ligand, and the gel was crystallized for 2.5 days. Liu et al. [4] further revealed that Pd single-atom catalysts confined in ZSM-5 showed high catalytic activity in the semi-hydrogenation of phenylacetylene. This study aims to prepare single platinum atoms supported on MFI zeolite and evaluate their catalytic performance in hydrocracking.



Scheme 1: Schematic illustration for the synthesis procedures of Pd_1@ZSM-5 by the seed-assisted growth method, Catalytic performance of Pd_1@ZSM-5, PdO/ZSM-5, and ZSM-5 in semi-hydrogenation of phenylacetylene and TOF values comparison of different catalysts for semi-hydrogenation of phenylacetylene under their optimal reaction condition [4].

2. Experimental

$[Pt(EtNH_2)_4]I_2$ will be synthesized by adding K_2PtCl_4 to an excess ethylamine solution and characterized using ^{13}C and ^{1}H NMR, as well as FTIR spectroscopy. The synthesized complex will then be incorporated into the MFI synthesis gel and crystallized to form Pt atoms within the MFI zeolite framework. The resulting zeolite will be characterized followed by catalytic performance in hydrocracking processes (**Scheme 2**).



Scheme 1: Layout of project

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Notes

Oral presentation: OP13

Suppression of CH4 formation in Mn and Fe partially substituted LaCoO3 during the Preferential Oxidation of CO in H_2 Streams

Noluvuyo Ndila and Patricia Kooyman

Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch, 7700, South Africa,
E-mail: ndlnol010@myuct.ac.za

Keywords: SGDs, fuel cells, CO-PROX, perovskite oxides catalysts

Abstract

Today's energy production relies heavily on fossil fuels, leading to significant environmental challenges, including climate change [1]. To mitigate these issues, the United Nations has prioritized the development and provision of sustainable, dependable, and clean energy as part of its Sustainable Development Goals (SDG 7 and 13) [1]. Proton exchange membrane fuel cells (PEMFCs) are among the leading sustainable energy sources and play a crucial role in the energy transition process. Currently, 95% of H2 production is via steam reforming; however, this H2 must be purified to reduce the CO concentration before its utilization in PEMFCs [1]. CO deactivates the Pt catalyst of fuel cells [2]. Preferential oxidation of carbon monoxide (CO-PROX) is one of the most effective methods for H2 purification for fuel cells [2]. Cobalt-based catalysts are highly active for CO-PROX. However, studies have shown that during the time on stream, Co3O4 catalysts deactivate via the reduction of Co3O4 to metallic Co at temperatures above 175℃ [2,3]. Metallic Co is active for CO methanation, which consumes the desired H2 product [2,3].

To address the deactivation of cobalt-based catalysts, this study investigates the stabilization of Co3+/Co2+ cations in a perovskite oxide matrix (LaCoO3) to overcome overreduction to metallic cobalt. Additionally, we investigate the effect of partially substituting Co3+ with Mn3+ (LaCo1-xMnxO3±δ) or Fe3+ (LaCo1-xFexO3±δ), where x = 0, 0.1, 0.15, 0.2, on the activity, selectivity, and phase stability of the catalysts during CO-PROX. XRD, EDS, BET, and ICP-OES characterized the structural properties of the catalysts. The redox kinetics of the catalysts were investigated via TPR/TPO cycles using TGA. TGA and iodometric titrations were used to determine the oxygen non-stoichiometry of the catalysts. The correlation of the catalyst structure with catalytic performance was investigated via in situ XRD.

XRD patterns showed no diffraction lines related to impurities related to Mn and Fe. The unit cell volume increased with increasing Mn3+/Fe3+ content because they have a bigger ionic radius than Co3+. EDS showed a homogeneous distribution of La, Co, Mn/Fe, and O, which confirms the successful incorporation of Mn and Fe in LaCoO3. The oxygen non-stoichiometry increases with increasing substituent content. The catalytic performance evaluations showed that the catalytic performance improves with the incorporation of Mn and Fe. LaCo0.85Mn0.15O3 achieved 99.9% at 220℃, LaCo0.85Fe0.15O3 achieved 90% conversion at 310℃, and LaCoO3 achieved a maximum CO conversion of 58% at 300℃. Additionally, for LaCoO3 and LaCo0.85Fe0.15O3, there was negligible CH4 formation, while for LaCo0.85Mn0.15O3 onset of CH4 occurred at 330℃. The B-site partial substitution increases the hybridization of the O-2p band center and the B-site metal cation 3d-band center [4]. Increased hybridization signifies improved covalency, which makes electron transfer to and from the metal center easier, improves the lattice oxygen activity and mobility, thus improving catalytic performance [4]. These catalysts can potentially replace conventional cobalt-based catalysts as they exhibit improved catalytic activity and stability.

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Notes

Oral presentation: OP14

Hydrogenolysis of polyolefins into liquid hydrocarbons over a bimetallic silica supported nickel-molybdenum catalyst

Carol Dlamini,[a] Chelsea Tucker,[c] Hendrik Van de Bovenkamp,[b] Mzamo Shozi[d] and Pinkie Ntola[a]

[a] *Department of Chemistry, Durban University of Technology, P.O. Box 1334, Durban 4001, South Africa, E-mail: 21829499@dut4life.ac.za.*
[b] *Department of Chemical Engineering, University of Groningen, Nijenborgh 4, 9747 AG, Netherlands.*
[c] *Herbert H. Dowweg, 5, 4542 NM Hoek, Netherlands.* [d] *School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X54001, Durban 4000, South Africa.*

Keywords: polyolefins, chemical upcycling, hydrogenolysis, nickel catalysts

Abstract

Catalytic hydrogenolysis has emerged as a promising technique for chemical recycling of polyolefins. This process involves the selective cleavage of C-C bonds in a hydrogen-rich environment under relatively mild conditions, converting plastic waste into valuable hydrocarbons that can serve as fuel and chemical feedstocks [1]. However, a key challenge lies in developing cost-effective and efficient catalysts that favour the production of liquid-range hydrocarbons over low-value gaseous products, such as methane. Ni-based catalysts have demonstrated strong activity in polyolefin hydrogenolysis, although the high production of methane remains a significant problem [2]. Recent progress in bimetallic catalysts has offered strategies to mitigate this issue [3]. In this study, $NiMo/SiO_2$ was evaluated for the hydrogenolysis of polyethylene and compared to Ni/SiO_2 under mild conditions of 300 °C and 30 bar of H_2. After 18 h, Ni/SiO_2 completely converted polyethylene into gaseous and liquid products, with methane accounting for 36 % of the products. In contrast, $NiMo/SiO_2$ exhibited a much lower conversion of 9 % to gaseous products. Notably, the selectivity for methane was nearly equal to that of propane, unlike Ni/SiO_2, which produced methane as the dominant gaseous product. This shift in product distribution suggested that the addition of Mo suppressed the demethylation tendency of Ni, though at the expense of catalytic activity. XRD data, together with H_2-TPR, confirmed the incorporation of Mo into the Ni lattice structure, indicating a structural modification that altered Ni's catalytic behaviour. Although conversion was reduced for the bimetallic catalyst, these findings pave the way for future catalyst refinement and design.

Table 1: Gaseous yield for Ni/SiO_2 and $NiMo/SiO_2$

Catalyst	C_1 yield	C_2 yield	C_3 yield
$15Ni/SiO_2$	36.10	3.59	3.01
$15Ni5Mo/SiO_2$	4.53	0.25	4.63

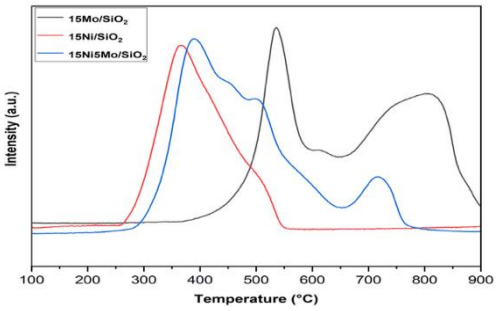

Figure 1: H_2-TPR results of

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Notes

Oral presentation: OP15

Photocatalytic degradation of ciprofloxacin through persulfate activation by NiCo-C catalyst

P.J. Mafa[a],*, M.E. Malefane[a], F.Opoku[b], B.B. Mamba[a], A.T. Kuvarega[a]

[a]*Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida, 1709, Johannesburg, South Africa.*
[b]*Department of Chemistry, Kwame Nkrumah University of Science and Technology, Kumasi, Ghana*
mafa.027@gmail.com

Keywords: photocatalysis, persulfate, charge transfer, ciprofloxacin, mechanism.

Abstract

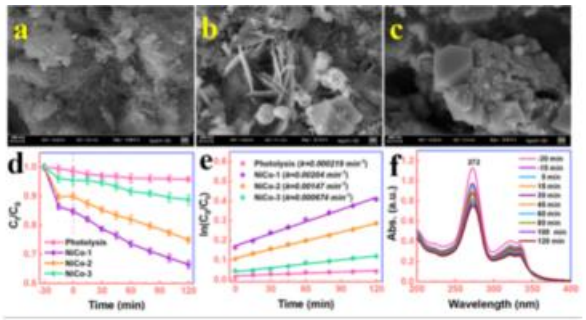
Antibiotics such as ciprofloxacin (CIP) have found a very important use in human health and animal husbandry, but their excessive use ends up causing havoc in aquatic life, and this kind of pollution is considered the most dangerous environmental challenge [1]. The CIP antibiotic in water is associated with negative health effects, and its removal is paramount.

Photocatalysis using semiconductors has appeared as a powerful technology that is green for the treatment of CIP-contaminated waters [2]. The combination of photocatalysis and persulfate activation is a more plausible route for the degradation of pollutants. The process of persulfate photocatalysis relies on efficient activation by breaking down the O–O bond in persulfate material [3]. Heterogeneous activation using metal-based catalysts such as Co3O4, NiO, NiCo2O4, carbon, etc., is regarded as an efficient way to break the O–O bond [4]. This work sought to find effective and efficient photocatalysts from nickel, cobalt, oxygen, and carbon for the heterogeneous activation of persulfate toward the degradation of CIP pollutants.

The photocatalysts were prepared by sequential calcination of the precursors at 500 °C for 7 h to yield the three catalysts. After the synthesis step, the photocatalysts were characterized, and Figure 1 exemplifies the integrity of the materials. Scanning electron microscopy (SEM) images illustrate flower-like, fibrous, and pentagonal morphology as seen in Figure 1a-c. Ramana analysis indicates the presence of defects with ID/IG and D' peak. The prepared catalysts were evaluated for photocatalytic degradation using CIP (10 ppm, 100 mL) as a model pharmaceutical pollutant. NiCo-1 exhibited removal efficiency of 1.34 and 2.98 times higher than NiCo-2 and NiCo-3, respectively (Figure 1d). The rate constants of NiCo-1, NiCo-2, and NiCo-3 were found to be 0.00204 (R2=0.991), 0.00147 (R2=0.997), and 0.000673 min-1 (R2=0.973) as shown in Figure 1e. Figure 1f depicts the reduction of the CIP peak at 272 nm as degradation time increases. The improved performance of NiCo-1 was linked to high charge migration rates as confirmed by electrochemical analysis. Although the NiCo-1 catalyst displayed improved performance as compared to NiCo-2 and NiCo-3, the degradation efficiencies are far below 50% and this calls for more improvement to achieve high degradation efficiencies. Therefore, the next step is the explore the activation of peroxydisulfate toward attaining high CIP removal efficiencies.

A collage of images of plants and a graphDescription automatically generated with medium confidence

Figure 1. (a-c) SEM images of NiCo-1, NiCo-2, and NiCo-3, (d) CIP degradation efficiency in different systems, (e) Kinetic plots, and (f) UV-vis spectra of CIP degradation.



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Notes

Oral presentation: OP16

Towards a Sustainable Future – Synthesis, Characterization, and Catalytic Evaluation of Conventional SSZ-13 with Varying Si/Al Ratios

Bevan George and Patricia J. Kooyman

Centre of Catalysis Research, Department of Chemical Engineering, University of Cape Town, Rondebosch, Cape Town, South Africa,

E-mail: GRGBEV001@myuct.ac.za.

Keywords: SSZ-13, methanol-to-hydrocarbons, DME conversion, sustainability, gLFG

Abstract

To combat climate change, reducing reliance on fossil fuels is essential. However, global energy demands—especially in emerging economies—still depend heavily on them. The GreenQUEST project, funded by the German government, aims to develop a sustainable alternative to cooking fuels like coal, wood, and LPG by converting captured CO_2 and green hydrogen into liquefied fuel gas (gLFG). This is achieved through the catalytic conversion of dimethyl ether (DME) and green hydrogen using a Pd/solid acid bifunctional catalyst. The project's scientific goal is to assess whether the DME-to-gLFG reaction (analogous to the methanol-to-hydrocarbon (MTH) reaction) can yield an economically viable product stream. The methanol-to-hydrocarbons (MTH) process currently uses SAPO-34, a CHA-type material, due to its effective product selectivity [1]. However, SAPO-34's weak acidity requires operation at high temperatures (400–500°C) to offset its diffusion limitations [2]. These high temperatures are acceptable in coal-based economies but make renewable methanol routes economically unsustainable.

SSZ-13, which also adopts the CHA framework, offers stronger acidity than SAPO-34 and thus promises improved reactivity at lower temperatures [2]. However, its high acidity also makes it prone to deactivation by coking. While introducing mesoporosity has been studied to mitigate this, our study focuses on tuning the Si/Al ratio (SAR) of SSZ-13 to find an optimal balance between acidity, catalytic activity, and stability.

SSZ-13 samples with SARs of 15, 20, 25, and 30 were synthesized using a direct hydrothermal method, followed by Pd impregnation. These samples were characterized using NH3-TPD, XRD, BET, ICP, and TEM to evaluate acidity, crystal structure, surface area, composition, and Pd dispersion. The catalytic performance of each was evaluated in the DME to gLFG reaction.

The study aims to understand how varying the SAR in conventional SSZ-13 influences catalytic behaviour and to identify the optimal SAR that minimizes deactivation while maintaining high activity — a key requirement for economically viable low-temperature gLFG production

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Noted

Oral presentation: OP17

Degradation of ciprofloxacin and sulfamethoxazole in water using an ozonation/persulfate system under solar irradiation.

Tankiso Johannes Masangane, Motsa Machawe Mxolisi and Alex Tawanda Kuvarega

Institute for Nanotechnology and Water Sustainability, College of Science, Engineering, and Technology, University of South Africa, Florida 1709, Johannesburg, South Africa.

64028224@mylife.uisa.za.ac

Keywords: Advanced Oxidation Processes (AOPs), Ozonation, Persulfate, Pharmaceuticals, Solar Irradiation, Hydroxyl Radicals, Sulphate Radicals, Wastewater.

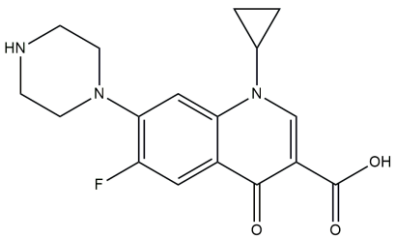
Abstract

Pharmaceutical contaminants such as ciprofloxacin (CIP) and sulfamethoxazole (SMX) present significant environmental and public health risks due to their persistence in water and resistance to conventional treatment. This study evaluated the degradation of CIP and SMX using an ozone-based advanced oxidation process (AOP) under natural solar irradiation (85,200 lux) in a 15 L borosilicate glass reactor with a 10 cm ceramic gas diffuser. Experiments were conducted at 25°C, with ozone introduced at controlled dosage rates. Key parameters assessed included ozone dosage (250–1000 g/m³), pH (2–10), initial concentrations (10–60 ppm), and persulfate (PS) dosage (0.045 mmol/L).

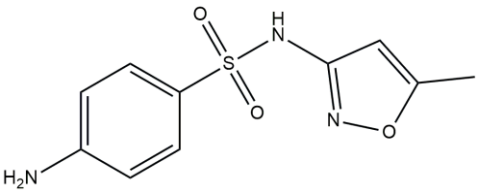
Solar irradiation alone contributed minimally to CIP degradation, while higher ozone dosages (500–1000 g/m³) achieved up to 97% CIP degradation in 60 minutes. Increased initial contaminant concentrations reduced degradation efficiency, while alkaline conditions (pH 10) improved degradation rates to 98% for CIP and 88% for SMX. The addition of 0.045 mmol/L PS further accelerated degradation, achieving over 90% CIP degradation within 15 minutes. A preliminary cost analysis estimated the chemical cost at $0.0036 per litre run, with the potential for significant reduction through reactor optimisation. The scavenger quenching experiments confirmed that both •OH and $SO_4^{\bullet-}$ are the dominant reactive species driving CIP degradation.

The results demonstrate the effectiveness and adaptability of the O_3/PS system for antibiotic degradation, highlighting the importance of operational parameter optimisation for enhanced performance and cost efficiency.

Figure 1: Studied antibiotics



Ciprofloxacin (CIP)



Sulfamethoxazole (SMX)

Notes

Oral presentation: OP18

Synthesis of Pd/SAPO-34 catalysts for the conversion of dimethyl ether to green Liquified Fuel Gas for clean cooking in Africa.

K. S. Nene[1], S. J. Roberts[1], N. Fischer[1], J. C. Q. Fletcher[1] & S. Raseale[1]*

*shaine.raseale@uct.ac.za
[1]*Catalysis Institute, University of Cape Town, Rondebosch, Cape Town, 7700*

Keywords: green Liquified Fuel Gas, Pd/SAPO-34 catalyst, Dimethyl ether

Abstract

Liquefied petroleum gas (LPG) is an easy to store, highly portable, efficient, and clean burning cooking fuel with the potential to substitute the heavily polluting solid fuels (e.g., coal and biomass) prevalently utilised in low-income households in Sub-Saharan Africa. However, LPG remains fossil-derived, prompting the pursuit of renewable alternatives such as Green Liquefied Fuel Gas (gLFG), which can be synthesized from captured CO_2 and green H_2. To date, the potential route for gLFG synthesis involves the hydrogenation of co-fed CO and/or CO_2 through sequential multiple reactions-methanol formation, dimethyl ether (DME) synthesis from methanol, and subsequent conversion of DME to gLFG-typically performed in a "one-pot" approach over a hybrid catalyst [(Cu/ZnO/ZrO_2/Al_2O_3)/Pd-H-Beta] [1], [2], [3]. While convenient, this approach yields a complex product stream with significant water and coke precursors (e.g., polymethyl benzenes) formation, leading to rapid catalyst hydrothermal instability and deactivation.

To address these challenges we propose an unbundled, multi-stage sequential process that allows optimization of each individual reaction step under its optimal operating conditions with intermittent water removal. While the other initial reaction steps are well-understood and close to or already industrially implemented, the DME-to-gLFG step is still poorly understood and is the focus of this study [4]. Prior work identified Pd/H-Beta as a promising bifunctional catalyst, yet its hydrothermal instability emanating from acid sites interaction with water formed in situ limits performance. Chabazite Silicoaluminophosphate (SAPO-34) zeolites, with milder acid sites and conceivably superior hydrophobicity, may offer enhanced hydrothermal stability than aluminosilicate zeolites which lack Phosphorus in their framework [5].

In this work, we present the synthesis of SAPO-34 with tuneable acidity via Si/(Si+Al+P) ratio adjustment and subsequent Pd impregnation to form Pd/SAPO-34 catalysts. Structural properties, acidity, and hydrothermal stability are characterized, and catalytic performance in the DME hydrogenation to gLFG is evaluated in a fixed-bed reactor. The results will demonstrate the impact of acid sites modulation on product selectivity and stability, offering insights for the development of robust catalysts for renewable fuel synthesis.

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Notes

Oral presentation: OP19

Quantification of Operando Metal Nanoparticle Morphological Dynamics Using Machine Learning and Digital Image Processing

Thomas Neff, Dr. Kyle Abrahams, and Prof. Patricia J Kooyman

Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch, 7700, South Africa,
E-mail: nfftho001@myuct.ac.za, kyle.abrahams@uct.ac.za, and patricia.kooyman@uct.ac.za

Keywords: Nanoparticle, machine learning, image processing, silhouette-fitting

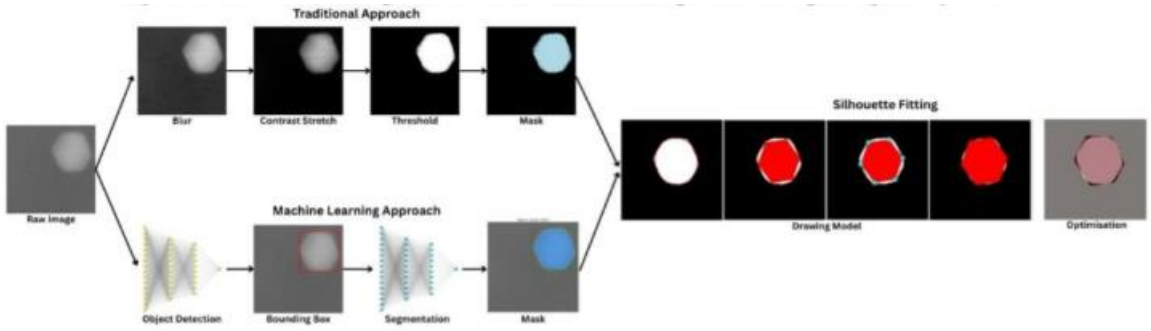
Abstract

The catalytic performance and activity of metal nanoparticles (mNPs) depend upon their size and structure. In specific reactive environments, the surface structure of a mNP is dynamic due to the changing interfacial free energies between the environment and the mNP's surface terminations [1]. This complex structure-performance relationship can be studied using operando transmission electron microscopy (TEM) [1, 2]. 2D TEM time series allow for the visualisation of the dynamic behaviour of mNPs.

Manual quantitative analysis of morphology changes is inherently subjective, inconsistent, and inefficient. Computational techniques offer more consistent and automated methods for quantifying morphology changes. Silhouette fitting, developed by Roobol (2014), provides a method for measuring shape dynamics by quantifying the degree of rounding at a mNP's corners to infer information about its overall degree of roundness [2]. A high degree of rounding at the corners implies a rounder mNP, while less rounding implies a facetted particle. By processing individual frames in a time series, the shape evolution of the mNP can be tracked over time with parameters such as temperature and partial pressure.

This study discusses a workflow designed to automate the quantification and classification of mNP shape changes. Image segmentation is employed as the first step in this workflow, which can be achieved using either traditional digital image processing (DIP) techniques, such as thresholding, or machine-learning techniques (Fig. 1). When using a machine-learning approach a mNP is first detected using YOLO, an object detection model, and is then segmented using the SAM2 model, for zero-shot segmentation [3, 4, 5]. Downstream from segmentation, a drawing model and subsequent optimisation produce a silhouette of the original mNP (Fig. 1). This provides a reconstruction and measurement for the roundness of the mNP. mNPs can, therefore, be classified as round or facetted, and the extent of this classification can be quantified. As a complete tool, this workflow can aid in the study of the structure-performance relationship of mNPs.

Figure 1: Workflow for quantification of metal nanoparticle morphological dynamics.



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Notes

Oral presentation: OP20

Implementation of Biocatalysis technologies on an industrial scale in South Africa.

Lucia Steenkamp, Chris van der Westhuyzen and Ntsoaki Mosina

Chemicals Cluster, Biomanufacturing, CSIR. Meiring Naude Road, Pretoria, 0001, South Africa,
E-mail: lsteenkamp@csir.co.za.

Keywords: biocatalysis, commercialisation, bio-economy, circular economy.

Abstract

The bio-economy in South Africa is defined as any biotechnological activities and processes which can be implemented on commercial scale and are creating revenue. The South African Government has identified the bio-economy to be a significant contributor to the country's economy by 2030 in terms of the gross domestic product (GDP). Biocatalysis has been identified in the Decadal Plan as one of the important areas in South Africa which will contribute to the Bio-economy. The CSIR is hosting the Industrial Biocatalysis Hub with funding from the Technology Innovation Agency (TIA) and the Department of Science, Technology and Innovation (DSTI). One of the main activities of the Hub is the development of new or improved technologies for commercialization in collaboration with large companies and SMME industry partners. Complete circular economy technologies are also developed.

The use of biocatalysis in commercial processes is gaining momentum as the processes can be carried out under very mild conditions and in organic solvents as well as aqueous environments, with enzymes and biocatalytically active cells. The technologies are renewable and sustainable. Biocatalysis is the ultimate green technology and conforms to at least 10 of the 12 Principles of green chemistry. Waste is normally reduced significantly or completely eliminated.

Some of the biocatalysis technologies developed by the CSIR for industry which will be discussed in detail include (-) Ambrafuran and Orris butter for the fragrance industry as well as products for the cosmetics market, which include Aloesin, a natural skin lightener. A technology to produce free fatty acids, using an immobilised enzyme instead of alkaline hydrolysis at high temperatures, used in the mining industry to float and recover rare minerals will also be discussed. A platform technology has also been created for bioconversion of nitro containing substrates to amine products, which with classical chemical synthesis can potentially result in explosive reactions. The amine compounds are very important in the pharmaceutical and veterinary industries as 70% of these compounds have an amine active group. Biocatalysis is also extremely valuable in the circular economy where waste streams are turned into valuable products. An example is the beneficiation of the whole citrus fruit to create products for the biocide, insecticide, bioplastics and food sectors. A promising technology was also developed from paper and pulp waste as ruminant feed for an industry partner.

Noted

Oral presentation: OP21

Influence of catalyst preparation and Mn promotion on model Co-based FT catalysts for Fischer-Tropsch Synthesis

Revana Chanerika,[a]* Shabaaz Abdullah,[a] Mohamed I. Fadlalla,[b] Denzil Moodley,[c] and Michael Claeys[a]*

[a]*Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch, 7700, South Africa*
[b]*Research and Technology, Energy Operations and Technology, Sasol South Africa, Sasolburg 1947, South Africa*
E-mail: revana.chanerika@uct.ac.za and michael.claeys@uct.ac.za

Keywords: Fischer-Tropsch synthesis, cobalt, manganese, solid solutions, Co-Mn interface.
This work was supported by the German Federal Ministry of Research, Tec

Abstract

Achieving net-zero emissions hinges on transforming the transportation sector, which remains heavily reliant on fossil-derived fuels and is responsible for roughly 25% of global energy-related CO_2 emissions [1]. Fischer–Tropsch synthesis (FTS) offers a promising deviation from this dependency by enabling the direct conversion of renewable syngas into clean-burning transportation fuels [2]. Within this context, the CARE-O-SENE project unites science and industry to pioneer next-generation catalysts aiming to improve productivity and offer precise control over product selectivity, specifically targeting green synthetic kerosene. Cobalt catalysts have been one of the long workhorses of low-temperature Fischer-Tropsch synthesis (LTFTS) for jet-fuel-range hydrocarbons, yet their performance is often limited by water-induced deactivation [3] – their long-term stability and selectivity remain under constant optimisation. Manganese promotion offers a compelling path forward when incorporated into the cobalt lattice, however, the formation of Co-Mn solid solutions (SS) is traditionally associated with limited FT activity due to poor reducibility [4].
Here, as part of the CARE-O-SENE initiative, we challenge this convention. By adopting carefully designed synthesis routes and characterisation conditions, we show solid solution catalysts (with enhanced Co-Mn interaction) capable of overcoming the reduction barrier (Fig. 1) where support effects impede the observed Co0 sintering occurring in the unsupported material (from Rietveld refinement).

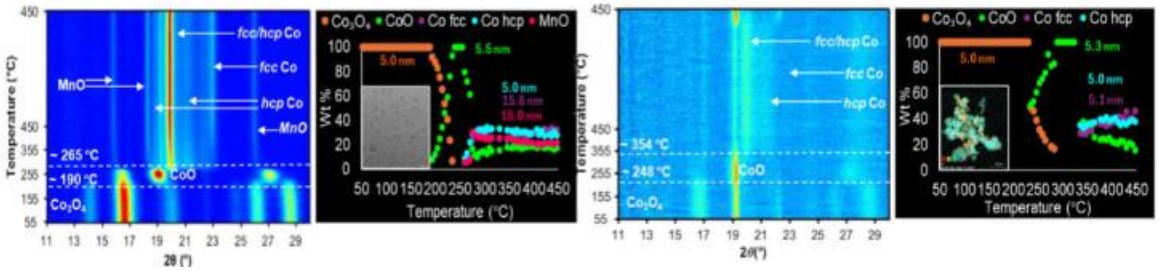

Figure 1. In situ XRD plots and Rietveld refinement of unsupported (left) and supported Co-Mn catalysts (right).

With the tailored electronic environment at the active sites of the Co-Mn interface in the SS catalyst, we aim to unravel the origins of the Co-Mn synergy in these catalysts under realistic FT conditions. These findings coupled with in situ X-ray diffraction and other complementary characterisation techniques will drive the rational design of robust, high-throughput catalysts that offer potential to promote favourable hydrogenation and chain-growth pathways and transform an often-overlooked FT catalyst class into a competitive, inexpensive alternative for large-scale, clean kerosene production.

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Notes

Oral presentation: OP22

Covalent immobilisation of xylanase on carboxyl-activated chitosan-coated magnetic nanoparticles for animal feed treatment

Justin B. Safari [a,b] Vincent J. Smitha and Brett I. Pletschke[b]

[a]*Department of Chemistry, Rhodes University, P.O. Box 94, Makanda 6140, Eastern Cape, South Africa, E-mail: safaribazibuhejustin@gmail.com*

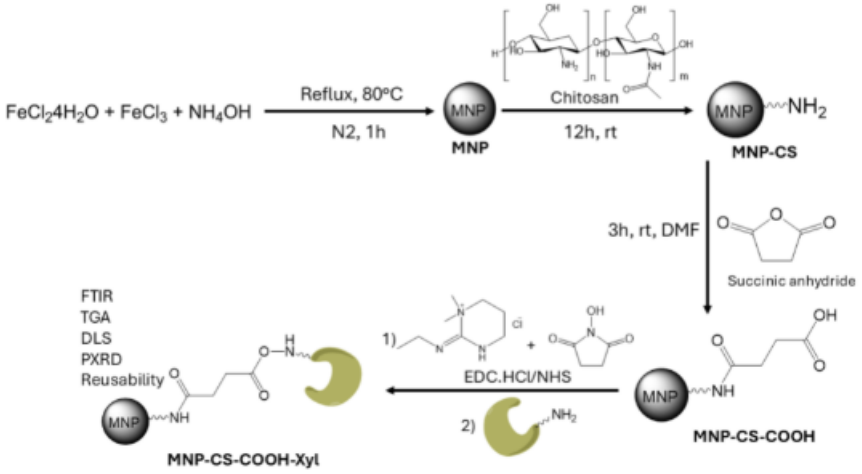
[b]*RU Node of the Industrial Biocatalysis Hub (IBH), Department of Biochemistry, Microbiology and Bioinformatics, Rhodes University, P.O. Box 94, Makanda 6140, Eastern Cape, South Africa.*

Keywords: immobilisation, xylanase, magnetic nanoparticles, animal feed

Abstract

Improving the digestibility of animal feed is essential for raising the feed efficiency, growth performance and nutrient absorption of livestock [1]. In this study, xylanase was covalently immobilised onto carboxyl-activated chitosan-coated magnetic nanoparticles (CC-MNPs) to develop a stable and reusable biocatalyst for hemicellulose degradation in animal feed. Magnetic nanoparticles were synthesised via co-precipitation, coated with chitosan, and functionalised with carboxyl groups using succinic anhydride to enable covalent enzyme attachment through carbodiimide-mediated activation. The immobilisation process was optimised by varying the enzyme concentration, the mass of nanoparticles and activation time, achieving a maximal activity recovery of close to 100%. Characterisation of the produced biocatalyst by FTIR, PXRD, DLS, and TGA confirmed successful coating, functionalisation, and enzyme immobilisation, while magnetic responsiveness facilitated rapid separation and reuse. The immobilised xylanase displayed enhanced thermal and pH stability compared to the free enzyme, retaining over 50% activity after six reuse cycles. In vitro feed degradation assays demonstrated a significant increase in the release of reducing sugars, highlighting its potential to improve fibre digestibility in monogastric diets. In addition, the xylo-oligosaccharides produced exhibited a prebiotic effect. This study presents a robust and magnetically recoverable xylanase system with promising applications in the sustainable processing of animal feeds.

Figure 1: Immobilisation of xylanase.



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Notes

Oral presentation: OP23

Light at the end of the channel: Washcoating of a monolith for photocatalytic hydrogen generation in an optical fibre monolith reactor

Noor Zara Hassan,[a] Naomi Harrisankar de Oliveria[a] and Eric van Steen[a]

[a]*Catalysis Institute, University of Cape Town, Cape Town, 7700, South Africa,*
E-mail: HSSNOO005@myuct.ac.za

Keywords: photocatalysis, water splitting, green hydrogen, monolith reactor, optical fibre, zeta potential

Abstract

Photocatalytic water splitting offers an alternative method of producing green hydrogen that uses sunlight directly, rather than via electricity, as is the case with water electrolysis. Photocatalysis involves the excitation of an electron in a semiconductor, resulting in the co-generation of a hole in the valence band. These electrons and holes can participate in the desired redox reactions or recombine and thus decreasing the efficiency. TiO2 is considered a benchmark photocatalyst, which is cheap, non-toxic and stable under photocatalytic reaction conditions. However, it has a wide band gap thus requiring UV light to excite its electrons [1]. CdS has emerged as an alternative with a smaller band gap allowing for the use of the more prevalent visible light [2].

Photocatalytic reactors are usually carried out in a slurry reactor, with a light source at a single point – either from a lamp or LEDs. One of the main issues with this configuration is shading, which occurs when catalyst particles block each other from receiving light [3]. Using a monolith reactor, with the catalyst fixed to the walls, optical fibres can be used to deliver light through each individual channel, ensuring the even distribution of the light over the catalyst layer. Light only penetrates up to a certain depth of the catalyst, meaning that there is an optimal layer thickness, after which any additional catalyst does not participate in the reaction.

In this study, both TiO2 and CdS were tested in a batch slurry reactor under UVA light at various intensities, as well as under visible light for the CdS. Changing the catalyst concentration resulted in the observance of the shading effect. TiO2 was then deposited on to a cordierite monolith by washcoating, which involves dipping the monolith in an aqueous suspension of the catalyst, removing the solution with airflow, drying and calcination. The acceptable concentration range to perform zeta potential measurements, which is a measure of the surface charge, was established for TiO2 and cordierite. Particles in suspensions with zeta potentials of a high magnitude, i.e. a strong surface charge, repel each other, causing them to remain stable, whereas settling occurs in suspensions with a zeta potential of a small magnitude. The relationship between the zeta potential and pH for each of these substances was used to determine the pH at which the TiO2 has an opposite charge to the cordierite, causing the catalyst to be attracted to the monolith surface. The washcoating was carried out at different slurry concentrations (2, 5, 10, 15, 20 wt.-%), pH (3, 4.5, 6), and calcination temperatures (450°C, 550°C, 650°C). The results show a linear increase in the average catalyst layer thickness with slurry concentration, allowing for specific thicknesses to be targeted. Adherence tests were performed in an ultrasonic bath to indicate slurry conditions which resulted in the lowest mass loss of catalyst from the monolith. Monoliths coated with higher slurry concentrations (15 and 20 wt.-%) showed a significantly higher loss of catalyst. The monoliths were also examined using SEM to evaluate the homogeneity of the catalyst layer. It was found that the layers of the initial monoliths were very uneven, with some sections containing very thick layers, while others had virtually no catalyst. Another issue observed was the cracking of the catalyst layer that occurred during drying. This led to an investigation into modifying various aspects of the washcoating procedure, such as the use of a glass layer as a smoother base for catalyst deposition, and multi-cycle washcoating. The multi-cycle process resulted in the creation of more homogenous layers that did not have cracks. The layer was observed to be consistent across the channels, as well as down the length of the monolith.

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Notes

Oral presentation: OP24

Green Hydrogen Production via Proton Exchange Membrane (PEM) Water Electrolysis.

Claudelle Sybilline Anensong Djadock,[a] and Shawn Gouws[a]

[a] *Department of Chemistry, Nelson Mandela University, PO Box 77000, Gqeberha, 6031 South Africa*
E-mail: s232290091@mandela.ac.za

Keywords: hydrogen production, PEM water electrolysis, electrocatalysts, analytical and electrochemical characterization, hydrogen safety.

Abstract

Energy is vital for development. It enables investments, innovation, and new industries that generate jobs, drive inclusive growth, and support shared prosperity on a sustainable planet. The limitation of fossil energy sources arises from their damaging environmental impact, especially due to significant greenhouse gas emissions, such as CO_2 and CH_4, released during production and combustion [1-2]. Therefore, exploring alternative energy sources to replace fossil fuels or enhancing their efficiency is essential for fostering economic growth while decreasing harm to the climate and environment [3].

This study summarizes the key factors surrounding the production of green hydrogen through PEM water electrolysis. Eleven colors of hydrogen are reported to exemplify various approaches to hydrogen production, either as a primary source or as a by-product. The different water electrolysis technologies currently available include Proton Exchange Membrane Water Electrolysis (PEMWES), Alkaline Water Electrolysis (AWES), Anion Exchange Water Electrolysis (AEMWES), and Solid Oxide Water Electrolysis (SOWES). Their comparisons are made to demonstrate why PEMWES is more favourable than other water electrolyzers. Material testing parameters and performance indicators, including activity, selectivity, and stability of the electrochemical cell built with OER catalysts/electrodes, are evaluated using diverse analytical techniques such as X-Ray Diffraction (XRD), X-ray Fluorescence (XRF), Scanning/Transmission Electron Microscopy (SEM/HR-TEM), and XPS analysis, in addition to electrochemical techniques like Cyclic Voltammetry (CV), Linear Scan Voltammetry (LSV), Electrochemical Impedance Spectroscopy (EIS), and Chronopotentiometry (CP)We conclude the study with an outline of safety aspects during PEM hydrogen production.

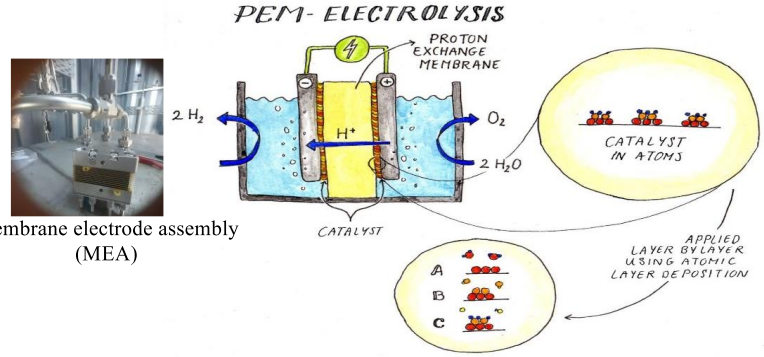

Fig. 1 PEM water electrolysis for Hydrogen production

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Notes

Oral presentation: OP25

Heteropore Conjugated Organic Reticular Subnano-Crystal for Photocatalytic Water Splitting

Ruijuan Zhang,[a,b] Shanlin Qiao,[b] Yali Yao[a] and Xinying Liu[a]

[a]*Institute for Catalysis and Energy Solutions, University of South Africa, Florida, South Africa, E-mail: 13568027@mylife.unisa.ac.za.*
[b]*College of Chemistry and Pharmaceutical Engineering, Hebei University of Science and Technology, Shijiazhuang, China.*

Keywords: conjugated reticular oligomers, covalent organic frameworks, photocatalytic water splitting, polymer dots, two-dimensional heteropore polymers.

Abstract

2D COF based photocatalysts exist as insoluble and difficult-to-process blocks, the layered stacking buries active sites, hindering water molecule access, while crystal defects restrict charge carrier migration/penetration. The well-defined sub-nanostructures with distinct configurations (C2, C3) can construct multiple pathways and intramolecular electric fields, which promote electron separation and transfer. Hence, we develop a kind of heteropore conjugated reticular oligomers (CROs) subnano-crystals with well-defined structures, which can be regarded as a defect-free COFs segment. These sub-nanometer dots ensure sufficient exposure of active sites, enhance processability, form a "homogeneous catalyst" and consequently increase the accessibility of water molecules. Accordingly, the photocatalytic performance of series CROs is up to 129.33 μmol h–1, improving 3–5 times over bulk COFs. Theoretical calculation shows that: Electron transfer number (ET) increased from 0.43 to 0.99 e, charge transfer distance (D) increases from 2.467 to 10.319 Å, while electron–hole overlap integral (Sr) decreases from 0.495 to 0.023, and exciton binding energy (Eb) decreases from 6.28 to 4.28 eV. The statistical product and service solutions (SPSS) method indicates that extending electron–hole separation distances and reducing exciton binding energy play a pivotal role in achieving effective electron delocalization and efficient charge transfer, thus significantly promoting the photocatalytic process.

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Notes

Oral presentation: OP26

Pd-NiO-C Triple-Junction Interface Electrocatalyst Supported on Metal-Organic Framework for Efficient Glycerol Oxidation in Alkaline Fuel Cell.

Makhaokane Paulina Chabalala,[a] Nobathembu Faleni [b,] and Nobanathi Wendy Maxakato[a]

[a] *Department of Chemical Sciences, University of Johannesburg, Doornfontein 2028, South Africa,*
E-mail: nmaxakato@uj.ac.za
[b] *Department of Chemistry and Physical Sciences, Walter Sisulu University, South Africa*

Keywords: ZIF-8, Synergistic Electrocatalysis, Multi-interface structure, Glycerol Oxidation Reaction, Alkaline media.

Abstract

Metal-organic frameworks (MOFs) have received significant research attention as promising catalyst support materials due to their high surface area and porosity, enhancing activity through increased electrocatalyst surface area. In this study, Palladium nanoparticles (Pd NPs) were deposited on primary support material consisting of Nickel oxide (NiO) and carbon nanotubes (CNTs) through the microwave-assisted polyol method to form Pd/NiO-CNTs. The as-prepared material was then successfully impregnated on the surface of the zeolitic imidazolate framework-8 (ZIF-8) secondary support through the capillary impregnation method, forming a binary metal-based Pd/NiO-CNTs@ZIF-8 electrocatalyst with multiple interfaces. The Pd/NiO-CNTs@ZIF-8 electrocatalyst exhibited high catalytic activity for glycerol oxidation in alkaline media, achieving a high current density of 4195.81mA mg_{Pd}^{-1}, the most negative onset potential, good reaction kinetics, and long-term stability. This remarkable performance is attributed to the double support materials (NiO-CNTs and ZIF-8), the bifunctional mechanisms of the triple-junction interfaces, synergistic effect, and strong metal-support interactions provided by NiO, CNTs, and ZIF-8.

Notes

Oral presentation: OP27

From Greenhouse to Green Fuel: Light-Driven Methane-to-Methanol Conversion over Pt/TiO2 and Pt/WO3 Catalysts.

Chiamaka Amejum[a] Amonyea and Eric van Steen[a]

[a]*Department of Chemical Engineering, University of Cape Town, South Lane, Rondebosch, 7700, South Africa, E-mail: amnchi003@myuct.ac.za.*

Keywords: photocatalysis, methane oxidation, platinum-based catalysts.

Abstract

Methane is a potent greenhouse gas with a warming potential 28 times greater than carbon dioxide over a 100-year timescale, contributing significantly to global warming when emitted from anthropogenic sources such as landfill sites [1]. Its direct conversion into value-added products such as methanol and formaldehyde offers a sustainable route to mitigating methane emissions, while producing useful products. However, current industrial methane-to-methanol approaches involve severe operating conditions – particularly high temperatures for the reforming step - resulting in an increase in the overall carbon footprint [2].

Photocatalysis, which harnesses solar energy to drive reactions under milder conditions, has emerged as a promising alternative [3]. Yet, current photocatalytic systems encounter a selectivity-conversion trade-off, often yielding undesired reaction intermediates, as well as deep oxidation products – CO2 and CO [2,4]. Tungsten trioxide (WO3), a visible-light responsive semiconductor, offers moderate oxidation power, potentially limiting overoxidation [5]. However, like many metal oxides employed in photocatalysis, pure WO3 suffers from rapid charge carrier recombination, necessitating modifications such as metal deposition, amongst other techniques, for enhanced performance [6]. Density functional theory suggests that platinum can play an important role in catalysing methane to methanol by providing active sites for oxygen adsorption and methoxy specie formation (in the presence of water), lowering activation energies [6,7].

In this study, the photocatalytic and thermocatalytic oxidation of methane was investigated over 0.5wt% Pt/TiO2 (rutile) and 0.5wt% Pt/WO3 catalysts in a continuously operating slurry reactor. Comparative experiments were conducted under both illuminated (using LEDs of predefined photon energies) and dark conditions at matched system temperatures (50–180ºC) and pressure (22 bar), in the presence of water and molecular oxygen. The effects of illumination on methane conversion, product selectivity, and reaction kinetics were evaluated. Apparent activation energies were calculated from Arrhenius plots for both the light-assisted and thermally driven reactions. Interestingly, the light-assisted reactions had an observed lower activation energy and improved selectivity toward methanol and formaldehyde by suppression of overoxidation pathways. This is attributed to the surface plasmon resonance (SPR) effect of platinum particles, which promotes charge separation and generates energetic (hot) electrons which facilitate C-H bond activation on the catalyst surface [8].

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Notes

Oral presentation: OP28

Polyaniline Composites for Electrocatalytic Hydrogen Production

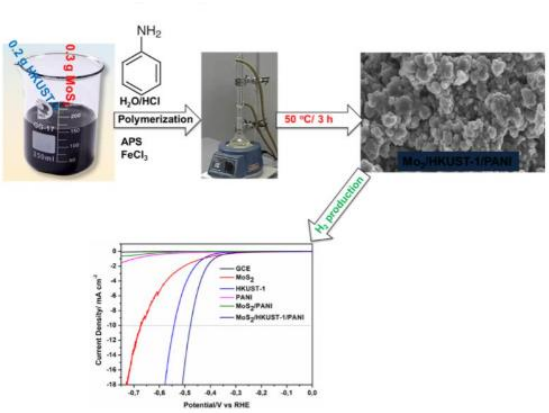
Kabelo E. Ramohlola[a, b], Miranda M. Ndipingwi[a], Kwena D. Modibane[b,c] , Emmanuel I. Iwuoha[a]

[a]*SensorLab (University of the Western Cape Sensor Laboratories), Faculty of Science, University of the Western Cape, Bellville 7535, Cape Town, South Africa*
Email: 6305580@myuwc.ac.za
[b]*Department of Chemistry, School of Physical and Mineral Sciences, Faculty of Science and Agriculture, University of Limpopo, Polokwane 0727, South Africa*
[c]*DSI-NRF SARChI Chair in Photocatalytic Hydrogen Production, Department of Chemistry, School of Physical and Mineral Sciences, University of Limpopo (Turfloop), Polokwane, Sovenga 0727, South Africa.*

Keywords: Metal Organic Frameworks, Electrocatalysis, Hydrogen Evolution Reaction

Abstract

A search for an abundant and cheap electrocatalyst to replace the expensive and scarce precious metal-based electrocatalysts for hydrogen evolution reaction (HER) is critical for realization of hydrogen as an energy carrier [1,2]. Herein, molybdenum disulphide-copper based metal organic framework/polyaniline (MoS2/HKUST-1/PANI) ternary composite was synthesized following a simple in-situ chemical oxidative polymerization of aniline in the presence of already hydrothermally synthesised MoS2 and HKUST-1 pristine materials. Several analytical techniques were used to evaluation the formation and structure properties of the ternary composite. The x-ray photoelectron spectroscopy results were in agreement with the morphological and structural characterization techniques and further confirming the wrapping of MoS2 and HKUST-1 by PANI. Optical studies displayed an increase of direct and indirect band gaps the ternary composite but closer to the one of PANI homopolymer suggesting the ternary composite exhibited good conductivity, which is an essential property for HER. The electrochemical characterization presented that the ternary composite possessed a diffusion-controlled nature with a twelve-fold increase in the electrochemical surface area of as compared to PANI homopolymer. The prepared MoS2/HKUST-1/PANI composite exhibited excellent HER properties with a Tafel slope of 44.7 mV.dec-1 and low charge-transfer resistance as well as turnover frequency of 4.0 mol H2 per second at 750 mV potential versus reversible hydrogen electrode (RHE). Most importantly, it only needed 110 mV overpotential vs RHE to reach the current density of 10 mA.cm-2. Additionally, MoS2/HKUST-1/PANI ternary composite achieved superior stability over other prepared electrocatalysts. For the first time, employing MoS2 and HKUST-1 to the backbone of polyaniline for the construction of the edge-rich integrative ternary nanocomposite has successfully achieved an outstanding HER performance.



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Notes

Oral presentation: OP29

Construction of oxygen deficient NiAl-LDH-nanocomposites for enhanced photocatalytic hydrogen evolution via water splitting.

Mametja Sense, Mmelesi Olga[a], X. Liu[a], and Gorimbo Joshua[a]

[a]*Institute for Catalysis and Energy Solutions, College of Science, Engineering and Technology, University of South Africa, Florida Park, 1709 Johannesburg, South Africa*
E-mail correspondence: 22469567@mylife.unisa.ac.za

Keywords: Photocatalysis, defects, hydrothermal, chemical reduction, photocatalytic activity

Abstract

Recently, hydrogen has received remarkable scientific attention as a renewable resource in energy applications since the current energy production processes include combustion of non-renewable resources, highly contributing to the effect of global warming due to great emission of greenhouse gases [1]. This study addresses the production of hydrogen through photocatalytic water splitting, a cleaner alternative to methods such as gasification and steam methane reformation, which emit a large quantity of carbon dioxide and thus undermining the environmental sustainability goal. Photocatalysis is defined as the enhancement of a photoreaction by employing light as illustrated in Figure 1. While several photocatalysts have been explore for hydrogen evolution, this study focuses double-layered hydroxides (LDHs) due to their desirable properties such as distinctive layered structures, cost effectiveness, modifiable compositions, and facile synthesis. However, their large band gap makes it difficult for the promotion of electrons from the valence band to the conduction band, which results in poor photocatalytic activity. To mitigate this, defect engineering (oxygen vacancy) proved to be one of the most efficient techniques to enhance photocatalytic activity [2]. As a cost-effective alternative for platinum (Pt), nickel (Ni) and aluminium (Al) were embedded within LDH to form NiAl-LDH, followed by chemical reduction using different concentrations of sodium borohydride (NaBH4) to construct oxygen vacancy. FTIR, Raman, and XRD showed successful formation of the nanocomposites and reduced peak intensities due to the removal of oxygen. The UV-VIS-DRS spectra and Tauc plots revealed enhanced light absorption capacity as well as reduced band gap energy respectively. Interestingly, the introduction of oxygen vacancies increased the quantity of active sites and reduced Tafel slope, indicating faster reaction kinetics.

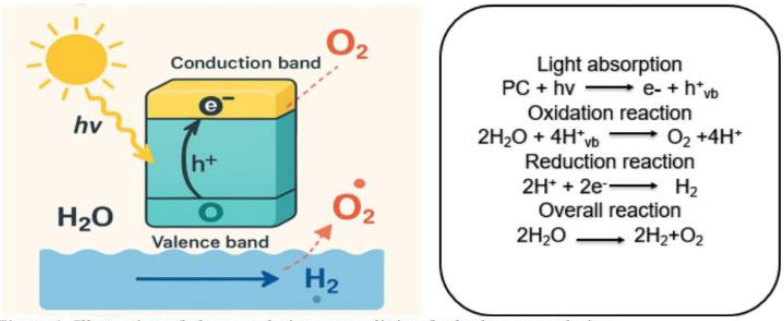

Figure 1. Illustration of photocatalytic water splitting for hydrogen evolution.

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Notes

Oral presentation: OP30

A Direct Catalyst Coated Membrane for Proton Exchange Membrane Water Electrolysis using a Slot-die Coating Method

Jatin Parbhoo[a], Francois Van Schalkwyk[a] and Rhiyaad Mohamed[a]

[a]*Department of Chemical Engineering, Upper Campus, University of Cape Town, Rondebosch, 7700, South Africa,*
E-mail: prbjat001@myuct.ac.za.

Keywords: slot die coating, proton exchange membrane electrolysis, catalyst coated membrane.

Abstract

Green hydrogen can be used as an energy carrier to decarbonise various sectors. Proton exchange membrane water electrolysis (PEMWE) is a promising technology for the large-scale production of green hydrogen. At the core of a PEMWE device is the catalyst coated membrane (CCM). Here, the water splitting, oxygen evolution (at the anode), and hydrogen evolution (at the cathode) reactions take place.
Currently about 4.5% of the total electrolyser plant cost is made up of the time-consuming CCM manufacturing process alone (excluding materials) [1]. Roll-to-roll setups have been shown to reduce manufacturing costs for thin film products in other industries [2]. Such a setup often makes use of a slot die coater as shown in Figure 1. A slot die coating method to coat PEMWE CCMs could therefore prove useful.

Figure 1: A roll-to-roll coating setup [3]

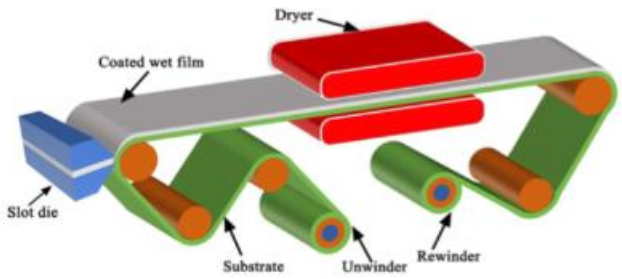
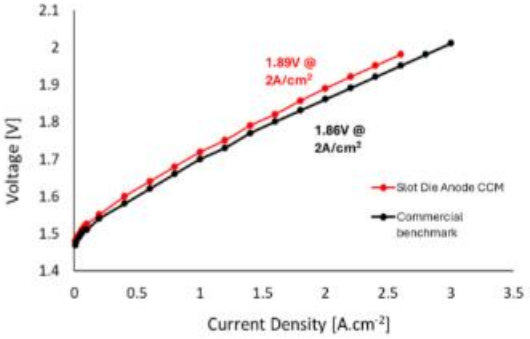


Figure 2: Polarization curve



This study aims to slot die coat the anode catalyst layer (CL) to produce a CL with minimal defects (associated with slot die coating) and ultimately to produce one that performs electrochemically on par with industry standards.
The industry standard anodic catalyst material is iridium oxide (IrO2). This material is expensive and scarce. An oxide material was used for developing the initial coating method. The experimental process consisted of formulating a catalyst ink and coating it on a substrate/proton

exchange membrane. Initial trial coating showed that coating at a high ink solid content (>25wt%), produced layers that best met the desired metal loadings. However, these layers often showed signs of cracking and other defects. Various technical hurdles pertaining to the coating system were also experienced and these needed to be overcome to establish a more reliable coating method. IrO2 based inks were successfully slot die coated to produce anodes and the CCMs were electrochemically characterised.

The slot die coated anode CCMs were able to produce hydrogen gas, but as is shown in Figure 2, its electrochemical performance was slightly lower than the benchmark CCM. Further study is being conducted to increase its performance as well as reduce defects in the coated layer.

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Notes

Oral presentation: OP31

Highly Efficient Ruthenium Based Catalysts Supported on Modified Al_2O_3 for Ammonia Decomposition for Green Hydrogen Production

Mamello Maliehe[a], Tshepo Dipheko[a], Thulani Nyathi[a], and Michael Claeys[a]

[a]*Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch 7700, Cape Town, South Africa*

Email(s): mlhmam006@myuct.ac.za. (Mamello Maliehe)
michael.claeys@uct.ac.za (Michael Claeys)

Keywords: NH_3 decomposition, Ru catalysts, modifiers, electronegativity

Abstract

The global pursuit for carbon-neutral energy solutions has identified green hydrogen as a promising clean and versatile energy carrier. Ammonia (NH_3) emerging as a promising hydrogen carrier due to its high hydrogen content (17.8%), well understood synthesis, and carbon-free decomposition pathway. This study investigates the catalytic decomposition of ammonia over ruthenium (Ru) based catalysts. Ru-based catalysts have been found to be highly active in ammonia decomposition.

A series of Ru-based catalysts supported on modified alumina (Ru/M-Al_2O_3, where M is Ba, La, Mn, Si, and W) were synthesized using wet impregnation technique. The loading of Ru, and M, were 2 wt% and 5 wt%, respectively. Characterisation techniques, such as BET surface area analysis, XRD, TEM, H_2-TPR, TPD, were used to study the physicochemical properties of the catalysts. Catalytic performance during ammonia decomposition reaction was evaluated in a fixed-bed reactor at 500 °C and at 1 atm.

BET experiments revealed that the surface area increased in the order Al_2O_3 > Ba-Al_2O_3 > Mn-Al_2O_3 > La-Al_2O_3 > Si-Al_2O_3 > W-Al_2O_3. The CO_2-TPD experiments of the M-Al_2O_3 supports revealed that addition of modifiers with a low electronegativity, namely, Ba, La and Mn increased the basicity of the support. Conversely, Si and W, modifiers with high electronegativity, lowered the basicity of the support. The optimized catalyst achieved near-complete ammonia conversion at 500 °C for the production of green hydrogen. This supports the green hydrogen value chain by finding ways to store, transport green hydrogen, and integrating it into future green energy systems.

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Notes

Oral presentation: OP32

Homojunction of graphitic carbon nitride for efficacious chlortetracycline degradation via peroxydisulfate activation

Mhlengi Jali,[a]Potlako J. Mafa,[a]Muthumuni Managa,[a]Xolile Fuku[a] and Alex T. Kuvarega[a]

[a]*Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology, University of South Africa, Florida, 1709, Johannesburg, South Africa,*
E-mail: 68066066@mylife.unisa.ac.za

Keywords: Black graphitic carbon nitride, Yellow graphitic carbon nitride, Z-Scheme homojunction, chlortetracycline hydrochloride.

Abstract

Graphitic carbon nitride photocatalyst has gained popularity for environmental applications. The present work evaluates the black (B-GCN) and yellow (Y-GCN) graphitic carbon nitride homojunction for the photocatalytic degradation of chlortetracycline hydrochloride (CTCH) in water under visible light irradiation. The conditions for optimal degradation were determined as catalyst dosage = 20 mg; peroxydisulfate (PDS) dosage = 0.17 mmol; solution pH = 10.05. The photocatalytic system without any additives was able to degrade 85% in 120 minutes. With the addition of PDS, the system underwent a remarkable change, showing 96 % degradation in 30 minutes. The catalyst showed excellent stability throughout five cycles of reuse, as it maintained degradation efficiencies of above 90 %. Moreover, application of the catalyst to real wastewater yielded promising degradation levels of 91%, suggesting the potential of the catalyst in environmental remediation. Experiments on trapping reactive species revealed that photogenerated holes (h^+) were the predominant active species for degradation. According to Mott-Schottky analysis, UV-Vis DRS and scavenger experiments, a Z-scheme charge transfer mechanism was proposed, benefiting charge separation and redox capability

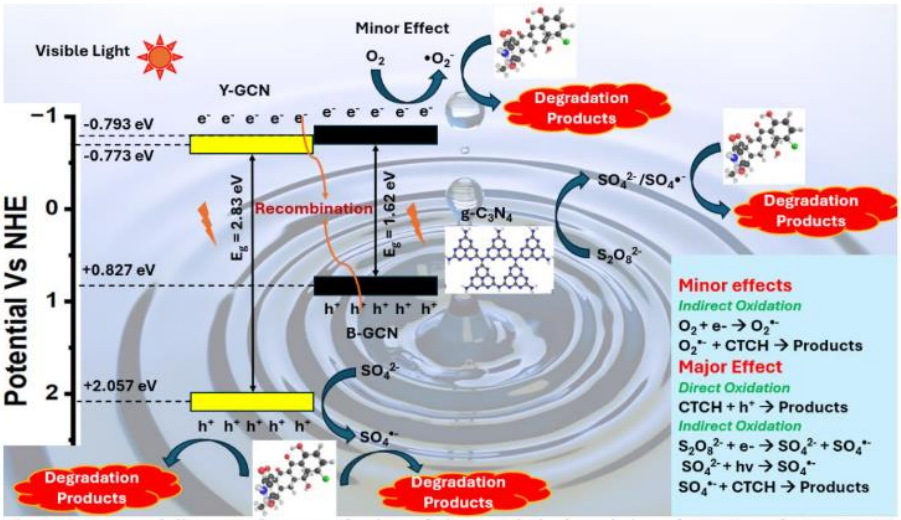


Figure 1: Proposed direct Z-scheme mechanism of photocatalytic degradation of CTCH on the B-GCN/Y-GCN catalyst.

Notes

Oral presentation: OP33

Macroporous resin grafted with Perylene diimide side-chains for efficient photosynthesis of H_2O_2

Jiangbo Guo[a], Xinying Liu[a], Yali Yao[a] and Xudong Yu[b]

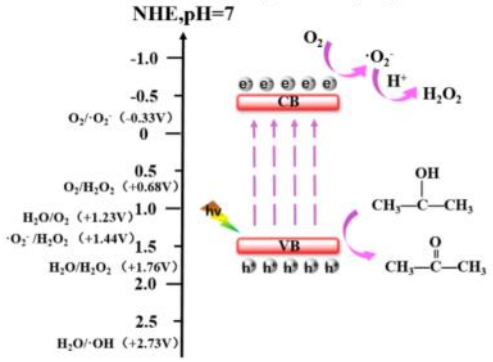
[a]*Institute for Catalysis and Energy Solutions, University of South Africa,1710, Private Bag X6, Florida, South Africa*
13523937@mylife.unisa.ac.za
[b]*Hebei Provincial Key Laboratory of Photoelectric Control on Surface and Interface, and College of Science, Hebei University of Science and Technology, Yuxiang Road 26, Shijiazhuang 050080, PR China*

Keywords: photocatalysis, macroporous resin, hydrogen peroxide, perylene diimid.

Abstract

Hydrogen peroxide, as an important chemical, is widely used in the chemical, pharmaceutical, textile, and environmental industries. However, traditional industrial production method has high energy consumption, high cost, and is not environmentally friendly. Photosynthesis, a green method, has attracted the attention of researchers. It is significant to develop a photocatalyst that high efficiently converts superoxide radicals to hydrogen peroxide. However, traditional photocatalysts still face two challenges, 1) Poor O2 adsorption. 2) Slow photogenerated carrier separation and transfer. In this work, we introduce perylene diimide (PDI) units into macroporous resin polymer chains using sulfamide bonds as linkers to produce three photocatalysts named PSS-AM-PDI, PSS-HA-PDI and PSS-EDA-PDI. In the grafted resin, PDI molecules linked to the polymer chains form a short-range π-π stacking interaction, which not only shortens the charge migration distance and reduces the charge recombination efficiency, but also expanding the spectral absorption range. In addition, sulfamide bond, as a polar oxygen functional group, can not only extract electrons to accelerate the separation of photogenerated carrier and electron/proton transport, but also improve hydrophilicity and oxygen adsorption via hydrogen bonding. The experimental results indicate that PSS-EDA-PDI efficiently synthesizes H2O2 through the two-step 2e- ORR process. PSS-EDA-PDI exhibits the highest light-driven H2O2 production rate among the three photocatalysts, reaching 6141 umol g−1 h−1 in the presence of isopropanol as a sacrificer, superior to most reported PDI-based photocatalysts.

Figure 1: Mechanism of PSS-PDIEDA photocatalytic production of H_2O_2.



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Notes

Oral presentation: OP34

Ultra-stable catalyst for electrocatalytic oxygen evolution reaction: triphenylphosphine derived P modified $NiFe_2O_4$-TiO_2

Siyabonga Patrick Mbokazi[a], Tarekegn Heliso Dolla[b], Haitao Zheng[c], and Nobanathi Wendy Maxakato[a]

[a]*Department of Chemical Sciences, University of Johannesburg, Doornfontein 2028, South Africa*
[b]*Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering and Technology, University of South Africa (UNISA), Private Bag X6, Florida, 1710, South Africa*
[c]*Energy Centre, Council for Scientific and Industrial Research (CSIR), PO Box 395, Pretoria 0001, South Africa.*
Email:siyabongambokazi141@gmail.com

Keywords: Oxygen vacancies/defects, composites, phosphatized metal oxides, oxygen evolution reaction, electrocatalysts.

Abstract

The rational design of high-performance electrocatalysts is essential for promoting the industrialization of water electrolyzers. Herein, a solvothermal method was implemented for the fabrication of $NiFe_2O_4$ nanocubes coupled with an oxidative pyrolysis approach of $NiFe_2O_4$, TiO_2, and triphenylphosphine to form a P-$NiFe_2O_4$-P-TiO_2 nanocomposite with enhanced conductivity and optimized electronic configurations [1], [2]. Triphenylphosphine introduced phosphorus modifications, probed defects on P-NiFe2O4-P-TiO2 by triggering lattice distortions, and created oxygen vacancies on NiFe2O4 and TiO2, which greatly enhanced the conductivity and charge-transfer efficiency of that nanocomposite. Additionally, the phosphorus species on P-$NiFe_2O_4$-P-TiO_2 served as electron acceptors, which enhanced the catalytic activity through high-valent metal generation in oxygen electrocatalysis [3], [4], [5]. As expected, P-$NiFe_2O_4$-P-TiO_2 demonstrated efficient catalytic activity with an overpotential of only 294 and 321 mV at 10 and 50 mA/cm² for OER in 1 M NaOH. Meantime, the alkaline water electrolyzer assembled with P-$NiFe_2O_4$-P-TiO_2 as the working electrode requires a voltage of only 1.583 V to achieve a water-splitting current density of 10 mA/cm², which surpasses that of IrO_2 along with good stability over 50 h. This work puts forward a simple approach based on elemental doping and vacancy engineering for the design of effective and enduring catalysts for alkaline-based water electrolyzers.

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Noted

Oral presentation: OP35

Automotive Paint Slugde Ash: A potential catalyst to carbonaceous materials pyrolysis

Athi-enkosi Mavukwana,[a]

[a]*Department of Chemical and Materials Engineering, University of South Africa, Cnr Christiaan de Wet & Pioneer Ave, Roodepoort, South Africa,*
E-mail: mavukae@unisa.ac.za.

Keywords: Pyrolysis, Automotive Paint Sludge, biomass, fluid catalytic cracking.

Abstract

In the work we seek to conduct various experiments studying the synergy of co-thermal treatment of automative paint sludge (APS) with other selected carbonaceous materials. Automotive paint sludge is one type of sludge generated during the painting process in the automotive industry, primarily composed of residues from paint application. The composition of this sludge typically includes volatile organic compounds (VOCs), heavy metals, pigments, and non-recyclable materials, which pose significant environmental concerns if not managed properly. The potential of five different automotive paint sludges as a feedstock for pyrolysis was evaluated using ultimate analysis, XRF, ICP-MS and TGA analysis. The XRF and ICP results confirmed that the mineral elements contained in the different APS sludges have a similar composition to the major commercial catalysts such as zeolites and fluid cracking catalysts (FCC). Mineral compounds such as SiO2, Al2O3, K2O, FeO, CaO, MgO, Na2O, Fe2O3 or various combinations of the same, are catalysts that have been explored to reduce the amount of tar and improve biol-oil and syngas production during gasification and pyrolysis of solid carbonaceous materials. The different APS sludges contain these minerals in varied compositions and thus it would be of great value to investigate the synergy of incorporating APS in co-pyrolysis and co-gasification with other solid waste. As such the thermal decomposition of automotive paint sludge under inert and air atmosphere and three heating rates was also investigated. This was done to understand the mechanism of different APS sludges decomposition for process targeting during the conceptual design of thermal treatment processes. The overall, the findings of this study shows that the clear coat sludge and base coat sludge can be disposed of through by pyrolysis. Whereas the primer coat, electro coat and phosphate sludges would find suitable use in civil engineering applications, or as catalysts. Therefore, there should be no kinetic limitations to the co-gasification of these materials.

Notes

Oral presentation: OP36

Advanced HEA Catalysts for CO_2 Hydrogenation: Unlocking Methanol Selectivity through Catalyst Engineering

Lebohang Macheli[1]*, Gerard M. Leteba[2], Yibo Tang[3], Jiabing Chen[3], Sarah L. George[2], Candace I. Lang[2], Xiaojun Lu[3]*, Linda L. Jewell[1]*

[1]*Department of Chemical and Materials Engineering, University of South Africa, Florida 1709, Johannesburg, South Africa, E-mail: machelg@unisa.ac.za*
[2]*Centre for Materials Research, Department of Mechanical Engineering, University of Cape Town, Rondebosch 7708, Cape Town, South Africa*
[3]*School of Chemical Engineering and Pharmacy and Key Laboratory for Green Chemical Process of Ministry of Education, Wuhan Institute of Technology, Wuhan 430205, China*

Keywords: methanol synthesis, High entropy alloys, CO2 hydrogenation

Abstract

The catalytic hydrogenation of CO_2 to methanol presents a sustainable pathway for carbon utilization. In this work, Pt-Pd-Ni-Cu-Mn-Au high-entropy alloys (HEAs) were synthesized using triphenylphosphine (TPP) or oleylamine (OAm) to control nanoparticle morphology and surface composition. X-ray diffraction confirmed single-phase FCC HEAs, while XPS revealed that TPP-derived HEAs possessed higher surface Cu content, correlating with improved methanol selectivity. Hydrogen temperature-programmed reduction showed stepwise reduction of Cu, Mn, and Ni oxides, influenced by surfactant and calcination treatment. Catalytic testing in a fixed-bed reactor at 240 °C and 40 bar demonstrated that TPP-derived catalysts achieved superior methanol yields compared to OAm-derived counterparts. In situ DRIFTS identified carbonate and formate intermediates, supporting a stepwise CO_2 hydrogenation mechanism via C_1 oxygenates. These results demonstrate that surfactant-controlled synthesis enables tunable surface-active sites in HEAs, offering a rational pathway for designing robust catalysts for efficient and selective CO_2-to-methanol conversion.

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Notes

Oral presentation: OP37

Parametric optimization of a catalytic lab-scale pyrolysis system for enhanced hydrogen generation from pine wood residues

Mithayelanga Mazitshana[a], Johann Gorgens[b], Azwihangwisi I. Mabuda[c], Philani P. Mpungose[a]

[a]*Department of Chemistry, Cape Peninsula University of Technology, Bellville, Western Cape, 7535, South Africa, E-mail: 217256597@mycput.ac.za.*
[b]*Department of Chemical Engineering, Stellenbosch University, Stellenbosch, 7599, South Africa.*

Keywords: pyrolysis, biomass, central composite design.

Abstract

Hydrogen is a key energy carrier in transitioning to a sustainable energy future due to its environmental, economic, and social advantages. Biomass-derived hydrogen offers a renewable and clean pathway for addressing global energy challenges. In this study, the aim is to improve the efficiency and sustainability of hydrogen production from renewable biomass, contributing to cleaner energy systems and reduced reliance on fossil fuels. Among thermochemical methods, pyrolysis shows strong potential for converting biomass into hydrogen-rich gases. This study focuses on optimizing hydrogen production from pine wood through pyrolysis. A Central Composite Design (CCD) was applied to predict optimal process conditions and to determine the required number of experimental runs. Key variables such as temperature, heating rate, and feedstock-to-catalyst ratio were investigated. In addition, different types of catalysts were evaluated for their effectiveness in enhancing hydrogen yield and reducing tar formation. Product characterization was carried out using thermogravimetric analysis (TGA) and gas chromatography-mass spectrometry (GC-MS

Notes

Oral presentation: OP38

Influence of Phase Transitions in Indium-based catalysts for the catalytic performance in CO_2 hydrogenation to methanol

Nick Herrmann,[a] *Wijnand Marquardt,*[b] *Guillermo Martín Atanes,*[c] *Joaquín Grassi,*[c] *Nico Fischer,*[b] *and Jakob Albert* [a]

[a] *Institute of Technical and Macromolecular Chemistry, University of Hamburg, Bundesstrasse 45, 20146 Hamburg, Germany, E-mail: nick.herrmann@uni-hamburg, jakob.albert@uni-hamburg.de* [b] *Catalysis Institute, University of Cape Town, Chemical Engineering Building, Rondebosch, South Africa* [c] *Energy Lab, Campus Universitario de Vigo, 36310 Vigo (Pontevedra) Spain*

Keywords: Methanol synthesis, CO_2 reduction, Indium catalysis, Phase transition, in-situ XRD.

Abstract

The valorisation of CO_2 and the production of sustainable methanol with green hydrogen is a frequently discussed approach to reduce industry emissions and store energy from intermittent renewables in an easy to store liquid fuel. Traditionally, methanol is synthesised with a copper-based catalyst using syngas. Since the copper catalyst exhibits deactivation in the use of CO_2 as a feedstock, more resistant catalysts based on indium have been developed.

The reaction network on neat indium oxide has been well investigated and described in literature before.[1,2] The promoting effect of a suitable support material and noble metals on the catalysis are generally well described, enhancing catalyst productivity. We could already show that neat indium oxide undergoes a dehydration-rehydration pathway converting it to indium hydroxide between 250 and 275 °C. [3]

This In_2O_3 to $In(OH)_3$ equilibrium is dependent on the reaction conditions, especially on the amount of water formed either by methanol synthesis or RWGS, yet the influence of the support material and promoting metals have not been explored. To investigate the phase change, the different catalyst materials were observed by in-situ XRD. The catalysts were exposed to the reaction atmosphere of 15% conversion and heated up steadily.

The in-situ XRD shows that the phase of neat indium oxide remains stable even at higher conversion, while neat indium hydroxide undergoes a phase shift at around 250 °C confirming previous studies. Regarding the zirconia-supported catalyst, the phase change occurred already at 125 °C under a hydrogen atmosphere showing a significant effect of the support (Figure 1).

With this phase change figured out we performed catalytic experiments and confirmed that with the proper treatment, the catalyst productivity was improved significantly (Figure 2).

Figure 1: in-situ XRD of $In(OH)_3/ZrO_2$ under H_2 atmosphere.

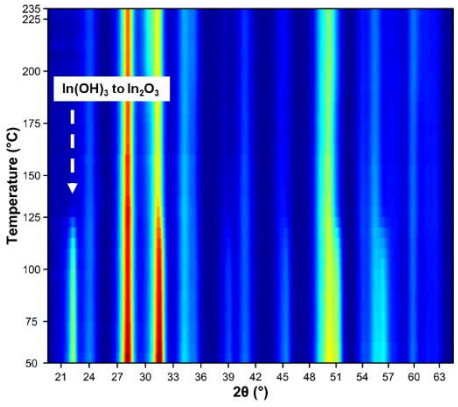
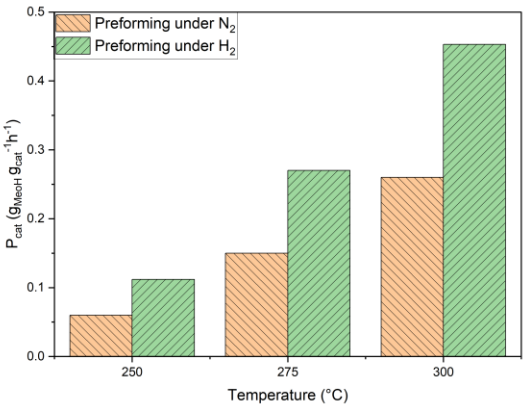


Figure 2: Increased productivity of In_2O_3/ZrO_2 after H_2 preforming at 200 °C.



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Notes

Oral presentation: OP39

Adsorptive desulfurization of diesel fuel using activated carbon from waste biomass (Carica papaya-PVA).

Beatice Makasi[a], Linda Jewell[b], Liberty Mguni[a], Yali Yao[a],*

[a]*Institute for Catalysis and Energy Solutions (ICES), University of South Africa, 29 Pioneer Avenue and Christian De Wet, 1710, Florida, Private bag X6, South Africa,*
[b]*Department of Chemical Engineering, University of South Africa, 29 Pioneer Avenue and Christian De Wet, 1710, Florida, Private bag X6, South Africa,*
E-mail:19218079 @mylife.unisa.ac.za.

Keywords: Waste biomass, Activated Carbon, Synthesis, Model Diesel, Adsorbent, Adsorptive Desulfurization, Adsorption capacity, MOFs, DBT.

Abstract

Combustion of fossil fuels results in the emission of various air pollutants such as sulfur oxides, which results in acid-rain by reacting with the air moisture, photochemical smog, which is detrimental to human health and the environment, corrosion problems in pumping, pipeline, and refinery equipment due to the oxyacid formation and catalytic poisoning of converters in automotive engines. Deep desulfurization of these fuels is a necessity to support the UN Sustainable Goal 7 and Goal 15 on affordable clean energy and climate action [1]. Adsorptive desulfurization has shown to be the most environmentally friendly, cost effective, simple and efficient method for deep desulphurization as compared to the conventional method, which utilizes expensive oxidants. ADS utilises different types of adsorbents which include zeolites, activated carbons (AC), and metal-organic-frameworks (MOFs). Activated carbon (AC) has gotten lots of research attention due to its steady adsorption performance, superior mass transfer, cost effectiveness, different pore sizes (microporous, mesoporous and macropores) for adsorption of various sulphur compound sizes, and large surface area for ample reactions to occur. Activated carbon (AC) from renewable and low-cost waste biomass is very economical and prevents environmental degradation [2].

This research focused on the synthesis of low-cost adsorbent (AC) from Carica Papaya waste biomass for adsorptive desulfurization. The adsorption efficiency of the AC is as shown in Figure 1.below. The highest sulfur removal was observed at approximately 55% for DBT in 1000ppm model diesel for both catalysts at 25˚C,800rpm in a batch reactor.

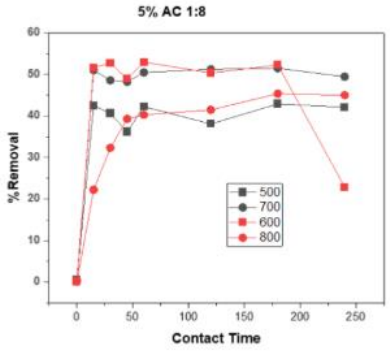

Figure 1: Adsorption efficiency of 5 % AC 1:8 @ 25℃,800 rpm,1000 ppm DBT.

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Notes

Oral presentation: OP40

Alkaline Earth Metal Promotion of Cu Surfaces for CO_2 Hydrogenation to Methanol: Structure–Phase–Function Relationships for Selective Catalysis

Tumelo Sethosa[a], Thobani Gambu[a] and Eric van Steen[a]

[a]*Catalysis Institute, Department of Chemical Engineering, University of Cape Town, South Lane, Upper Campus, Rondebosch, 7700, South Africa*
Email: sthtum002@myuct.ac.za

Keywords: Molecular Modelling, Alkaline Earth Metal, Phase Diagram, Promotion, CO2 Hydrogenation

Abstract

Reducing CO_2 to methanol offers a dual benefit; it enables sustainable fuel production and provides a practical liquid hydrogen carrier thanks to methanol's high hydrogen content, physical properties, and compatibility with existing distribution infrastructure [1,2] all while retaining methanol's central role as a versatile feedstock in the chemical industry. The benchmark $Cu/ZnO/Al_2O_3$ catalyst is typically operated at 200-250 0C [3,4] and struggle with poor CO_2 activation and low selectivity [5]. Our work addresses this challenge by investigating how alkaline earth metals, specifically magnesium, can be used to tune Cu surfaces for improved CO_2 activation and methanol selectivity. Starting from the catalytic limitations of bare Cu(111) and Cu(100) and building on prior DFT and microkinetic modelling studies [6,7,8], we focus on four key intermediates, viz; CO_2, H, CO, and methoxy, that govern activity and selectivity. Improving the adsorption and transformation of these species requires promoter phases that can interact favourably with both the surface and the reactants.

To determine which Mg-based phase (oxide, hydroxide, carbonate) is stable under reaction conditions, we used a two-stage approach. First, we perform global structure optimization using a genetic algorithm with CHGNet [9] as a machine-learned relaxer to identify the most stable MgCxOyHz/Cu(hkl) configurations. We then calculated their Gibbs free energies via density functional theory (DFT) and constructed surface phase diagrams.
Our findings show that Mg-based promoters can shift adsorption energetics in the desired direction enhancing CO_2 and H adsorption, suppressing CO desorption, and promoting methoxy hydrogenation (Figure 1). These effects reveal a distinct promotional mechanism at MgO–metal interfaces, pointing to a possible complementary role for Mg-based promoters alongside or in place of traditional ZnO systems [6,10]. Further comparative studies are needed to assess their efficacy relative to established $Cu/ZnO/Al_2O_3$ catalysts.

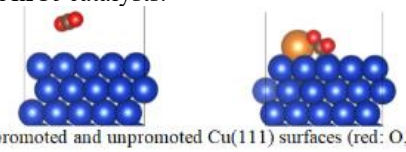

Figure 1: CO_2 adsorption on magnesium promoted and unpromoted Cu(111) surfaces (red: O, brown: C, orange: Mg, and blue: Cu).

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Notes

Oral presentation: OP41

A sustainable and efficient mechanochemical protocol for the synthesis of Schiff base derivatives

Simnikiwe Nogqala[a], Rosalyn Klein[a], and Xavier Siwe-Noundou[b]

[a]*Department of Chemistry, Rhodes University, Drosty Rd, Makhanda, 6139,*
E-mail: snogqala97@gmail.com,
[b]*Sefako Makgatho Health Sciences University, Pretoria 0204, South Africa*

Keywords: Mechanochemical imine synthesis, Silica sulfuric acid (SSA) catalyst, solvent-free mechanochemistry

Abstract

Mechanochemical synthesis has emerged as a sustainable and efficient alternative to conventional solution-phase protocols in organic chemistry [1]. Herein, we introduce a convenient, affordable, and solvent-free mechanochemically assisted protocol for the preparation of imine (azomethine) derivatives, using sulfuric acid adsorbed on silica gel (silica sulfuric acid, SSA) as a recyclable solid acid catalyst in a planetary ball mill.

Under controlled planetary ball-milling conditions, equimolar mixtures of amines and carbonyl containing reagents were ground with SSA at ambient temperature, without any solvent. For comparison, analogous runs were performed using acetic acid as the catalyst under identical milling conditions. The conventional reflux method (in solution with SSA) was employed in parallel to benchmark performance. Catalyst recycling was evaluated by recovering SSA after reaction, washing, and reusing it for a total of six successive runs, with yields recorded at each cycle.

The mechanochemical SSA protocol yielded up to 83%, markedly exceeding the maximum of 68% obtained under conventional reflux conditions. In contrast, acetic acid yielded only 63% under mechanochemical conditions, underscoring the enhanced acidity and catalytic efficiency of solid-supported sulfuric acid under grinding. The SSA catalyst retained high activity throughout six cycles, showing only a minimal decline in yield, which highlights its robustness and reuse potential. These findings align with the known mixing and thermal effects of ball milling that favour condensation equilibria under solvent-free conditions [2].

This novel SSA-ball-mill method offers a superior, eco-friendly, and cost-effective route to imine derivatives compared to traditional reflux. Key advantages include higher yields, solid acid catalysis, solvent elimination, and efficient catalyst recyclability. The protocol thus provides a compelling alternative for both academic and industrial synthesis of azomethine compounds, advancing the fields of green chemistry and mechanochemical organic synthesis.

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Notes

Oral presentation: OP42

Thermocatalytic activity of UiO-66 on CO2 hydrogenation to methanol

Tani J. Monene[a] and Mduduzi N. Cele[b]

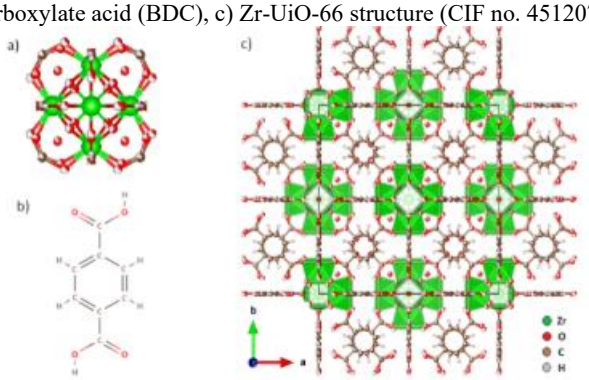
[a]*School of Physical and Chemical Sciences, Faculty of Natural and Agricultural Sciences, North-West University (Mafikeng Campus), Private Bag X 2046, Mmabatho 2735, South Africa; 33018308@mynwu.ac.za*

Keywords: UiO-66, green methanol, CO2 hydrogenation.

Abstract

Carbon dioxide (CO2) is increasing continuously in the atmosphere due to the burning of fossil fuels, contributing to global warming and other natural disasters [1]. CO2 conversion is one of the most promising methods for reducing CO2 in the atmosphere to produce sustainable chemicals, fuel, and renewable energy [2]. Metal-organic frameworks (MOFs) are attractive catalysts in CO2 utilization due to their high surface area and the tunability of metal nodes and organic ligands [3, 4]. The conversion of CO2 to green methanol using the modified Zr-UiO-66 catalysts at moderate operating conditions is one of the promising applications. The UiO-66 catalysts were synthesized using a co-precipitation method incorporating copper, calcium, and manganese to promote the CO2 conversion and high methanol selectivity. The synthesized Zr-UiO-66, Cu/Zr-UiO-66, Ca/Zr-UiO-66, CaCu/Zr-UiO-66, Mn/Zr-UiO-66, and MnCu/Zr-UiO-66 catalysts were characterized using FTIR, XRD, and TGA. The XRD and FTIR confirmed the successful synthesis of all the UiO-66 catalysts by providing XRD patterns and functional groups corresponding to the standard UiO-66 MOF. The TGA analyzed the thermal stability of synthesized UiO-66 catalysts, and they were all thermally stable up to 482 °C. The current aspects of the study include further characterization and testing of the modified UiO-66 catalysts in CO2 conversion to methanol.

Figure 1: UiO-66 catalyst structure, a) octahedral cluster with 12 carboxylate groups to the zirconium atom, b) 1,4-benzene-dicarboxylate acid (BDC), c) Zr-UiO-66 structure (CIF no. 4512072).



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Notes

Oral presentation: OP43

The nitrilase mechanism: A proposal based on experimentally determined structures and molecular modeling

Dewald van Heerden,[a] Erik Eppinger,[b] Trevor Sewella and Roger Hunter[a]

[a]*Structural Biology Research Unit, University of Cape Town, Rondebosch, South Africa,*
E-mail: dewald.vanheerden@uct.ac.za.
[b]*Institut für Mikrobiologie, Universität Stuttgart, Germany.*

Keywords: nitrilases, molecular dynamics, catalytic dyad.

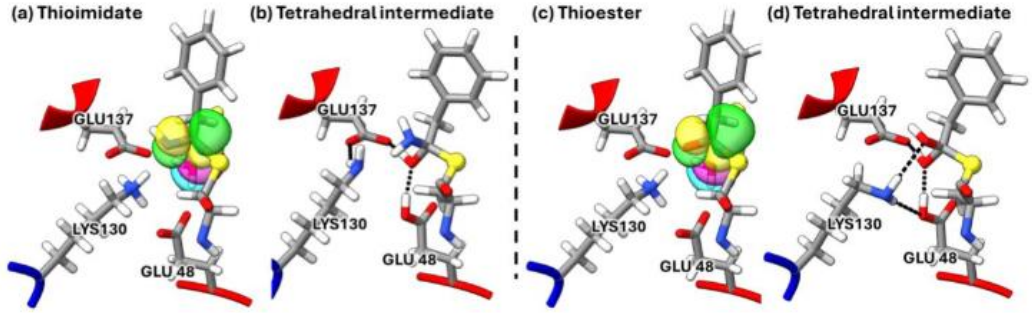
Abstract

The nitrilase superfamily, which includes amidases, are thiol enzymes that catalyse the hydrolysis and condensation of non-peptide, carbon–nitrogen linkages. There are several possible applications for nitrilases in biotechnology, including the chemo-, regio- and enantioselective synthesis of carboxylic acids from nitriles.[1]

Sequence and structural homology with other superfamily members has identified a conserved active site grouping comprising a cysteine, two glutamates, and a lysine. All postulated nitrilase and amidase mechanisms involve the covalent modification of the cysteine. However, current generation modelling tools do not allow for the facile modelling of such residues. To address this shortcoming, we developed a procedure that enables the geometric optimisation of covalent intermediates using the Interactive Structure Optimization by Local Direct Exploration (ISOLDE) package[2] incorporated in UCSF ChimeraX. In addition to coordinates that conventional docking programs rely on, ISOLDE employs electron density to minimize protein structures.

The dominant hypothesis for the nitrilase reaction is that it proceeds via a thioimidate formed on the catalytic cysteine. The thioimidate is then hydrolysed to form a thioester with the release of ammonia. The thioester is further hydrolysed to form the ultimate carboxylic acid product.[3] In the amidase reaction, the thioester formation is proposed to follow nucleophilic attack by the cysteine on the amide carbonyl carbon followed by the release of ammonia. However, our work involves a detailed geometrical and energetic appraisal of these mechanisms. Recently determined three-dimensional structures of plant and bacterial nitrilases together with mutational and biochemical studies have enabled an interrogation of the nitrilase mechanism that was hitherto impossible.[4,5] Herein, we use molecular dynamics simulations and natural bond orbital analysis to describe a novel unified mechanism operating in the catalysis propagation for both nitrilases and amidases that relies an arming/disarming process of a glutamate/lysine catalytic dyad for driving the hydrolysis.

Figure 1: Natural bond orbitals of the phenylacetonitrile (a) thioimidate and (c) thioester intermediates, showing the overlap between the p-type lone pair of a water and the π-type C=O and C=N antibonding orbitals, respectively, affording the corresponding tetrahedral intermediates shown in (b) and (d).



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Notes

Oral presentation: OP44

The effect of copper in iron-based CO_2-hydrogenation catalysts

Lan Lin Wang[a], Nicholas S. Featherstone[a], Eric van Steen[a]*

[a]*Catalysis Institute, University of Cape Town, 7700, Cape Town, South Africa,*
E-mail: eric.vansteen@uct.ac.za

Keywords: CO_2-hydrogenation, iron, copper, promoters

Abstract

CO_2 is a major contributor to climate change, where the increase in the atmospheric CO_2 concentration can be attributed to anthropogenic activities. Carbon capture, storage, and utilisation techniques are promising approaches to mitigate the environmental impacts caused by CO_2 and greenhouse gas emissions. CO_2 hydrogenation (or CO_2-Fischer-Tropsch, CO_2-FT) may utilise captured CO_2 from point sources or direct air capture (DAC) to form useful chemicals. These include renewable fuels, which are expected to be valuable hydrogen and energy carriers in the future, as well as forming olefins, the backbone of the chemical industry. Within iron-based catalysts for the Fischer-Tropsch (FT) synthesis or CO_2-FT, one or more promoters may be present, including structural promoters such as silica, electronic promoters such as potassium, and reduction promoters such as copper. These are extensively used to enhance the performance of the catalysts. Copper specifically is traditionally believed to be a reduction promoter. However, the addition of copper to iron-based FT catalysts shows enhanced activity, and selectivity towards longer chain hydrocarbons. Similar trends have been seen for CO_2-FT.

In this study, three different iron-copper-based catalyst systems are examined, viz. copper ferrite ($CuFe_2O_4$), delafossite ($CuFeO_2$), and co-precipitated iron-copper systems. Within the latter, different loadings of copper are targeted, i.e., 100Fe/0Cu, 100Fe/5Cu, 100Fe/50Cu, 100Fe/100Cu, 0Fe/100Cu. Physical mixtures with the same copper loadings were also made to test the effect of intimacy on the iron-copper system.

The synthesised catalysts were reduced and carburised in-situ to form the active phase, after which, the performance of the activated catalysts was be evaluated in a fixed-bed CO_2-FT reactor operated at 280°C, 20 bar, H_2:CO_2 = 3:1. The catalysts were tested at a constant catalyst mass, as well at a constant iron loading. The catalysts were characterised using various techniques such as XRD (of the precursor, activated, and spent sample), TPR, ICP-OES, and TGA., as the iron is understood to be the active phase (though copper is an active metal for methanol formation).

Copper does indeed assist in the reduction of iron and thereby potentially assist in the stabilisation of the active iron carbides. However, contrary to what has been reported, the presence of copper does not aid the activity nor the selectivity. Rather, the presence of copper decreases the activity and promote the formation of methane. This may be rationalised by the role of copper to supply hydrogen to the catalytic active phase. Under CO-hydrogenation conditions, this will increase the rate of CO-dissociation, but under CO_2-hydrogenation conditions sufficient hydrogen is already present and supply of more hydrogen will favour methane formation (see the Sabatier plot in Figure 1).

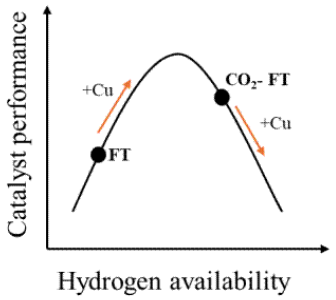


Figure 1: Effect of copper on catalyst performance

Notes

Oral presentation: OP45

A Chemoenzymatic Synthesis of Amide-Containing Quinazolin-4(3H)-one Derivatives

Mudzuli M. Maphupha,[a] Dean Bradya and Charles B. de Koning[a]

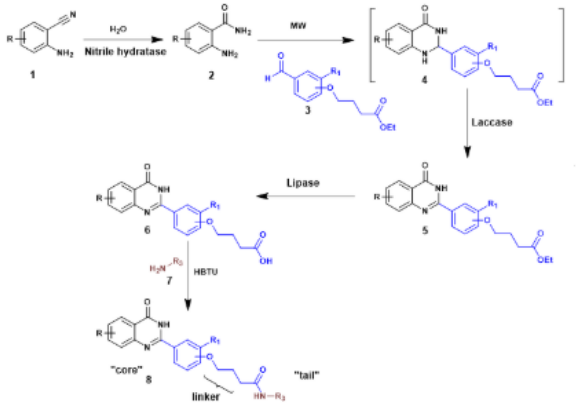
[a]*School of Chemistry, University of the Witwatersrand, Johannesburg, South Africa;*
E-mail: mudzuli.maphupha@wits.ac.za

Keywords: Biocatalysis, N-heterocycles, Laccase, Lipase, Nitrile hydratase

Abstract

Because of advances in molecular biology and biotechnology, the role of enzymes in synthetic organic chemistry has expanded significantly [1]. These advancements have enabled the development of biocatalytic processes that are rapidly replacing traditional chemical methods [2]. Considering the growing global focus on sustainability and climate change, it is increasingly imperative for synthetic chemists to adopt synthetic approaches that align with the principles of green chemistry [3]. The ability to design enzyme-based transformations that are both efficient and environmentally friendly positions biocatalysis as an essential tool for chemical synthesis [1-3].

In line with the growing importance of sustainability in chemical processes, this study explores the synthetic potential of three key biocatalysts: laccases, nitrile hydratases, and lipases. Laccases, multi-copper oxidases, facilitate the oxidation of a broad range of phenolic-related substrates using molecular oxygen and releasing water as a byproduct [4]. Nitrile hydratases are metalloenzymes that catalyse the hydration of nitriles to amides [5]. Lipases catalyse the hydrolysis of carboxyl esters and are highly versatile [6]. Collectively, these biocatalysts exemplify how nature-inspired catalysts can support the transition toward greener and more sustainable synthetic chemistry.



Scheme 1: Chemoenzymatic route for the synthesis of quinazolin-4(3H)-one derivative containing an amide moiety.

Herein, we present a multi-enzyme method for synthesising novel quinazolinone compounds from aminonitriles using biocatalysis (Scheme 1). We efficiently catalysed the hydrolysis of aminonitriles to aminoamides using whole cells containing nitrile hydratase, followed by a novel laccase/DMSO oxidative cyclisation of aminoamides to quinazolinone esters. The esters were then hydrolysed to their corresponding acids with immobilised lipase (CAL B), and finally, HBTU was used to catalyse the direct amidation of the acid products, producing the target amide-containing quinazolin-4(3H)-one derivatives in excellent yields. The target compounds contain a quinazolinone moiety and could potentially be useful as anti-tubercular or anti-cancer agents.

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Notes

Oral presentation: OP46

Hydrogen permeability of reinforced polyamide 12 composites modified with CNTs as a hydrogen permeation barrier lining in pipelines and tanks

Habib Mouadili[a], Sigwadi, Rudzani[a], Ledwaba Kabelo[a], DABACHI Mohamed Amine[b], Touhami Mokrani[c].

[a]*Department of Materials and Chemical Engineering College of Science, Engineering and Technology, University of South Africa. Private Bax X6, Johannesburg1710, South Africa*

[b]*Advanced Systems Engineering and Innovation Laboratory, Electrical and Mechanical Engineering Department, Faculty of Science and Technology, Hassan First University, Settat, Morocco*

[c]*Institute for Catalysis and Energy Solutions (ICES). University of South Africa. College of Science, Engineering and Technology, Private Bax X6, Johannesburg1710, South Africa.*

Abstract

This study investigates the fabrication and performance of polyamide 12 (PA12) composites reinforced with carbon nanotubes (CNTs) functionalized using different oxidants, including Fe_2O_3, CuO, MoO_3, and La_2O_3, to enhance their hydrogen barrier properties. CNT loadings ranging from 0.06125% to 1 wt% were incorporated into the PA12 matrix. FTIR spectroscopy confirmed successful chemical modification and improved CNT dispersion, while stress–strain testing and thermal stability analyses validated the material modifications and revealed strong interactions between the polymer matrix and the CNTs. Permeability parameters namely the diffusion coefficient (D), hydrogen solubility (S), and the permeability coefficient (Pe) were measured for both neat PA12 and CNTs-reinforced composites to evaluate their influence on hydrogen permeability. Permeability tests conducted at different temperatures enabled the determination of activation parameters, including the activation energy of permeability (Epe), the activation energy of diffusion (E_D), and the enthalpy of sorption (ΔH_s). The results demonstrate that chemically functionalized CNT-reinforced PA12 composites are promising candidates for high-performance liners in hydrogen storage tanks and pipelines, offering a recyclable and thermally stable alternative to conventional materials. In particular, incorporating 1 wt% Fe_2O_3-functionalized CNTs into the PA12 matrix significantly enhanced barrier performance, effectively preventing hydrogen diffusion across the membrane.

Keywords: Hydrogen permeation ; Polyamide 12 ; Carbon nanotubes ; Thermoplastic composites ; Chemical functionalization ; Hydrogen storage liners.

Notes

Oral presentation: OP47

Microwave synthesis and characterization of cobalt ferrite for application in photocatalysis.

Olga K. Mmelesi*, Xinying Liu

Institute for Catalysis and Energy Solutions, College of Science Engineering and Technology, University of South Africa, Florida Science Campus, South Africa

Keywords: Cobalt ferrite, microwave, Photocatalysis, Magnetic

Abstract

The study of spinel ferrite nanoparticles (SFNPs) has drawn a lot of attention lately, primarily because of its many applications in various fields of study, low bandgap energy, high capacity for adsorption of contaminants, and magnetic characteristics. In the presence of various fuels, cobalt ferrite nanoparticles (CFNPs) were created by the microwave approach [1,2]. X-ray diffraction, UV–vis Diffuse Reflectance Spectroscopy, X-ray photoelectron spectroscopy, high resolution transmission electron microscopy, and the Physical Property Measurement System were used to characterise the stability, magnetic properties, particle size, and structural variations of the synthesised NPs. The NPs that were synthesised with L-arginine had the highest saturation magnetisation (Ms), measuring 126.7 emu/g. The Ms, physical, and chemical characteristics of CFNPs have been shown to be significantly impacted by the synthesis conditions, which require further investigation in subsequent studies. In photocatalysis for the destruction of organic contaminants, the synthesised CFNPs' photocatalytic qualities were evaluated in water splitting for hydrogen evolution and degradation of pollutants.

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Notes

Oral presentation: OP48

Impact of Support on the Performance of Platinum Catalysts in Methane Oxidation

Shaista Ali, [a] Sinqobile V.L. Mahlaba, [a] Same Malatji, [a] Zibusiso Nhachengo, [a] Eric van Steen [a]

[a] *Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Private Bag X3, Rondebosch 7701, E-mail: alxsha020@myuct.ac.za.*

Keywords: methane, oxidation, platinum, trickle bed reactor, support

Abstract

The platinum-catalysed, selective oxidation of methane in the presence of water offers an attractive route to activate and functionalize methane [1]. The support plays an important role in the obtained activity [1-3], as differences in the support may affect the platinum dispersion, the hydrophobicity of the support may affect the distribution of water over the catalyst, and the acidity of the support may affect the product selectivity.

In this study platinum was supported on 4 different support materials, viz. C, SiO_2, ZSM-5, and TiO_2 and their catalytic efficiency was determined in a trickle bed reactor. The product was analysis using an on-line GC-FID equipped with a methanizer. The catalytic activity was determined as a function of the inlet ratio of water to methane keeping the methane space velocity (as well as the linear gas velocity) constant. The fresh and used catalysts were characterized using Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) spectroscopy, Thermogravimetric Analysis, powder X-ray Diffraction (pXRD), chemisorption, Scanning Electron Microscopy- Energy Dispersive X-ray (SEM-EDX) and Transmission Electron Microscopy (TEM) for changes of surface chemistry of support upon reaction. The maximum methane conversion 6.7 % was observed with Pt/SiO_2 with highest selectivity of formaldehyde (23 %) and some methanol (1 %).

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Notes

Oral presentation: OP49

Microwave-assisted catalytic decomposition of plastic waste: catalyst evolution, magnetite-driven heating, and dual-product valorisation

Motlokoa Khasu,[a] and Nico Fischer[a]

[a]*The Catalysis Institute Department of Chemical Engineering, South Lane Upper Campus, University of Cape Town, Private Bag X3, 7701 Rondebosch, South Africa, Tel: +27 21 650 4467 / 3279.*
Email:motlokoa.khasu@uct.ac.za

Keywords: carbon nanotubes, magnetite, microwave-assisted, pyrolysis

Abstract

Microwave-assisted catalytic decomposition presents a promising route for valorising plastic waste into high-value products. This study investigates the use of FeAlOx catalysts for the decomposition of high-density polyethylene (HDPE) under oxygen-deficient microwave conditions. The incorporation of magnetite (Fe_3O_4) enables efficient microwave absorption, facilitating rapid and localized heating. During the reaction, iron species actively participate in hydrocarbon cracking and hydrogen evolution, while simultaneously serving as nucleation sites for carbon nanostructure growth. Thermocatalytic and pyrolytic plastic decomposition have been widely studied but often suffer from high energy demand and limited selectivity. Recent literature suggests that microwave irradiation significantly enhances energy efficiency, particularly when used with magnetic or dielectric susceptors such as Fe_3O_4 or SiC. Magnetite, in particular, has shown superior microwave absorption due to its mixed-valence iron oxide structure, enabling volumetric heating and rapid catalyst activation.

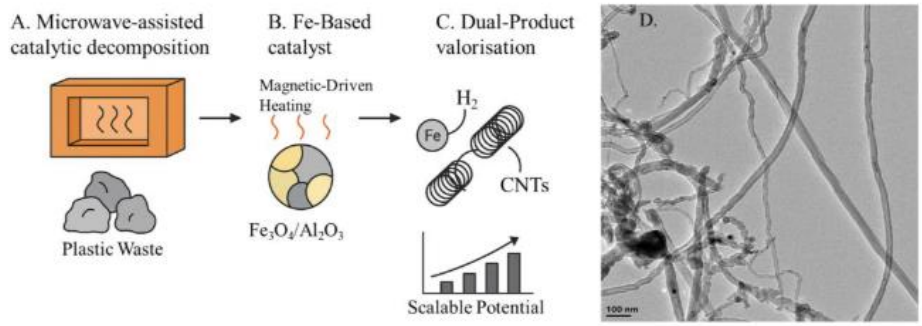

Figure 1: Schematic representation of the microwave-assisted catalytic decomposition of plastic waste and dual-product valorisation, and TEM image of multi-walled carbon nanotubes.

Iron-based catalysts are known to undergo dynamic phase changes under reaction conditions, with transitions from Fe_3O_4 to Fe^0 or iron carbides playing a central role in hydrogen release and carbon growth. However, prolonged use can lead to nanoparticle encapsulation by graphitic carbon, hindering reusability. Initial cycling tests in this study reveal that the catalyst retains activity over multiple runs, although quantitative evaluation of iron loss and phase stability across extended cycles is ongoing. The dual production of hydrogen and graphitic carbon offers a strong value proposition in the context of circular economy and decentralized waste-to-resource platforms. Hydrogen is increasingly recognized as a clean fuel, while carbon nanotubes and related nanostructures have emerging applications in cement-hardening, electronics, and energy storage. The combination of simple catalyst, microwave efficiency, and multiproduct value supports the scalable potential of this technology for addressing the global plastic waste crisis.

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Notes

Oral presentation: OP50

Unravelling Anion Effects in the Structure of Ruthenium(II) Arene Pyridyl-Triazole Complexes: Implications for Transfer Hydrogenation Catalysis

Cassiem Joseph,[a] Izak Kotze,[b] Andrew Swarts[b] and Selwyn Mapolie[a]

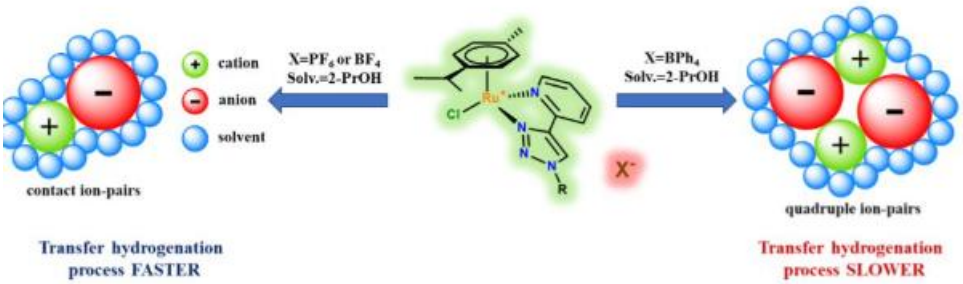
[a]*Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag 1, Matieland, 7601, Stellenbosch, South Africa. E-mail: cjoseph@sun.ac.za.*
[b]*Molecular Science Institute, School of Chemistry, University of the Witwatersrand, Johannesburg-Braamfontein, 2050, South Africa.*

Keywords: ruthenium catalysts, transfer hydrogenation, ion-pairing

Notes

Transition-metal complexes, particularly those based on Ru(II), continue to play a pivotal role in the advancement of homogeneous catalysis due to their robust reactivity profiles and tunable coordination environments [1]. Among these, cationic half-sandwich Ru(II) arene complexes have garnered interest not only for their catalytic potential in hydrogenation and related processes but also for their rich solution-phase behavior arising from ion-pairing phenomena [2]. The pairing of the metal cation with various counterions can significantly influence both the structure and reactivity of these systems. In particular, weakly coordinating anions such as BF_4^-, PF_6^-, and BPh_4^- are commonly employed to stabilize cationic complexes, but their impact on metal–substrate interactions and catalytic efficiency remains underexplored [1-3]. This is especially critical for systems where subtle changes in steric or electrostatic environments can affect the accessibility of the metal center.

Recent efforts have shown that the extent and nature of ion-pairing are strongly solvent-dependent and can manifest in multiple forms - from contact ion-pairs to solvent-separated aggregates - each influencing the behaviour of the complex in catalysis [4]. In this context, we investigated a series of Ru(II) arene complexes supported by pyridyl-1,2,3-triazole ligands bearing BPh_4^-, PF_6^-, or BF_4^- counterions to systematically probe their ion-pairing tendencies using PGSE NMR, NOE spectroscopy, X-ray diffraction, and conductivity studies [5]. Our findings reveal that the BPh_4^- analogue forms tight ion aggregates (even in polar solvents like MeCN), while the PF_6^- and BF_4^- complexes exhibit looser or solvent-separated ion pairs. These structural insights were directly correlated with catalytic data in transfer hydrogenation, where complexes with weaker ion-pairing (e.g., PF_6^-) showed enhanced activity, suggesting that counterion selection is not merely a structural detail but a functional design element in catalyst optimization.



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Notes

Oral presentation: OP51

Biphasic Hydroaminomethylation of Olefins Catalysed by Pyridyl-triazole Ruthenium Complexes

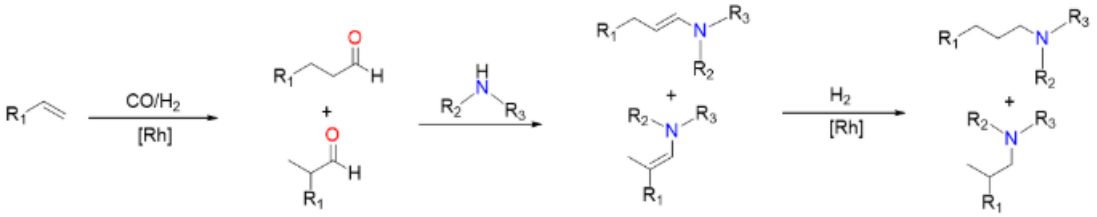
Lydia Christoph[a] and Selwyn Mapolie[a]

[a]*Department of Chemistry and Polymer Science, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa, E-mail: lchristoph@sun.ac.za*

Keywords: Hydroaminomethylation, hydroformylation, ruthenium, biphasic, recycling.

Notes

Amines constitute an important class of compounds with widespread application in the preparation of pharmaceuticals, dyes, and surfactants among various fine and bulk chemicals.[1,2] They are commonly synthesised via substitution reactions using alkyl halides, reactions which often result in low yields and substantial amounts of organic waste.[1] The yield and efficiency of amine syntheses can be improved using tandem catalytic processes, such as the hydroaminomethylation (HAM) reaction, which allows for the synthesis of amines from widely available and affordable alkenes.



Scheme 1: General reaction scheme for the hydroaminomethylation of olefins.

HAM is conventionally catalysed by rhodium complexes bearing bulky phosphine ligands. Such systems normally afford high conversions and selectivity towards the desired amine products.[2–4] However, due to the high cost of rhodium, the use of alternative metals has attracted interest. Ruthenium presents an attractive alternative due to its notable hydrogenation activity. In this study, a new aqueous biphasic system for the hydroformylation and HAM of olefins was developed. Pyridyl-triazole ligands were synthesised from affordable starting materials via simple reaction procedures and were modified via the incorporation of a polyethylene glycol (PEG) tether to enhance their solubility in water and enable catalyst recycling.

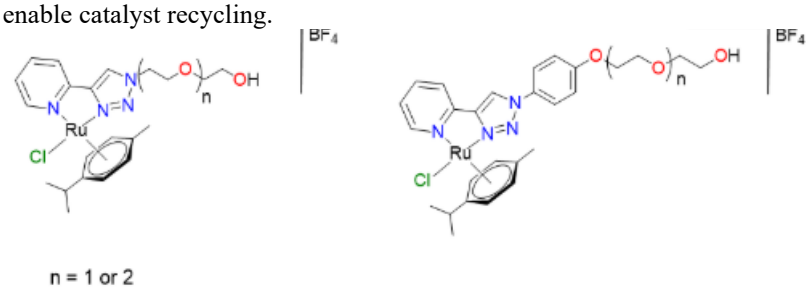


Figure 1: Structures of new pyridyl-triazole ruthenium(II) complexes.

These ligands were used to prepare four novel water-soluble ruthenium(II) complexes which were fully characterised using various analytical techniques. The complexes were evaluated as pre-catalysts in the aqueous biphasic hydroformylation and hydroaminomethylation of 1-octene as a model substrate. Key reaction parameters which included time, temperature, catalyst loading, and syngas pressure were optimised systematically. The complexes displayed promising catalytic activity and recyclability, demonstrating their potential as environmentally-friendly catalysts. Furthermore, the HAM of 1-octene with piperidine was coupled to the water-gas-shift reaction, which involves the conversion of carbon monoxide and water to CO_2 and H_2. In doing this, the reactions could be carried out purely under CO pressure without the need for the use of hydrogen gas directly.

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Notes

Oral presentation: OP52

Manganese-cobalt-oxide constructed in hybrid nitrogen doped carbon nanotubes-carbon nano onions as cathode electrocatalysts for rechargeable zinc-air battery

Ludwe L Sikeyi[a], Nithyadharseni Palaniyandy[a], Mkhulu M Mathe[a] and Soorathep Kheawhom[b]

[a]*Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering, and Technology, Florida Science Campus, University of South Africa, Roodepoort 1709, South Africa,*
E-mail: esikeyll@unisa.ac.za.
[b]*Department of Chemical Engineering, Faculty of Engineering, Chulalongkorn University, Bangkok 10330, Thailand.*

Keywords: N-CNT@CNO, cathode electrocatalysts, electrode fabrication, cycling performances, zinc-air battery.

Abstract

Zinc-air batteries (ZABs) are a promising energy storage technology that has gained increasing interest for their high energy density, cost benefits, and safety, as well as their abundant supply of zinc (Zn) and environmental friendliness [1]. The primary reactions that comprise the charging and discharging processes in ZABs are the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) [2]. To enhance both ORR and OER activities, researchers have focused on designing proficient bifunctional electrocatalysts [3]. The N-CNT@CNO hybrid nanocomposite material was synthesized by an assisted hydrothermal method. Herein, the one-pot synthesis technique is introduced as an efficient and low-cost method for the preparation of electrocatalysts based on bimetallic Mn-Co-O nanometer-scale particles distributed over a hybrid carbon support N-CNT@CNO structure. This hybrid structure, Mn-Co-O/N-CNT@CNO, successfully enhances conductivity and active site accessibility, thereby enhancing ORR and OER reactions. The Mn-Co-O/N-CNT@CNO hybrid demonstrates excellent bifunctional activity, characterized by a notable ORR's half-wave potential of 0.74 V and an OER's onset potential of 1.5 V with a potential gap (ΔE) of 0.94 V. When employed in a ZAB, the battery achieves a peak power density of 17 Mw cm^{-2} and maintains cycling stability for over 93 h at 10 mA cm^{-2}.

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Notes

Oral presentation: OP53

Identification of High-Entropy Alloy Descriptors for CO_2 Methanation: Catalyst design using Machine learning

Liberty L Mguni[a], Andrew Ndhlovu[b], Yali Yao, Bogdan Dorneanu[c], Harvey Arellano-Garcia[c]

[a]*Institute of Catalysis and Energy Solutions (ICES), University of South Africa, Florida campus, Johannesburg 1710, South Africa,*
[b]*Evolutionary Genomics Group, Department of Botany and Zoology, University of Stellenbosch, Private Bag X1, 7602, Matieland, South Africa.*
[c]*Department of Process and Plant Technology, Brandenburg University of Technology (BTU) Cottbus-Senftenberg, Cottbus, Germany*

Keywords: High-Entropy Alloy, multi-objective optimization, machine learning

Abstract

Carbon dioxide hydrogenation offers a sustainable approach to mitigate climate change by converting CO_2 into value-added fuels such as methane (CH_4), which benefits from existing infrastructure and broad utility [1]. This study focuses on the rational design and optimization of high-entropy alloy (HEA) catalysts for CO_2 methanation, leveraging their compositional flexibility and thermal stability. Literature data were analysed to identify key performance descriptors, followed by multi-objective optimization using NSGA-II and fuzzy logic to define ideal property windows. Notably, weighted Pauling electronegativity (EN) was a more reliable predictor of catalytic behaviour than Mulliken EN, with values above 1.2 correlating with improved activity. Additionally, smaller weighted atomic radii (1.1–1.6 Å) and low ΔR values enhanced CH_4 selectivity, likely due to reduced lattice strain and better structural coherence. Over 2 million alloy compositions were computationally screened using this optimized descriptor space, yielding 8614 promising candidates (0.43%). An experimental analysis of a few selected alloys showed great promise, with an activation energy (Ea) for the process ranging between 45 and 71 kJ/mol, which is lower than the Ea of the widely used catalyst Ni/Al_2O_3 at 75 kJ/mol. The catalyst, however, showed low selectivity towards methane. This approach demonstrates a potential data-driven framework for catalyst discovery, capable of rapidly narrowing vast chemical spaces to identify novel, high-performance HEAs for CO_2 hydrogenation.

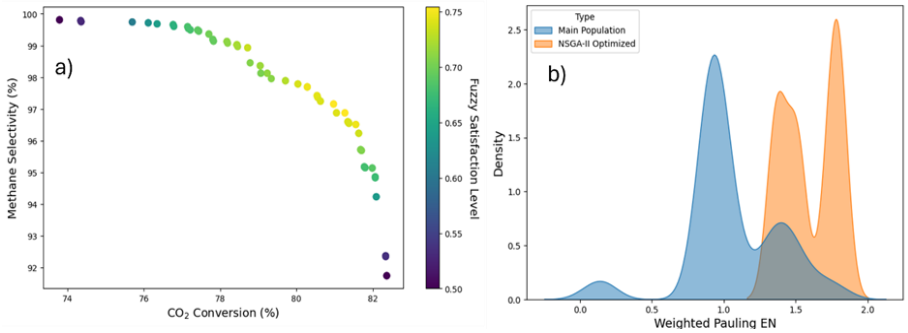

Figure 1 a) NSGA II Pareto front results and the property distribution for promising alloys b) Weighted Pauling EN

Reference

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Notes

Oral presentation: OP54

Approaching photocatalysis from a different angle: Low energy waves a game changer.

Ngonidzashe Masunga[a], Vijaya S. Vallabhapurapu[a], Bhekie B. Mamba[b]
Corresponding author: masungn@unisa.ac.za

[a]*University of South Africa, Florida Science Campus, College of Science Engineering and Technology, Physics Department, South Africa*
[b]*University of South Africa, Florida Science Campus, College of Science Engineering and Technology, Institute for Nanotechnology and Water Sustainability, South Africa*

Keywords: Low energy waves, Photocatalysis, magnetic field, Thin-film, Organic pollutants

Abstract

In the search for environmentally clean technology for the effective removal of organic pollutants from water and a clean way of producing hydrogen from water, visible-light-driven photocatalysis has gained a lot of attention. However, the application of this promising technology at the industrial scale has been limited due to the high cost involved, low efficiency, and difficulty in recovering and reusing the photocatalyst. In this work, the impact of low energy waves (LEW) on tailoring the physical, optical, and electrochemical properties of the thin film photocatalysts during and after synthesis was discussed. Additionally, the incorporation of LEW in a photocatalytic reactor to activate the photocatalyst and as an energy source was explored. The photocatalytic activities of the produced thin films towards organic pollutants in water and hydrogen evolution were discussed. The possibility of recovery and reuse of thin-film photocatalysts, the principles of LEW heating, and the advantages and demerits of LEW heating were deliberated. Lastly, the gaps that are still open for research and the way LEW should be incorporated in photocatalysis to pave the way for the industrial application of this technology were proposed. Overall, the incorporation of LEW energy in photocatalysis offers significant opportunities for advancing the field and addressing pressing environmental and energy challenges. Continued research and development in this area will likely yield novel catalyst designs, improved process efficiencies, and expanded applications, ultimately contributing to a more sustainable and cleaner future

Acknowledgements

The University of South Africa is to be commended for making all the resources required for this project work available to the authors

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Notes

Oral presentation: OP55

From Black Box to Profiles: Advancing Catalysis Research with the Profile Reactors

Dr. Aldo Conti,[a]

[a]*AC Scientific*

Keywords: reactions, reaction mechanism, Iso-potential spectroscopy, Spatially resolved profiling

Abstract

Understanding catalytic processes requires experimental tools capable of resolving spatial and temporal variations inside working reactors. The Compact Profile Reactor (CPR), developed by Reacnostics, addresses this need by enabling high-resolution operando profiling of catalytic fixed beds under industrially relevant conditions. The CPR integrates micrometer-precision capillary sampling with simultaneous temperature and concentration measurements, while maintaining mechanical robustness for operation up to 20 bar (80 with a stainless steel reactor tube) and 700 °C. Crucially, the design allows for optical access and direct coupling to advanced spectroscopic techniques such as diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), thereby overcoming the limitations of conventional operando cells that often compromise either kinetic accuracy or spectroscopic quality.

A key feature of the CPR is its compatibility with iso-potential operando spectroscopy, which separates the catalytic reactor from the spectroscopic cell while maintaining the same local chemical potential. This approach ensures that catalyst structure, adsorbate populations, and reactivity observed spectroscopically are representative of the conditions inside the reactor. Applied to CO_2 methanation on Ni/Al_2O_3, iso-potential DRIFTS within the CPR enabled spatially resolved detection of surface intermediates, identifying formates as kinetically relevant species while carbonyls act largely as spectators. These insights, obtained directly under realistic flow and gradient conditions, demonstrate the power of the CPR to connect local chemistry with global reactor performance.

By combining robustness, modularity, and advanced operando spectroscopy, the Compact Profile Reactor establishes a versatile platform for mechanistic studies, catalyst development, and process optimization. Its ability to resolve gradients and correlate them with catalyst dynamics represents a significant advance in heterogeneous catalysis research.

Notes

Oral presentation: OP56

The development of Cu-based perovskites for application in CO2 hydrogenation to methanol

B.S. Xaba,[a] and P.R. Makgwane[a]

[a]*Institute of Catalysis and Energy Solutions, College of Science, Engineering and Technology, University of South Africa, Florida Campus, Johannesburg, 1709, South Africa,*
E-mail: xababs@unisa.ac.za

Keywords: carbon dioxide, hydrogenation, methanol, substituted perovskites.

Abstract

The intensification of catalytic processes that 70haract CO2 as a feedstock in the synthesis of value-added chemicals and fuels, such as methanol, dimethyl ether (DME), formic acid and hydrocarbons, holds the key to effective CO2 abatement, as CO2 is responsible for global warming [1, 2]. Catalytic hydrogenation of carbon dioxide presents a net-zero CO2 build-up and sustainable process to produce methanol, when green hydrogen is used (Figure 1). However, reported catalysts for methanol synthesis via CO2 hydrogenation still suffer from deactivation, resulting in activity loss due to Cu sintering or transformation of an active phase to an inactive species during the reaction. The commercial methanol synthesis uses syngas (CO/CO2/H2) as a feedstock over the Cu/ZnO/Al2O3 catalyst [3]. The atomic dispersion of Cu and thermal stability are some of the critical structural properties of the catalyst that can be significantly improved by employing perovskite catalysts, leading to enhancement in performance and thermal stability [4, 5]. In the current study, substituted Cu-based perovskites with the formula of SmxIn1-xCuyM1-yO3-δ (M = Zr or La) are 70haracteriz and 70haracterized using techniques such as XRD, BET, TGA, H2-TPD and CO2-TPD. These perovskites are evaluated in the CO2 hydrogenation to methanol reaction.

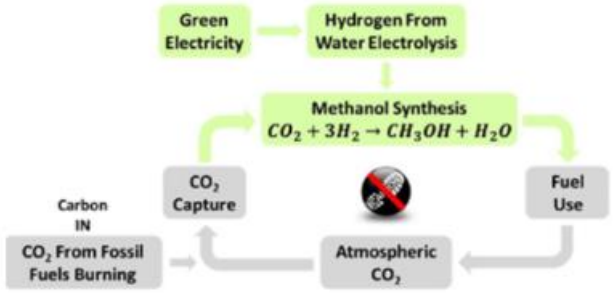

Figure 1: Methanol production pathway from green hydrogen and captured CO2 [6]

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Notes

Poster Presentation Session I: Catalysis, Materials, and Sustainable Innovation

Driving the Sustainable Development Goals through Advanced Catalytic Science

This session features pioneering research that advances multiple Sustainable Development Goals (SDGs), showcasing the catalytic strategies and material innovations shaping a more sustainable future. The posters span diverse applications from green hydrogen and biofuels to rare earth recovery and carbon capture each contributing to global sustainability targets.

Key SDG alignments include:

- ⚡ **SDG 7 (Affordable & Clean Energy):** Electrocatalysts for water splitting, PEMFC membrane development, and pilot-scale electrolysis systems for hydrogen production.
- 🌍 **SDG 13 (Climate Action):** CO_2 capture and conversion using MOFs, perovskites, and photocatalytic systems; thermodynamic analysis of calcination processes and methane oxidation.
- 🔄 **SDG 12 (Responsible Consumption & Production):** Upgrading of biomass-derived bio-oils, anaerobic digestion of wastewater, and valorization of coal ash and abattoir effluent.
- 🧪 **SDG 9 (Industry, Innovation & Infrastructure):** Zeolitic catalyst optimization, Fischer-Tropsch synthesis enhancements, and rare earth recovery for strategic materials.
- 🌱 **SDG 6 (Clean Water & Sanitation):** Development of gas sensors and conductive polymer composites for environmental monitoring and pollutant detection.
- 🧬 **SDG 3 (Good Health & Well-being):** Quantum dot synthesis for PET scanners and bioactive compound production with anti-obesity potential.

This session invites attendees to explore how catalytic science intersects with global development goals, offering molecular solutions to systemic challenges. Engage with presenters to uncover the mechanisms, materials, and multidisciplinary collaborations driving sustainable innovation.

Poster 1-1

Synthesis and Characterisation of OER Electrocatalysts for Green Hydrogen Production

Nzimeni Anele[a] , Claudelle Anansong[a], Shawn Gouws[a]

[a] *Department of Chemistry, Nelson Mandela University, Summerstrand, Gqeberha, 6001, South Africa, E-mail: s220664307@mandela.ac.za.*

Keywords: Oxygen Evolution Reaction, Proton Exchange Membrane (PEM) water electrolysis, metal-oxide catalyst.

Abstract

The development of durable and highly active oxygen evolution reaction (OER) electrocatalysts is crucial for enhancing the efficiency of green hydrogen production through proton exchange membrane (PEM) water electrolysis.[i] This study focuses on the strategic synthesis and characterisation of metal oxide-based alloyed systems of OER electrocatalysts, composed IrM oxides as bimetal, trimetal or multiple metal oxides (M= Ru, Ni, Mn, Ti, Co and Cu)[ii] prepared via various methods of synthesis, including Adam's Fusion method, Polyol method and Co-reduction polyol method to critically evaluate the influence of the synthetic route on the structure and performance of catalysts. Furthermore, the influence of calcination temperature (350 ℃ - 550 ℃) on the catalyst's particle size, crystallinity, surface area and morphology are systematically explored. Techniques such as X-ray diffraction (XRD), X-Ray Fluorescence (XRF), Scanning Electron Microscopy (SEM) and High-Resolution Transmission Electron Microscopy (HR – TEM) are employed for structural characterization. Cyclic Voltammetry (CV) and Linear Scan Voltammetry are utilised to evaluate the electrochemical performance of the synthesised catalysts in acidic media.[iii]

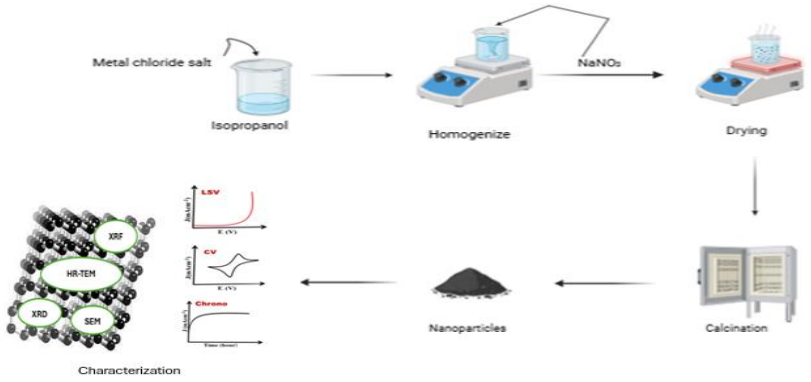


Figure 2: Schematic representation of the synthesis and characterisation of the electrocatalysts.

Notes

Poster 1-2

Visible-light-driven reductive carboxylation of unsaturated hydrocarbons and 1,3-dicarbonyl compounds with CO_2 catalyzed by Nickel(II) complexes

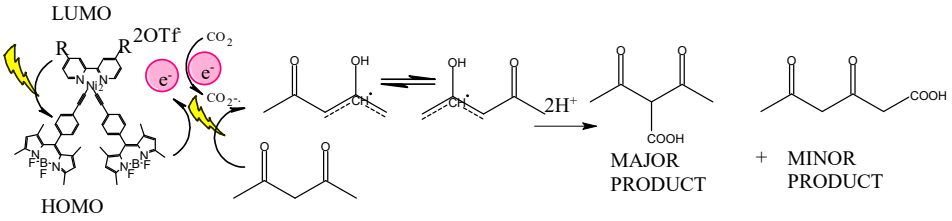
NT Nkala,[a] J Darkwa[a] and TA Tshabalala[a]

[a] *Department of Chemical Sciences, Faculty of Science, University of Johannesburg, P.O. BOX 524, Auckland Park 2006, Johannesburg, South Africa,*
E-mail: noxolonkala32@gmail.com

Keywords: carbon dioxide, carboxylic acids, photocatalysis, nickel complexes.

Abstract

The reliance on fossil fuels to meet the increasing global energy demand has resulted in a high concentration of carbon dioxide (CO_2) emissions, therefore the conversion of CO_2 into value-added chemicals and fuels under mild conditions has attracted considerable attention as a method to reduce CO_2 emissions and contribute towards the mitigation of global warming and climate change [1, 2]. In view of the significance of carboxylic acids and their derivatives in the production of pharmaceuticals, cosmetics, and polymers; CO_2 is an abundant, low-cost, and non-toxic C1 source for their synthesis [3]. Employing homogenous metal catalysts in traditional carboxylation reactions to achieve high selectivity and activity requires stoichiometric amounts of high energy reagents, harsh reaction conditions, and limited functional group substrates due to the thermodynamic stability and chemical inertness of CO_2 [4]. The introduction of visible-light-driven carboxylation offers gentle reaction conditions, a wide range of substrate compatibility, low catalyst loading, and easy product derivatization [5]. Pairing Ni(II) complexes with a well-known chromophore such as BODIPY (BDP) is advantageous since BDPs are known for their efficient light absorption, structural adaptability, adjustable electronic characteristics, and proficient charge transfer mechanisms [6]. For this reason, [Ni(BDP)] photocatalysts are synthesized, characterized, and applied in visible-light-driven reductive carboxylation with CO_2 reactions. This work aligns with three of the United Nation's Sustainable Development Goals. The design and development of novel catalytic materials relates to SDG 9 (Industry, Innovation, and Infrastructure). The application of these novel photocatalysts in visible-light-driven reductive carboxylation reactions with CO_2 aligns with SDG 7 (Affordable and Clean Energy) and 13 (Climate Action).



R = H, OMe, tBu

Scheme 1: Visible-light-driven reductive carboxylation of 1,3-dicarbonyl compounds with CO_2 mediated by Ni(II) complexes.

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Notes

Poster 1-3

CuPt nanoparticles in the selective, aerobic oxidation of methane

Zibusiso Nhachengo,[a] Sinqobile V.L. Mahlaba and Eric van Steen

[a]Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch, 7700, South Africa, E-mail: nhczib001@myuct.ac.za.

Keywords: CuPt nanoparticles, selective oxidation, platinum, formaldehyde, catalytic activity.

Abstract

Methane is a potent greenhouse gas, but it is at the same time an abundant clean source of energy and for the production of chemicals with the latter typically via the synthesis gas route, as the selective oxidation of methane to value-added chemicals such as methanol and formaldehyde, remains challenging. Platinum-based catalysts have been demonstrated to be effective in the selective oxidation of methane, but the reaction appears to be limited by the strong bonding of the product intermediate to the platinum surface [1]. Alloying platinum with another transition metal modifies the d-band configuration, and thus the strength of adsorption of intermediates, which may result in enhanced catalytic activity. For instance, Cu@Pt core-shell nanoparticles may be beneficial for this reaction as the compression of platinum in the shell will reduce the d-band centre, thus weakening the Pt-O bond which could increase the rate of reaction. Here, we investigate the catalytic performance of CuPt nanoparticles in the selective oxidation of methane.

CuPt nanoparticles were synthesized using a solvothermal method [2]. The metal precursors were mixed with benzyl ether, oleylamine and oleic acid. Water was removed from the solution under vacuum and the solution was rapidly heated to 300°C under N2 atmosphere for 1 hr. As a control, pure Pt and Cu-nanoparticles were synthesized using the same method. The nanoparticles were characterized by ICP-OES , TEM, XRD and FTIR to determine their composition and structural properties. The nanoparticles were dispersed on titania (rutile phase) to yield a metal loading of ca. 7%. Catalytic tests were conducted in a fixed bed reactor at 220°C and 20 bar in the presence and absence of steam (pO2=2 bar; pCH4=0.6 bar). The products were analysed using GC-FID equipped with a methaniser.

The removal of the surfactants, oleylamine and oleic acid, in the washing of the nanoparticles was monitored using FTIR. The XRD-pattern of the CuPt core-shell nanoparticles show the characteristic of the FCC-structure with the (111) reflection between 2θ value for FCC-Pt and FCC-Cu. This is typically observed upon alloying platinum with copper. The formation of an alloy rather than core-shell nanoparticles was confirmed using elemental mapping. Vegard's law was used to calculate the molar composition of Pt and Cu within the crystalline alloy with line-broadening used to determine the crystalline domain size. For instance, Cu1Pt2/TiO2, with an average crystalline domain size of 11.6 nm, showed in the TEM an average particle diameter of 10.2 nm. For initial tests, impregnated Pt and Cu supported on TiO2 were tested in the fixed bed reactor. The activity and selectivity of all synthesized CuPt core-shell nanoparticles supported on TiO2 will be compared with the activity and selectivity obtained over impregnated Pt/TiO2 (Pt-loading: 7.8 wt.-%; -rCH4 = 402 µmol/gcat/hr; SFormaldehyde = 81%) and Cu/TiO2 (Cu-loading: 4.9 wt.-%; -rCH4 = 114 µmol/gcat/hr; SFormaldehyde = 25%) in the selective oxidation of methane.

This study demonstrates the importance of Pt-based catalysts on the catalytic performance for the selective oxidation of methane. Future work will focus on fully understanding the synthesized CuPt core-shell nanoparticles on the catalytic performance for methane oxidation and exploring the underlying mechanisms to optimize catalyst.

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Notes

Poster 1-4

Sustainable BioFuel Production via One-Pot C-C Coupling and Hydrodeoxygenation of Biobased Compound over Versatile LaNi1-xCuxO3±δ Inorganic Perovskites.

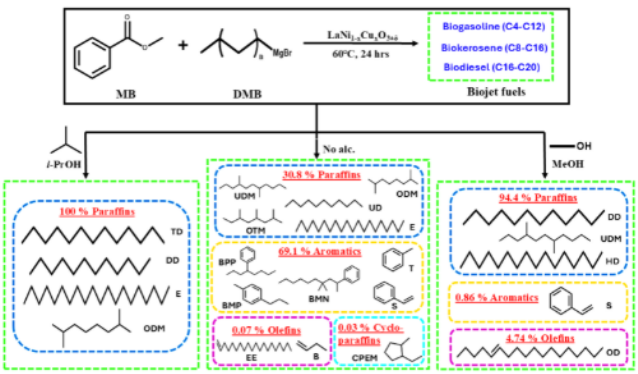
Hlengane Precious Mokwena[a], Sithandile Ngxangxa[b], Isaac N. Beas[c], Nangamso Nathaniel Nyangiwed, Hui Lie, and Ndzondelelo Bingwa[a]

[a]*Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering and Technology, University of South Africa, Florida Science Campus, Roodepoort 1709, E-mail: hlenganemokwena@gmail.com.*
[b]*Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, PO Box 524, Johannesburg, 2001, South Africa.*
[c]*Department of Natural Resources and Materials, Botswana Institute for Technology Research and Innovation, Maranyane House, Plot 50654 Machel Drive, Gaborone, Botswana.*
[d]*Department of Natural Resources and Materials, Botswana Institute for Technology Research and Innovation, Maranyane House, Plot 50654 Machel Drive, Gaborone, Botswana.*
[d]*Tshwane University of Technology, Department of Physics, 175 Nelson Mandela Dr, Arcadia, Pretoria, South Africa. e School of Thermal Engineering, Shandong Jianzhu University, Jinan, 250101, PR China.*

Keywords: perovskites, oxygen vacancies, carbon-carbon coupling, hydrodeoxygenation.

Abstract

Processing of biomass to energy chemicals starts from pyrolysis to oxygenated platform molecules that require hydrodeoxygenation (HDO) to biofuels. Also, the composition and carbon chain lengths from direct pyrolysis make direct utilization in specialized engines difficult due to compatibility issues. Therefore, tailormade carbon-carbon (C-C) coupling and hydrodeoxygenation of bioderived platform molecules become central to attainment of green and sustainable biofuels. In this work, the catalytic activity of LaNi1-xCuxO3±δ ($0 \leq x \leq 1$) perovskites was assessed in the attainment of biofuels, including biogasoline, biokerosene, and biodiesel. The acquired results suggest that the metal ratios of the B-site cations (B and B`) significantly influence the catalytic performance of the perovskites in the conversion of biobased compound to biofuels. Notably, the synthesized LaNi0.5Cu0.5O3±δ perovskites demonstrated efficient one pot C-C coupling and HDO of methyl benzoate and dodecylmagnesium bromide, a Grignard reagent, achieving 58.1% conversion and 100% selectivity towards fuel hydrocarbons at relatively low temperatures (60 to 90 °C). While reactions involving a Grignard reagent normally yield oxygenated products, for the first time the as-synthesized catalysts demonstrated a highly efficient one-pot C-C coupling and dehydration of the biofuel intermediates. Thus, this study provides valuable insights into the design of effective perovskite catalysts for sustainable synthesis of biofuels by looking at the effect of different alcohols as reaction media. Furthermore, this work presents the first use of a Grignard reagent for chain length extension in sustainable synthesis of biofuels.



Scheme 1: Summary of product distribution of biofuel components from one-pot C-C coupling and HDO of MB without alcohol and with the addition of MeOH and i-PrOH over the prepared LaNi1-xCuxO3±δ ($0 \leq x \leq 1$) perovskites.

Notes

Poster 1-5

Photocatalytic C-H carboxylation of unsaturated hydrocarbons and dicarbonyl compounds with CO2 promoted by Ru(II)-bodipy complexes

Tinyiko Baloyi,[a] James Darkwa and Thandeka Tshabalala

[a]*Department of Chemical Sciences, Research Centre for Synthesis and Catalysis, University of Johannesburg, P O Box524, Auckland Park 2006, Johannesburg, South Africa.*

Keywords: Dicarbonyl, hydrocarbon, carbon dioxide, carboxylation, photocatalyst.

Abstract

The use of carbon dioxide as a sustainable C1 source in the direct carboxylation to construct new C-C bonds has been a great challenge in keeping the environment eco-friendly [1]. CO2 is abundant, inexpensive, and non-toxic and is widely known due to its anthropogenic causes [2]. Carboxylic acids are one of the most important compounds in organic synthesis and industrial synthesis; however methods that have been put in place to produce these valuable commodities have proved to further increase the amount of CO2 in the atmosphere, such as the direct carboxylation methods, which is a reaction that has poor functional group tolerance, uses high stochiometric amounts of high energy reductants and uses harsh thermal catalytic conditions such as high temperatures [3]. Thus, even if this reaction had functional group tolerance these reactions would require stoichiometric amounts of metallic reductants further causing an increase in the CO2 emissions as well as further increase the CO2 concentration in the atmosphere. Green chemistry has played a significant role in reducing CO2 emissions whereby photocatalytic carboxylation is used, which is a method that is environmentally benign and uses mild reaction conditions [4].

In this project novel ruthenium(II) bodipy complexes will be used as photosensitizers in the photocatalytic carboxylation of various unsaturated hydrocarbons and dicarbonyl compounds to give the corresponding carboxylic acids. This project aims to develop highly efficient method for CO2 fixation the synthesis of valuable and industrially important reagents by designing highly effective and efficient photocatalyst with a great light absorption, electron efficiency and capacity to CO2.

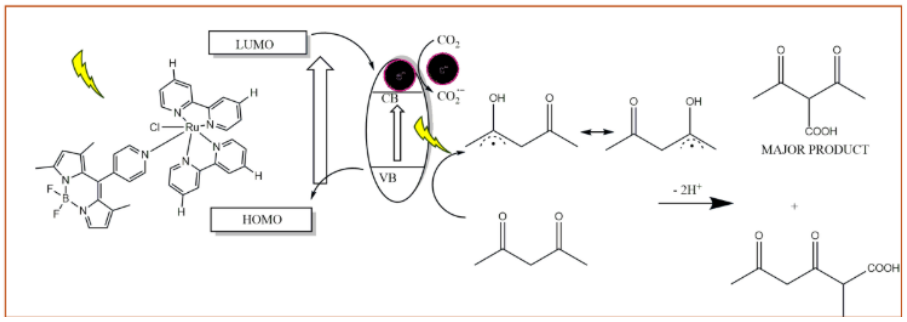


Figure 1: Proposed photocatalytic carboxylation of Ruthenium(II) complexes.

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Notes

Poster 1-6

The Effects of Different Supports over Co-Based Catalysts on the Ethylene Secondary Reaction in Fischer-Tropsch Synthesis condition

Chen Liu,[a] Yusheng Zhang[b] and Yali Yao[a]

[a]Institute for Catalysis and Energy Solutions, University of South Africa,1710, Private Bag X6, Florida, South Africa,
E-mail: 11744057@mylife.unisa.ac.za.
[b]College of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan Taoyuan Road (411201) , Hunan, PR China .

Keywords: FTS,ethylene hydrogenation, methane,Co, TiO_2, Al_2O

Abstract

During the gasification of primary carbon sources such as charcoal, natural gas, naphtha, and biomass, a significant amount of α-olefins is typically present in the resulting syngas.[1] In addition to linear alkanes, Fischer–Tropsch synthesis (FTS) products also contain α-olefins and oxygenates.[2] It is widely accepted that α-olefins, as primary FTS products, can be re-adsorbed onto the catalyst surface and undergo secondary reactions, thereby altering the overall product distribution. However, the reactivity of α-olefins under FTS conditions has not been systematically studied. To date, the influence of different catalyst supports on the types and products of α-olefin secondary reactions remains insufficiently understood. Various supports exhibit distinct behaviors in FT reactions; for instance, acidic and neutral Al2O3 differ in terms of surface sites, which in turn can affect catalytic performance. In this study, conventional inorganic oxide supports such as titanium dioxide (TiO2) and aluminum oxide (Al2O3) were employed. For comparison, the cobalt content was fixed at 15 wt% across all catalysts, and all samples were prepared using the conventional incipient wetness impregnation (IWI) method. To directly detect the products of ethylene hydrogenation and cleavage, deuterium was used as an isotopic probe. Methane with varying deuterium contents was analyzed by soft ionization mass spectrometry (MS) to investigate the underlying mechanism of ethylene hydrogenative cleavage and to elucidate the effect of support properties on this reaction.

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Notes

Poster 1-7

Macroporous resin grafted with Perylene diimide side-chains for efficient photosynthesis of H_2O_2

Jiangbo Guo[a], Xinying Liu[a], Yali Yao[a] and Xudong Yu[b]

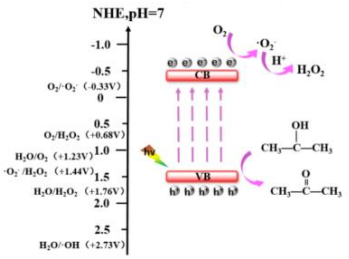
[a]*Institute for Catalysis and Energy Solutions, University of South Africa,1710, Private Bag X6, Florida, South Africa*
13523937@mylife.unisa.ac.za
[b]*Hebei Provincial Key Laboratory of Photoelectric Control on Surface and Interface, and College of Science, Hebei University of Science and Technology, Yuxiang Road 26, Shijiazhuang 050080, PR China*

Keywords: photocatalysis, macroporous resin, hydrogen peroxide, perylene diimid.

Abstract

Hydrogen peroxide, as an important chemical, is widely used in the chemical, pharmaceutical, textile, and environmental industries. However, traditional industrial production method has high energy consumption, high cost, and is not environmentally friendly. Photosynthesis, a green method, has attracted the attention of researchers. It is significant to develop a photocatalyst that high efficiently converts superoxide radicals to hydrogen peroxide. However, traditional photocatalysts still face two challenges, 1) Poor O2 adsorption. 2) Slow photogenerated carrier separation and transfer. In this work, we introduce perylene diimide (PDI) units into macroporous resin polymer chains using sulfamide bonds as linkers to produce three photocatalysts named PSS-AM-PDI, PSS-HA-PDI and PSS-EDA-PDI. In the grafted resin, PDI molecules linked to the polymer chains form a short-range π-π stacking interaction, which not only shortens the charge migration distance and reduces the charge recombination efficiency, but also expanding the spectral absorption range. In addition, sulfamide bond, as a polar oxygen functional group, can not only extract electrons to accelerate the separation of photogenerated carrier and electron/proton transport, but also improve hydrophilicity and oxygen adsorption via hydrogen bonding. The experimental results indicate that PSS-EDA-PDI efficiently synthesizes H2O2 through the two-step 2e- ORR process. PSS-EDA-PDI exhibits the highest light-driven H2O2 production rate among the three photocatalysts, reaching 6141 umol g−1 h−1 in the presence of isopropanol as a sacrificer, superior to most reported PDI-based photocatalysts.

Figure 1: Mechanism of PSS-PDIEDA photocatalytic production of H2O2.



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Notes

Poster 1-8

Dual Optimisation of Biogas Technology for Gas Production and Biofertiliser Generation.

Godfrey Mpho Lelaka[a], Baraka Celestin Sempuga[a], Linda Zikhona Linganisoa and Yao Yali[a]

[a]Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering, and Technology (CSET), University of South Africa (UNISA),
E-mail: 57648484@mylife.unisa.ac.za.
UNISA Science Campus, Corner of Christiaan de Wet Road and Pioneer Avenue, Florida, 1710, South Africa.

Keywords: Biogas, digestate, optimisation, biofertiliser, operating parameter

Abstract

With the aptitude to produce clean energy and a co-product rich in plant nutrients in the form of biofertiliser, biogas technology bargains a sustainable and multifunctional solution to the world's intensifying energy and agronomic demands. Nonetheless, substrate type, biodigester design, and other system operation factors are intertwined major impacts on the quality of the digestate as a fertiliser and the efficiency of biogas production. By appraising and refining the efficiency of anaerobic digestion (AD) systems under precise settings and concomitantly gauging the digestate's agricultural potential as a biofertiliser, this study seeks to harness the generation of biogas.

This study treasures circumstances that enhance methane yield and digestate nutrient content by combining co-digestion methods, such as mixing food waste with animal manure and agricultural residues, pH alteration, inoculum pre-treatment and temperature regulation. Over an approximately 60-day retention period, experiments will be carried out in a laboratory-scale Automatic Methane Potential Test System (AMPTS ®), tracking significant metrics such as the quantity of biogas, methane content, carbon-to-nitrogen (C:N) ratio, total solids (TS), and the volatile solids (VS) reduction.

The findings will demonstrate that, while preserving a steady archaeal activity, co-digestion of substrates (e.g. cow dung and food waste) at differing ratios can yield the most methane, estimated at above 65% methane concentration. The resulting digestate will be enriched with the high levels of the macronutrients, nitrogen (N), phosphorus (P) and potassium (K), NPK, that may be applicable as a soil improver and fertiliser. Furthermore, pre-treatment of feedstock with any available economic method, such as alkaline hydrolysis, will enhance the biodegradability of organic materials and produce more gas.

Additionally, to increase the biogas systems' energy efficiency, this optimisation procedure is hypothesised to promote a circular economy by reducing organic waste and improving the soil fertility through application of the co-product. Therefore, the experimental results will lend credence to the scalability of biogas technology for integrated energy-agriculture solutions in rural and peri-urban areas.

Notes

Poster 1-9

The Development of a High Performing and Durable MEA for PEMFCs.

Ursula Nyambi[a], Francois Van Schalkwyk[a] and Darija Susac[a]

[a]HySA Catalysis, Department of Chemical Engineering, University of Cape Town, South Lane, Rondebosch, Cape Town, 7700, South Africa,
E-mail: ursula.nyambi@uct.ac.za.

Keywords: PEMFCs, MEA, durability, performance.

Abstract

The global energy crisis, fuelled by the rising energy demand and the negative environmental impact of carbon dioxide emissions, has driven increasing interest in sustainable, clean energy alternatives. Renewable energy is a viable pathway to meet global energy needs and green hydrogen has become the foremost cited vector to unlock the potential sustainability thereof. In turn hydrogen fuelled proton exchange membrane fuel cells (PEMFCs) – recognized for their high-power density, high energy efficiency, zero CO2 emissions and versatility across a wide range of applications [1] – can decarbonise several hard-to-abate sectors. However, challenges related to cost and durability remain significant. This is due to primarily the membrane electrode assembly (MEA), which plays a crucial role in PEMFCs systems.

An MEA comprises of a proton-exchange membrane, platinum-group metals (PGM)-based catalyst layers and gas diffusion layers (GDLs). Platinum is a critical component in MEAs, and the advancement of this technology offers potential benefits for mineral beneficiation in South Africa, as it holds the world's largest platinum reserves. Despite their potential, MEAs face several challenges, including high PGM content, water management as well as the degradation of critical subcomponents induced by the dynamic operating conditions of PEMFC [1].

This project focuses on the development of an MEA solution for high power density, long-lifetime PEMFC applications. A first-generation MEA design was developed during 2024, comprising advanced South African catalysts and a combination of other best-in-class commercial components. Its performance and durability properties were assessed, in accordance with U.S Department of Energy (DOE) accelerated stress test protocols [2]. The extensive test campaign revealed both strengths and weaknesses of the first-generation platform and guided development efforts of the subsequent iteration. This presentation will introduce technology development progress of the next-generation MEA aimed at improving performance, efficiency and durability through the investigation of thinner membranes, advance GDLs and carbon corrosion resistant catalyst materials respectively.

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Notes

Poster 1-10

Design and Synthesis of Low-Valent Node Metal-Organic Frameworks for Carbon Dioxide (CO2) Capture and Hydrogenation

Onesimo Ntingana, Banothile Makhubela, and Banele Vatsha

Research Centre for Synthesis and Catalysis, Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park 2006, Johannesburg, South Africa,
e-mail: onesimontingana@gmail.com

Keywords: MOFs, CO2 capture and utilization, hydrogenation, low-valent metals, sulfur-based MOFs

Abstract

CO2 emissions from burning fossil fuels are one of the major contributors to high levels of CO2 in the atmosphere. As of June 2025, atmospheric CO2 emissions have reached 430 ppm,1 signaling concerns over air quality and inefficient use of fossil fuels, resulting in energetic carbon being emitted as CO2. CO2 capture, utilization, and storage (CCUS) is an engineering approach to reduce carbon emissions from industrial sources and the atmosphere.2 The captured CO2 can be used as a chemical synthesis precursor (Figure 1) or be stored securely in subsurface formations.2 Different porous adsorbents, such as zeolites, metal-organic frameworks (MOFs), and carbonaceous materials, such as amine-grafted silica and activated carbon, are being explored. Existing adsorbents have drawbacks such as low CO2 selectivity, high energy regeneration needs, moisture sensitivity, limited stability, and low CO2 absorption capacity.

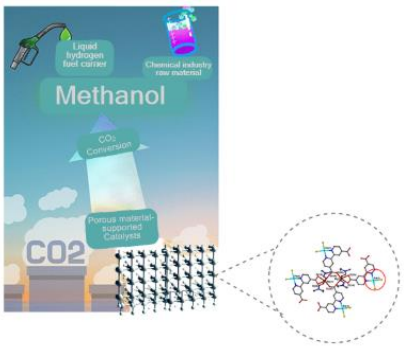

Figure 1. Illustration of CO_2 capture and hydrogenation to methanol using MOF adsorbent.

MOFs are promising materials for solid CO2 capture. These are crystalline nanomaterials of organic ligands and inorganic nodes extending infinitely into two or three dimensions through metal-ligand bonding.3 MOFs' porosity and surface area are defining characteristics of these versatile materials, with pore sizes ranging from a few Angströms to several nanometers (2 to 84 nm). Due to the diversity of ligands and the variability of metal atoms, their structure, pore size, functional groups, and coordination sizes, MOFs are tunable.4 Sulfur-based MOFs are being investigated for their potential in CO2 capture and hydrogenation. These MOFs demonstrate improved CO2 adsorption and adjustable catalytic activity for the hydrogenation reaction.5 They are soft, easily polarizable, and allow soft-soft metal-sulfur coordination, which is advantageous for CO2 capture and catalysis.6 This study uses sulfur-functionalized organic linkers to design and synthesize low-valent node MOFs for CO2 capture and hydrogenation.

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Notes

Poster 1-11

Fine-tuning the physical and chemical properties of zeolitic catalysts for ethanol dehydration to form ethylene

JTR Raphotle,a M Ngcobob and T.A Tshabalalaa

[a]*Department of Chemical Science, Faculty of Science, University of Johannesburg, P.O. BOX 524, Auckland Park 2006, Johannesburg, South Africa,*
E-mail: raphotlejtr@gmail.com.
[b]*Institute of Catalysis and Energy Solutions (ICES), College of Science, Engineering and Technology, University of South Africa,28 Pioneer Ave, Roodepoort, Private Bag X6, Florida 1709, South Africa.*

Keywords: Bioethanol, acid catalysts, zeolites, transition metals, bioethylene.

Abstract

The depletion of natural resources is a growing concern worldwide. This is due to growing industrialization and rapid population expansion, which increases the energy demand and puts significant strain on the world's limited resources [1]. This energy consumption, particularly from fossil fuels, is closely correlated with the concerning rise in greenhouse gas emissions, and these issues require instant attention [1]. It is necessary to design a process independent of fossil fuels, which lessens the rise in greenhouse gases and contributes to more sustainable energy. Alternatively, bioethanol is a renewable, sustainable energy source produced from the fermentation of biomass such as corn, sugar cane, etc. [2], [3]. It has recently drawn interest as a feedstock for the chemical industry, specifically to produce light olefins, especially ethylene, and other end products using a catalytic dehydration process. Using bioethanol as a feedstock in the production of light olefins is environmentally friendly and reduces the reliance on fossil fuels [3].

The dehydration of the bioethanol process is an acid-catalysed reaction, and it is very crucial to select a catalyst with high stability, activity, and selectivity. Among the reported catalysts based on metal-oxides, heteropolyacids, and molecular sieves, the H-ZSM-5 zeolite is a promising catalyst for the dehydration of bioethanol due to its porosity, availability of Lewis and Bronsted acidic sites, and other catalytic properties. However, its major drawback emanates from its highly acidic nature, leading to coke formation and catalyst deactivation [4]. As a result, several researchers have investigated methods, including desilication and dealumination, to balance the acidity of H-ZSM-5 for bioethanol dehydration to enhance the catalyst's stability and recyclability [5]. A viable strategy has been to add transition metals to the zeolites, which can enhance their hydrothermal stability and catalytic properties and so reduce the coking phenomenon [5].

In this study, H-ZSM-5 zeolite was synthesized hydrothermally in differing Si/Al ratios and modified with iron and nickel transition metals via the wet impregnation method. The obtained zeolitic catalysts were characterized using scanning electron microscopy-energy dispersive X-ray spectroscopy (SEM-EDS), transmission electron microscopy (TEM), powder X-ray diffraction (PXRD), X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FT-IR), Brunauer-Emmett-Teller (BET), and Thermogravimetric analysis (TGA). The synthesized modified zeolitic compounds formed potentially active, selective, stable, and recyclable catalysts for the sustainable bioethylene production from the dehydration process of bioethanol.

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Notes

Poster 1-12

Effect of palladium loading on zeolite Beta for light paraffin production from dimethyl ether

Lungelo Dlamini, Stephen Roberts and Jack CQ Fletcher

Catalysis Institute, Department of Chemical Engineering, University of Cape Town, South Africa
e-mail: dlmlun029@myuct.ac.za

Keywords: DME conversion, light paraffins, palladium, zeolite Beta

Abstract

The conversion of dimethyl ether (DME) to light paraffins (propane & butane, LPG) over zeolite Beta (H-BEA) catalysts suffers from rapid deactivation and undesired by-products such as heavy C5+ hydrocarbons [1]. Whereas the incorporation of palladium addresses these limitations in part, elevated hydrogen pressures are still required to promote intermediate olefin saturation, a consequence of which is concomitant undesired promotion of gasoline (C5+) yield [2 - 4].
So as to promote light paraffin selectivity and avoid byproduct C5+ yield, it is proposed to optimise Pd loading - both in terms of metal distribution and quantity.

H-BEA-150 (SiO_2/Al_2O_3 ~ 150) catalysts, both powders and industrial extrusions (1/16”), with Pd loadings in the range 0.01 – 0.5 wt%. are prepared by ‘incipient wetness and ion exchange methods using $Pd(NH_3)_4(NO_3)_2$.
Results of catalyst characterization by N2 adsorption, SEM, TEM, ICP-OES for surface area, porosity, morphology, metal particle size and distribution, and metal content, respectively, will be presented.
Catalytic performance, in respect of light paraffin production will be determined by the conversion of DME and hydrogen to hydrocarbon conversion at elevated temperature pressure.

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Notes

Poster 1-13

Upgrading Biomass-Derived Bio-Oil using Ni-containing Spinel Oxide: A cost-effective low-carbon pathway to biofuel production

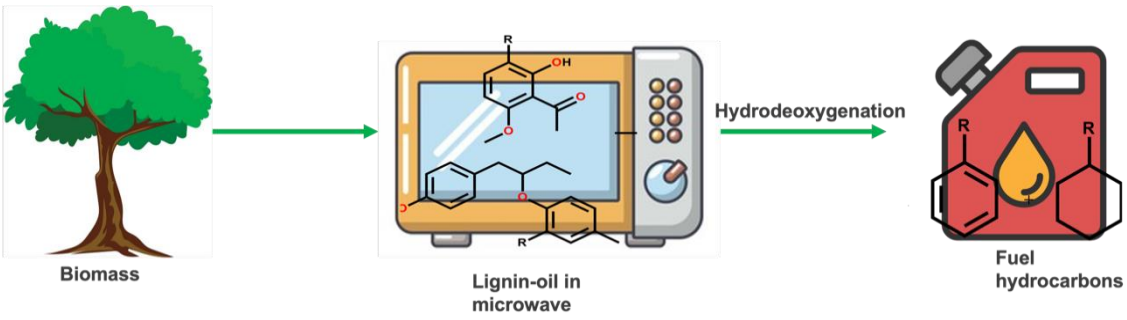
Lebohang Kekana,[a] Kabelo Ledwaba[b], Jairus L. Lamola[c], and Ndzondelelo Bingwa[a]

[a] *Institute for Catalysis and Energy Solutions (ICES), College of Science, Engineering and Technology, University of South Africa, Johannesburg, Florida Park, 1710, South Africa E-mail: lebo.mosia.ml@gmail.com.*
[b] *Department of Chemical Engineering, University of South Africa, Johannesburg, Florida Park, 1710, South Africa*
[c] *Sasol (Pty) Ltd., Research & Technology (R&T), 1 Klasie Havenga Rd, Sasolburg, 1947, South Africa*

Keywords: bio-oil upgrading, hydrodeoxygenation, mixed metal oxides, spinel.

Abstract

The hunt for sustainable and renewable energy sources has channelled much attention into exploring biomass-derived bio-oils as potential alternatives to fossil fuels. Crude bio-oil is chemically unstable, corrosive, and oxygen-rich, thus rendering it incompatible with the existing fuel infrastructures [1,2]. However, this can be remedied by means of hydrodeoxygenation (HDO) of bio-oil components to selectively remove oxygen-containing species and saturating the alkene and aromatic functionalities. This reaction is mechanistically challenging as it requires selectivity hydrogenation and deoxygenation pathways to occur synergistically [3]. Therefore, the nature of the catalyst that will facilitate this reaction is crucial in this reaction. This work showcases the use of Ni-based spinel oxides as catalyst used in upgrading lignin-derived bio-oil to biofuel in a microwave reactor. The Ni-based spinel oxides were holistically characterized and $NiMo_xO_4$ has a high surface area of 36.1 m^2/g. Microwave-assisted hydrodeoxygenation of lignin-oil in the presence of a Ni-based spinel catalyst is capable at accelerated catalysis owing to the heat emanating from within the reaction and preventing side reactions. Alkanes and arenes produced are useful chemicals in the production of fine chemicals and in the fuel market.



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Notes

Poster 1-14

Production of Alginate Oligosaccharides by Commercial and Recombinant (Flammeovirga AL2) Alginate Lyases for Potential Anti-Obesity Activity

Arryn L. Michaels[a], Coleen E. Grobler[a], Alaric Prins[b], Marilize Le Roes-Hill[b], and Brett I. Pletschke[a]

[a]*Department of Biochemistry, Microbiology and Bioinformatics, Rhodes University, Biological Sciences Building, Makhanda, 6139, South Africa,*
E-mail: inferno.michaels@gmail.com.
[b]*Applied Microbial and Health Biotechnology Institute, Cape Peninsula University of Technology, Bellville, 7535, South Africa.*

Keywords: alginate lyase, anti-obesity, alginate oligosaccharides, enzymatic hydrolysis, alginate

Abstract

Alginates are structural linear algal copolymer polysaccharides comprised of polyuronic acids, β-D-mannuronic acid (M) and α-L-guluronic acid (G), found in the cell walls of macroalgae. Alginates have been found to make up close to 40% of the dry weight of some brown seaweeds. Alginates are large molecules with high molecular weights, which means that despite the compound garnering a fair amount of attention for applications in the cosmetic and medical fields, the high molecular weight still limits its broader application.

Pancreatic lipase is responsible for the complete hydrolysis of all dietary fats, commonly in the form of triacylglycerides and diacylglycerides, into free fatty acids and monoacylglycerol. This makes it an ideal target when trying to treat obesity. Currently available treatments for obesity, such as orlistat, are effective, but result in poor patient adherence due to adverse side effects. Changing lifestyle factors such as diet and exercise are essential for managing this condition; however, many individuals struggle to maintain these changes over the long term. Sodium alginates have been shown to inhibit pancreatic lipase more moderately compared to current treatments. This may lead to a reduction in the adverse side effects patients experience [1].

Alginate oligosaccharides (AOS) are smaller alginate fragments, with lower molecular weights, which are known to have increased bioavailability as compared to the larger alginate molecule. The ideal method for producing AOS is through the enzymatic hydrolysis of sodium alginate using alginate lyases. There are very few alginate lyases available commercially - as such, a recombinant (Flammeovirga AL2) alginate lyase was included in this study [2].

The aim of our study was to use commercially available Sigma-Merck alginate lyase and the recombinant AL2 enzyme to produce AOS and test these compounds for their anti-obesity activity. The AOS were produced using commercial sodium alginate and were tested on synthetic p-nitrophenyl substrates for their potential to inhibit pancreatic lipase. The AOS should have improved inhibitory potential compared to sodium alginate, as enzymatic hydrolysis has the potential to introduce more diversity in the composition of the AOS, by exposing more of the G-unit portions of alginates, which are thought to be the main contributing factor for their inhibitory activity against pancreatic lipase.

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Notes

Poster 1-15

Hydrogenation of CO_2 to methanol over Fe modified Ce-MOFs

Keabetswe Raphoto,[a] Mduduzi. N. Cele [b]

[a]*School of Physical and Chemical Sciences, Faculty of Natural and Agricultural Sciences, North-West University (Mafikeng campus), Private bag X 2046, Mmabatho, 2745, South Africa,*
E-mail: 33223734@mynwu.ac.za

Keywords: Carbon dioxide, methanol, hydrogenation, iron, Ce-MOF.

Abstract

Carbon dioxide (CO2) is the main greenhouse gas and a major contributor to climate change and global warming [1]. The primary cause of the rise of CO2 emissions is the combustion of fossil fuels. The CO2 hydrogenation to methanol using Metal Organic Frameworks (MOFs) has been widely used due to their flexibility in synthesis and design, high porosity and large surface area [2]. MOFs have demonstrated outstanding potential regarding CO2 utilisation [3]. Methanol can be utilised as a chemical derivative of several chemicals, and it is a biodegradable and clean-burning fuel [4]. The MOFs of Ce-MOF, 1 % Fe/Ce-MOF and 2 % Fe/Ce-MOF catalysts were synthesised. The catalysts were characterised using Fourier transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). The FTIR results indicated significant peaks at 2972, 1721 and 1391 cm-1, confirming the Ce-MOF incorporation within all synthesised catalysts. It is evident from the XRD results that the intensity and crystallinity of the Ce-MOF, with peaks located at 2θ = 11.0 and 17.2°, are not affected by the presence of Fe modification in all catalysts.

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Notes

Poster 1-16

Recovery of Rare Earth Elements from coal ash

Praise Chikwadzea,[b], Lebohang Macheli[b], Joshua Gorimbo[a], Celestin Sempuga[a], Linda Jewell[b]

[a]*Institute for Catalysis and Energy Solutions, University of South Africa, c/o Pioneer Avenue and Christian De Wet, 1709, Florida, Private bag X6, South Africa,*
[b]*Department of Chemical and Materials Engineering, University of South Africa, c/o Pioneer Avenue and Christian De Wet, 1709, Florida, Private bag X6, South Africa,*
Email: praisechikwadze@gmail.com.

Keywords: Rare Earth Elements, ion exchange, coal ash.

Abstract

The research focuses on exploring the potential of coal ash as a source of rare earth elements (REEs). The increasing demand for REEs in advanced technologies such as catalysts, electronics, coupled with environmental and economic challenges associated with traditional mining, has driven the exploration of alternative sources of REEs. The study aims to investigate the potential for recovering REEs from coal ash leachates using ion exchange resins. Three coal ash samples from different power stations were leached using sulfuric acid, aqua regia, citric acid, and acetic acid at different concentrations, solid liquid ratio for 24 hours. The coal ash and leachates were subjected to XRF, XRD, and ICP-MS analysis to determine the mineralogical and chemical composition to identify the presence and concentration of REEs. Selective precipitation step has been considered for the removal of impurities such as iron, aluminium prior to ion exchange process. Two commercial ion exchange resins are investigated at varying pH, resin dosage, and contact time. The resin performance after multiple regeneration cycles will also be evaluated. The study will determine whether sodium citrate, EDTA can be used for elution of the REEs.

Notes

Poster 1-17

Establishing a slot-die coating operational procedure with alternative materials for proton exchange membrane water electrolysis

H.D. Neethling, S.P. du Preez, I.V. Pushkareva, and D.G. Bessarabov

HySA Infrastructure Centre of Competence, Faculty of Engineering, North-West University, Private Bag X6001, Potchefstroom, 2520, South Africa.
33756147@mynwu.ac.za

Keywords: PEMWE, catalyst ink, hydrogen, triple-phase boundary, catalyst layers

Abstract

Renewable energy sources, e.g., wind and solar, have grown rapidly in recent years. However, their intermittent nature creates challenges related to storage and uninterrupted power supply. A promising solution is to convert surplus renewable energy into hydrogen via proton exchange membrane water electrolysis (PEMWE). This method yields high-purity hydrogen (>99%) whilst excluding carbon from its life cycle. The generated H2 can subsequently be utilized in various applications, e.g., fuel cells, ammonia production, and petrol refining, by replacing H2 in existing processes with green H2 [1, 2].

Catalyst-coated membranes (CCMs) have limitations related to durability, cost and time-consuming manufacturing procedures. Therefore, efforts are focused on developing an operational procedure for direct coating of CCMs by slot-die coating. Slot-die coating is more favourable for roll-to-roll production of CCMs and less time-consuming than traditional coating techniques, e.g., spray coating[3]. The catalyst layers (CLs) are produced from ink formulations that form a three-dimensional intersecting network consisting of the catalyst, perfluoro sulfonic acid (PFSA) ionomer, and pores – collectively referred to as a triple phase boundary (TPB). The TPB is essential for achieving high-performance as it facilitates reactant and product transport to and from the catalyst active sites [4, 5].
Therefore, it is suggested to investigate the influences of different ink components and the formulation process on the stability and viscosity of the ink, as well as the morphology and uniformity of the fabricated catalyst layers. Due to the high cost of limited platinum group metals (PGMs), e.g., iridium and platinum used for CCM fabrication, we propose the use of alternative materials for catalyst ink formulations. These alternative materials can simulate the behaviour of the PGMs used traditionally, to establish the operational parameters for a slot-die coating procedure, e.g., pump rate, slot height, coating speed, and drying technique for the fabricated CCMs [2, 6].

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Notes

Poster 1-18

SYNTHESIS OF CONDUCTIVE POLYMER/ONION-LIKE CARBON COMPOSITES GAS SENSOR FOR THE DETECTION OF NH3 AT ROOM TEMPERATURE

Ketshepile Baabua[a], Manoko-Maubane NKadimenga Siziwe Gqoba[b], Cebisa Linganiso[b]

[a]Microscopy and Microanalysis Unit and the School of Chemistry, Private Bag 3, Wits 2050, Johannesburg, South Africa. Email:ketshepileb@gmail.com.
*[b]Centre for Carbon-nano Science Research, University of Witswatersrand, South Africa *Corresponding Author: Manoko. Maubane@wits.ac.za (M. Nkadimeng)*

Keywords: Onion-like carbons (OLCs), Conductive polymers, Polymer/OLC composites, Ammonia Sensing, Gas Sensor materials, Carbon nanomaterials

Abstract

Ammonia (NH_3) is mostly employed in industrial, agricultural, and medical applications, but its harmful effects and instability demand the development of effective, inexpensive detection devices. This study investigates the synthesis and use of conductive polymer/onion-like carbon (OLC) composites as gas sensors for ammonia detection at room temperature. OLCs were produced using an environmentally friendly, inexpensive flame pyrolysis method from waste cooking oil, providing an environmentally sustainable pathway to advanced carbon compounds. Three conductive polymers, such as polyaniline (PANI), polypyrrole (PPy), and polythiophene (PTH), were synthesized and combined with OLCs to determine their gas-sensing performance. The synthesized materials were characterized using BET, TEM, SEM, XRD, FTIR, TGA, and Raman to evaluate their morphological, structural, and surface properties. This work aims to determine the most active polymer-OLC combination with promising potential for room-temperature ammonia gas detection.

Notes

Poster 1-19

Catalytic activity of Ni modified ZIF-8 catalyst for methanol production from CO_2

A Dlodlo,[a] MN Cele[b]

[a]Department of Chemistry, North-West University, Mafikeng-Campus, Private Bag X 2046, Mmabatho2745, South Africa, E-mail: dlodloasiphelona@gmail,com.
[b]School of Physical and Chemical Sciences, North-West University, Mafikeng-Campus, Private Bag X 2046, Mmabatho2745, South Africa.

Keywords: carbon utilisation (CU), ZIF-8, hydrogenation, methanol.

Abstract

Carbon utilisation (CU) offers a sustainable route to convert CO_2 into valuable fuels and chemicals. Through catalytic systems, CU helps reduce atmospheric CO_2, supports a circular economy, and contributes to carbon neutrality.[1, 2]. The hydrogenation of CO_2 to methanol is a promising route for carbon capture and utilization. Metal–Organic Frameworks (MOFs), particularly Zeolitic Imidazolate Framework-8 (ZIF-8), offer high thermal stability, surface area, and tunable porosity, making them attractive as catalyst supports [3].

The ZIF-8 was synthesised and promoted with nickel (Ni) in order to investigate its potential application in CO_2 hydrogenation. The materials were characterised using Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). FTIR confirmed the successful formation of the ZIF-8 framework through the presence of the characteristic vibrational bands at 421 cm-1 attributed to Zn–N stretching, a band between 950 cm-¹ and 1350 cm-1 is associated with in-plane bending of the imidazole ring, and several bands between 1145 and 1584 cm-1 corresponding to C–N and C=N stretching. XRD confirmed the phase composition of ZIF-8 by showing prominent reflections at 2θ 7.3°, 10.4°, and 12.7°, indicating that crystallinity was still largely retained after the Ni modification. These preliminary results confirm the successful synthesis and modification of ZIF-8, supporting its potential use as a catalyst in methanol production from CO_2.

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Notes

Poster 1-20

Synthesis and Characterisation of CdS and CdSe quantum dots for PET scanners.

Muhleujehovah Mabuza,[a] James Keaveney [b] and Patricia J. Kooyman [a]

[a]Catalysis Institute, Department of Chemical Engineering, University of Cape, Rondebosch, Cape Town, 7700, South Africa,
[a]E-mail: mbzzin002@myuct.ac.za.
[b]Department of Physics, University of Cape Town, Rondebosch, Cape Town, 7700, South Africa.

Keywords: scintillator, quantum dots, cadmium, PET scanners.

Abstract

Positron emission tomography (PET) is an established imaging technique in nuclear medicine, where the accuracy of detection depends on the properties of the scintillator material. A scintillator is a material that converts high-energy radiation into visible light, which is then detected to form an image. The scintillators currently in clinical use, such as lutetium oxyorthosilicate (LSO) and bismuth germanate (BGO) are effective but are expensive to manufacture and difficult to scale [1]. Their high cost restricts widespread access to PET, limiting diagnostic capacity and equitable access to advanced imaging in hospitals, particularly in low- and middle-income regions. Developing lower-cost alternatives is therefore essential to expand clinical availability and improve patient outcomes.

Semiconductor quantum dots (QDs) provide a possible route toward more affordable scintillators. Their emission wavelength can be tuned through control of size and composition, allowing direct adjustment of optical properties to meet the requirements of PET detectors. Cadmium sulphide (CdS) and cadmium selenide (CdSe) QDs are of particular interest because their band gaps can be adjusted to achieve blue emission near 420 nm, which corresponds to the spectral sensitivity range of commonly used PET photodetectors. These materials are also well studied in the literature, providing a strong foundation for reproducible synthesis and characterisation.

This project focuses on the development of synthesis methods for CdS and CdSe QDs with controlled morphology and emission characteristics, using cadmium acetate dihydrate as a common cadmium precursor to ensure consistency across methods. The synthesis approaches under evaluation include hot injection, hydrothermal, solvothermal, microwave-assisted, and sonochemical methods, each adapted for gram-scale production. Planned characterisation include transmission electron microscopy, X-ray diffraction, photoluminescence spectroscopy, and inductively coupled plasma optical emission spectroscopy to establish particle size, crystallinity, optical properties, and elemental composition.

The work is currently centred on a critical review of synthesis strategies reported in literature and the design of methodologies suited to laboratory conditions. Future experiments will implement these methods, with the objective of producing CdS and CdSe QDs that can be incorporated into PET scintillators while meeting the requirements of scalability and optical performance.

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Notes

Poster 1-21

HySA Infrastructure Research Electrolysis Test Station: Advanced Research on Pilot Scale Water Electrolysis

Mr. H Brink, Dr A.S. Pushkarev, Dr I.V. Pushkareva, Mr C. Martinson, Mr S. Mamathuntsha, Prof D. Bessarabov

HySA Infrastructure Centre of Competence, North-West University, Faculty of Engineering, Private Bag X6001, Potchefstroom 2520, South Africa,
E-mail: hysa@nwu.ac.za.

Keywords: Green Hydrogen, Water Electrolysis, Proton Exchange Membrane, Test Station, Accelerated Stress Test.

Abstract

The decarbonization and sustainability of major industries, particularly the energy sector, are globally recognized as critical challenges. Green hydrogen has emerged as a promising energy carrier and storage medium to address these issues. Two of the greatest challenges facing green hydrogen production are cost and durability. To support innovations in novel materials and cell designs, advanced approaches for “in-situ” and “ex-situ” characterization of the cell itself or its components in realistic conditions are necessary.

There is a recognized need for an objective and comparative evaluation of electrolyser components and systems under conditions expected in future applications [1]. A wide range of operating conditions are expected during in-situ testing in order to simulate standard and abnormal operating conditions, such as accelerated stress tests (AST) [1]. The test station should be capable of these conditions, especially when upscaling is considered.

The HySA Infrastructure Research Electrolysis Test Station (HIRETS) was designed and constructed in-house to enable in-depth pilot-scale studies of water electrolysis on our proprietary cell and stack designs for proton exchange membrane water electrolysis (PEMWE). The HIRETS incorporates separate water circulation loops for the anode and cathode for various cell feeding modes. The continuous water quality and the test cell temperature management are ensured. Product gases (H_2 and O_2) are dried and analysed for purity in real-time. The system includes a wide array of instrumentation to monitor critical parameters such as temperature, pressure, flow rate, and water conductivity at key points along the anode/cathode loops and gas lines, making it a robust platform for studying the PEMWE at pilot scale.

The HIRETS offers a wide selection of operation modes for characterization and stress testing. These modes include constant current/potential, dynamic load cycling, and polarization curve measurement. When complemented with an external electrochemical workstation, more advanced characterizations, such as electrochemical impedance spectroscopy, can be performed. All of these measurements can be done while maintaining full control of temperatures and flow rates of feed/heating water.

In the presented study, we share the current progress of the project being executed on the HIRETS, where in-situ membrane degradation in a PEMWE cell via AST is studied.

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Notes

Poster 1-22

N-Formylation of Amines by CO_2 and H_2

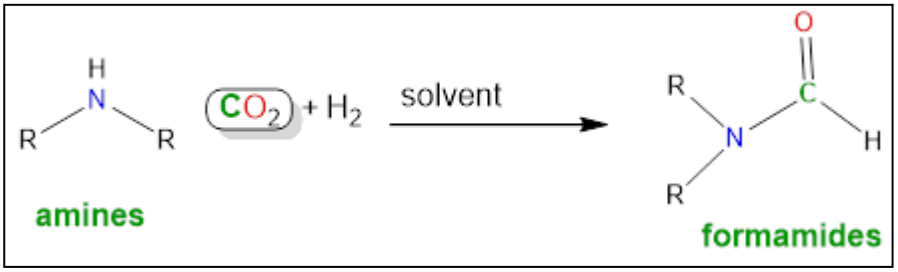
Kgabo Zwane,[a] and Prof. Banothile C. Makhubela[a]

[a] *Department of Chemical Sciences, University of Johannesburg, Auckland Park, South Africa.*

E-mail: zwane.kgabo99@gmail.com

Keywords: *N*-formylation, CO_2 utilization, formamides, solvent selectivity

Abstract



Carbon dioxide (CO_2) capture and utilization is vital for reducing greenhouse gas emissions while producing value-added chemicals. *N*-formylation directly transforms CO_2 into intermediates such as formamides, which are versatile in pharmaceuticals and can serve as precursors to CO for downstream fuel synthesis. Traditional methods often depend on transition-metal catalysts, motivating the need for greener alternatives [1-4].

Here, we demonstrate an approach to *N*-formylation of amines using CO_2 under optimized conditions. Reactions were carried out in mixed solvents, and products quantified by ^{1}H NMR. Linear and cyclic amines underwent efficient conversion to formamides, while aromatic amines, however, remained unreactive. Solvent composition significantly influenced product selectivity. An optimal solvent ratio balanced high conversion with maximum formamide yield. This study highlights a simple, scalable, and sustainable approach to integrate CO_2 utilization with C–N bond formation. By tuning solvent conditions, it is possible to steer product distribution between desired products. This work thus advances practical RCCUS strategies toward carbon circularity.

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Notes

Poster 1-23

Electrochemical Properties of KOH-Activated Onion-like Carbons Towards the Iodide/Triiodide Electrolyte for Application in DSSCs

Keneilwe Khoza[a], Grace Ngubeni[a] and Manoko Maubane-Nkadimeng[a,b]

[a] Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag 3, Johannesburg, 2050, South Africa, E-mail: 2326658@students.wits.ac.za. [b] Microscopy and Microanalysis Unit, University of the Witwatersrand, Private Bag 3, 2050, South Africa.

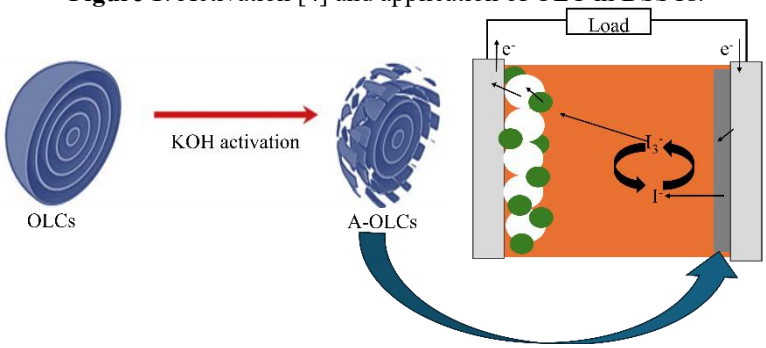
Keywords: OLC, KOH activation, counter electrode, catalyst, dye-sensitized solar cells

Abstract

The adverse impacts of non-renewable energy sources have made research into renewable substitutes increasingly imperative. Dye-sensitized solar cells (DSSCs) are among the most studied 3rd generation photovoltaics owing to their facile fabrication, flexibility, and competitive efficiency [1]. These employ platinum (Pt) as the state-of-the-art catalyst for the counter electrode (CE) due to its outstanding electrocatalytic properties. However, Pt's high cost and low abundance hinder their widespread application [1–2]. Carbonaceous materials have shown immense potential to replace Pt since they are abundant, stable, and display good electrical conductivity [3]. Nonetheless, studies show that when applied in DSSCs, the power conversion efficiency of carbon materials remains lower than that of Pt [3]. As such, there is a need to further develop and optimize nanocarbons as electrocatalysts.

This study approaches this by improving the electrochemical performance of onion-like carbons (OLCs) through the introduction of porosity and disorder to the material. OLCs were synthesized via flame-pyrolysis of waste engine oil and chemically activated using KOH at different OLC:KOH ratios (1:1–1:5). Structural analyses (XRD and Raman) confirmed the progressive introduction of disorder with activation, while BET surface area analysis revealed a significant increase in porosity, with the 1:4 activated OLC achieving the highest surface area of 1635 m^2/g. Moreover, electrochemical studies in the iodide/triiodide redox electrolyte demonstrated improved catalytic activity, with the reduction peak current density increasing from 3.6 mA/cm^2 (P-OLC) to 7.2 mA/cm^2 (A-OLC 1:4). Therefore, these findings underscore the potential of waste-derived activated OLCs as sustainable and cost-effective alternative CEs in DSSCs. Beyond advancing electrocatalysis, this research directly contributes to UN Sustainable Development Goals 7 (Affordable and Clean Energy), 12 (Responsible Consumption and Production), and 13 (Climate Action).

Figure 1: Activation [4] and application of OLC in DSSCs.



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Notes

Poster 1-24

Computational Investigation of Methane Oxidation Using a Single-Atom Catalyst of Transition Metals on $C_{24}N_{24}$ Fullerene

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Kwanele Ngubane,[a] Adedapo Adeyinka[b,] and Mafereka Mosoabisane[a]

[a] *Department of Chemical Sciences, University of Johannesburg, PO Box 524, Auckland Park, 2006, South Africa, E-mail: kwanelecynthia11@gmail.com*

[b] *Department of Chemical Sciences, University of Johannesburg, Auckland Park, 2006, South Africa.*

Keywords: Optimization, energy, reactions, metal, catalyst.

Abstract

This project aims to compare the catalytic performance of first-row transition metals (Mn, Fe, Co, Ni, Cu) and second-row transition metals (Ru, Rh, Pd) as single-atom catalysts supported on C24N24, using Density Functional Theory calculations. Among the metals examined (Mn, Fe, Co, Ni, Cu, and Ru), Ni [1] And Cu had the lowest energy barriers, while Ru had the highest. To explain these relative catalytic activities, the Activation Strain Model (ASM), which breaks down the activation energy into contributions from reactant distortion along the journey to the transition state and interaction energy at the transition state, was employed [2]. The increased distortion energies explained the difference in reaction barriers, where the C-H ΔE_{dist} of Ru is 2.6eV higher than Ni. Furthermore, the Quantum Theory of Atoms in Molecules (QTAIM) [3] was used to investigate the electron density topology and bonding properties at crucial points along the reaction pathway (reactant complex, transition state, and product complex). The analysis revealed that the lower electron density and Laplacian at TM-O and C-H Bond critical points of Co/Cu/Ni at TS correlate with their lower energy barrier. These findings indicate that, on the C24N24 support, first-row transition metals exhibit greater catalytic activity than their second-row counterparts, primarily due to their reduced reactant distortion requirements and more favourable electronic bonding properties at the transition state.

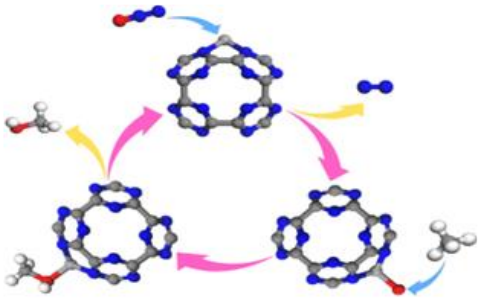

Figure 1: Graphical summary of the reaction.

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Notes

Poster 1-25

Thermodynamic Analysis of the Reducing Agent Effect on Calcium Carbonate Calcination and In-Situ Conversion

N. Moyo[a], B.C. Sempuga[a], L. Jewell[b], Y. Yao[a]*

[a]*Institute for Catalysis and Energy Solutions, University of South Africa, Roodepoort, 1709, South Africa*
[b]*Department of Chemical Engineering, University of South Africa, Roodepoort, 1709, South Africa*
20542658@mylife.unisa.ac.za

Keywords: reductive calcite calcination, in-situ conversion, syngas production, reverse water gas shift.

Abstract

Traditional exploitation of the calcium carbonate decomposition reaction, though of industrial significance, requires high temperatures and has been a dense contributor of anthropogenic CO2 emissions into the atmosphere. In this study, a thermodynamic analysis of the calcium carbonate calcination in reducing atmospheres i.e. hydrogen (H2), methane (CH4) and ammonia (NH3) was conducted, to combat both the high temperature requirements and greenhouse CO2 emissions. From the traditional calcination temperature of 864ºC, complete calcination in reducing atmospheres of molar feed ratio between reducing agent and calcium carbonate of 1, was realised at 785ºC, 703ºC and 755ºC, for H2, CH4 and NH3 respectively. Further increase of molar feed ratios promoted calcination temperature reduction, e.g. to 725ºC, 653ºC and 691ºC for H2, CH4 and NH3 respectively, at molar feed ratios of 3. Methane greatly impacted the calcination temperature; however, its decomposition impact is only activated at temperatures above 550ºC, contrary to that by H2 and NH3, which resulted in significant, low temperature decomposition rates especially at higher molar feed ratios i.e. at molar ratio of 10, temperature of 300ºC, 67.4% and 91.5% calcite decomposition rates were achieved in H2 and NH3 atmospheres respectively. CO2 emissions reduction was achieved with reducing atmospheres, facilitated by in-situ conversion of CO2 to methane at lower temperatures and CO at higher temperatures. Generally, increasing the mole feed ratio increased the reaction rate in all atmospheres, however, compromised the syngas quality, to ratios above 3, for direct utilization. As such, molar feed ratio between 1 and 3 was recommended for H2 and CH4, while with NH3, between 1 and 2.5. For H2 and CH4, direct utilization of the product gas is possible while the product gas from NH3 atmosphere is not suitable due to the diluent N2 gas, as such would need purification, compelling a cost benefit analysis to be considered when selecting NH3 as the reducing agent. To counter the carbon deposition experienced from CH4 atmosphere, a novel co-feeding of CH4 with NH3 is proposed in this study. Ultimately, it was displayed the advantageous utilization of the hydrogen donors, CH4 and NH3, as reducing agents, in place of the presently expensive green-hydrogen.

Notes

Poster 1-26

Poly (acrylic acid-co-vinyl sulfonic acid)-Polyether sulfone hydrogel immobilized with sulfonated graphene oxide as Proton Exchange Membrane.

Constatia Moyana,[a] Machodi Machaba[a], Orebotse Botlhoko[b] and Phumlani Msomi[a]

[a] Institute of Catalysis and Energy solution, University of South Africa, Christian De Wet & Pioneer Avenue, Florida, 17091, South Africa, E-mail: 67146325@mylife.unisa.ac.za. [b] Department of Chemistry, Auckland Park Kingsway campus, 2006, South Africa.

Keywords: Polymer, sulfonated, proton electrolyte, hydrogels.

Abstract

Fuel cells convert energy stored in fuels into electric power in an efficient and environmentally friendly manner if the fuel is continuously provided. Proton electrolyte fuel cells (PEMFCs) have attracted a lot of interest because they are environmentally friendly and efficient energy conversion devices that are expected to play a dominant role in future energy solutions. In the center of PEMs, there is a proton exchange membrane (PEM), which facilitates the H^+ conductivity, act as an electron insulator and prevent fuel crossover from anode to cathode. Current PEMs are unable to have a balance in properties to render then efficient and make the entire PEMFCs produce high power output. PEM limited commercialization is also hindered by high cost, swelling, limited thermal and mechanical stability. At high temperature the membrane water uptake decreases which leads to degradation, loss in ionic conductivity and low efficiency. This study aims to develop a novel hybrid hydrogel (instead of a membrane) to address the challenge by crosslinking polymer to get the desired properties and incorporate graphene-based nanomaterials to endure balanced properties. The as prepared poly(AA-co-PVSA) has been characterized using NMR, SEM and FTIR. The NMR showed the crosslinking of two polymers, the signal peaks around 1-1.5ppm (doublet) which shows the removal of double bond and presence of CH_3, the signal peaks around 1.85- 2.50 ppm (D, T, T) and signal peak around 4.30 ppm showing the CH_2 bond around aromatic region from the crosslinker agent. The SEM sulfonated graphene oxide shows the flaky, crumpled, multilayered structure and Sulfonated graphene oxide shows irregular folded and thick sheets. The EDS shows the presence of carbon 67.3wt%, oxygen 32.3wt% and the sulfonated graphene shows carbon 66.7 wt%, oxygen 32.1wt% and sulfonated graphene shows carbon 66.7 wt%. The FTIR shows the C-O stretch at 1700 cm^{-1}, C=O peak around 1450 cm^{-1}, C=C bond around 1650 cm^{-1} and O-H broad band around 3400 cm^{-1} confirms the chemical bond of graphene oxide. The FTIR spectra of sulfonated graphene oxide shows broad absorption peak at 3400 cm^{-1} for O-H, S=O bond stretches around 1350 cm, C-S band for S-H. These hydrogels are expected to enhance the proton conductivity while maintaining thermal stability and controlling swelling behaviour of hydrogel. These proposed multifunctional hydrogels are cost effective, environmentally friendly and expected to show superior mechanical properties compared to commercially available.

Notes

Poster 1-27

Anaerobic digestion of abattoir wastewater: A review of current practices, prospects for biochar-amended anaerobic digestion, and opportunities for upscaling

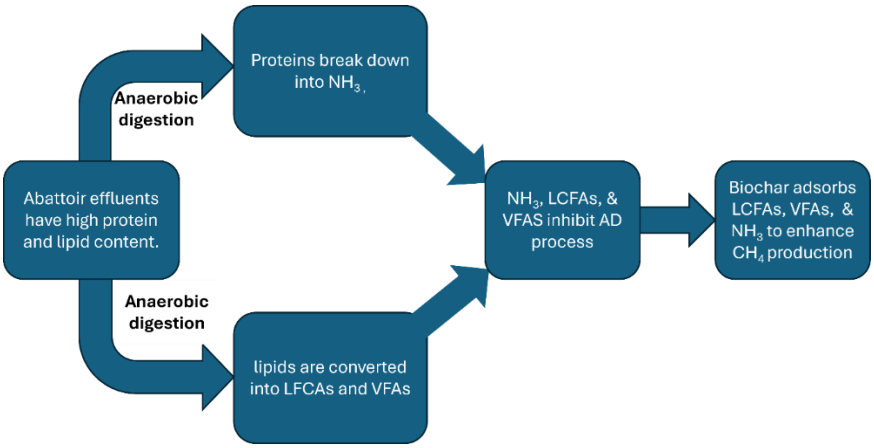
Kudzai Mutisi[a] Baraka Sempuga[a] and Mabatho Moreroa[a]

[a] *Institute of Catalysis and Energy Solutions, University of South Africa, Florida Park, Roodepoort, 1709, South Africa, E-mail: 50135082@mylife.unisa.ac.za.*

Keywords: structures, perspectives, reactions, metal, catalyst.

Abstract

The anaerobic digestion (AD) of abattoir effluents presents a sustainable solution for treating high-strength wastewater and producing renewable energy, however it is often hindered by process instability due to inhibitors such as ammonia, long-chain fatty acids (LFAs), and volatile fatty acids (VFAs). Biochar, a carbon-rich product of biomass pyrolysis, has emerged as an effective additive to mitigate these challenges by adsorbing inhibitory compounds, buffering pH, facilitating microbial attachment, and promoting direct interspecies electron transfer (DIET). This review integrates current knowledge on AD of abattoir wastewater, mechanisms of biochar action in AD systems, and the impacts of feedstock type, pyrolysis conditions, and reactor design on performance. The review highlights the prospects of biochar as an additive in the AD of abattoir effluents characterized by their high protein and lipid content. We also examine techno-economic and environmental considerations, expose the research gaps related to standardization, long-term effects, and scalable implementation, and propose future directions to optimize biochar-assisted AD for abattoir wastewater. The review emphasizes biochar's role in enhancing biogas yields, stabilizing microbial communities, and advancing circular-economy objectives.



Notes

Poster 1-28

Comparative Study of H_2 and Syngas as Reduction Gases for Iron-Based FT Catalysts

Phumelele Ngubane, Mpumelelo Mbatha, Francina Ramutsindela, Phathutshedzo Khangale, Joshua Gorimbo, Yali Yao*

Institute for Catalysis and Energy Solutions, University of South Africa, c/o Pioneer Avenue and Christian De Wet, Florida 1709, South Africa,
Email: yaoy@unisa.ac.za (Y Yao)

Keywords: Fischer-Tropsch Synthesis, water-gas shift, precipitated iron catalyst, FT catalyst activity; FT product selectivity

Abstract

Iron-based catalysts are cost-effective and highly active for both Fischer–Tropsch (FT) and water-gas shift (WGS) reactions, making them suitable for syngas feeds with low H_2/CO ratios. Catalyst activation via reduction is essential prior to FT synthesis, but using pure H_2 is costly and impractical for industrial use. This study explores the feasibility of using syngas as an alternative reducing agent at typical FT temperatures, comparing its impact on catalyst performance with that of H_2. Two fixed-bed reactors, each containing 1 g of precipitated iron catalyst, were reduced using either H_2 (330 °C) or syngas (230 °C) under identical flow conditions for 48 hours. Both reactors then underwent the same FT reaction protocol and were operated for over 7 months (>5000 hours). Catalyst activity, selectivity, and stability were systematically evaluated and compared.

Notes

Poster 1-29

Perovskites in Thermal Catalytic Organic Chemical Conversions

Rapelang Patala, [a] and Ndzondelelo Bingwa [a]

[a]*Institute for Catalysis and Energy Solutions (ICES), College of Science Engineering and Technology, University of South Africa, Florida Park, South Africa.*

Keywords: Heterogeneous Catalysis, Perovskite Oxides, Thermal Organic Transformations, C-C Coupling, Biomass Conversion, Defect Engineering.

Abstract

Perovskite oxides (ABO_3) have emerged as a highly versatile class of heterogeneous catalysts for thermal organic transformations, owing to their tunable redox properties, structural stability, and unique defect chemistry. This work explores the pivotal role of perovskites in catalyzing a wide array of reactions critical for sustainable chemistry, including C-C coupling (e.g., Suzuki, Heck), functional group transformations involving oxygen and nitrogen, and the upgrading of biomass-derived feedstocks [1]. We delve into the fundamental structure-activity relationships, emphasizing how strategic B-site doping and the engineering of oxygen vacancies can tailor acid-base characteristics and electron density to enhance catalytic activity and selectivity [2]. The discussion also covers the critical aspect of thermal activation of perovskite active sites and the challenges of catalyst deactivation, such as coking, alongside strategies to mitigate them. Furthermore, we examine the importance of reactor design and computational simulations in scaling up these catalytic processes. By synthesizing recent advancements and identifying key research gaps, this work underscores the significant potential of perovskite catalysts to drive innovation in South Africa and the global catalysis landscape, particularly in the quest for efficient and sustainable chemical production.

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ACS Energy Lett 5 (2020) 566–571.

Notes

Poster Presentation Session II: Catalytic Frontiers in Energy, Environment, and Biotransformation

Advancing the Sustainable Development Goals through Molecular Innovation

This session highlights the catalytic ingenuity driving progress across multiple Sustainable Development Goals (SDGs), from clean energy and water to responsible production and climate action. The featured posters span a rich array of topics, including:

- 🌱 **SDG 6 & 14 (Clean Water & Life Below Water):** Photocatalytic degradation of antibiotics and dyes, and detection of pharmaceutical residues in wastewater using MOFs and heterojunction nanomaterials.
- ⚡ **SDG 7 (Affordable & Clean Energy):** Hydrogen production via butanol reforming, ammonia decomposition, and CO_2 hydrogenation; membrane innovations for fuel cells and zinc-air batteries.
- 🧬 **SDG 9 (Industry, Innovation & Infrastructure):** Smart catalyst design for Fischer-Tropsch upgrading, hydroformylation, and Sonogashira coupling; enzyme engineering for regioselective hydroxylation and chiral synthesis.
- 🌍 **SDG 12 & 13 (Responsible Consumption & Climate Action):** Valorization of biomass and glycerol, green synthesis of platform chemicals, and sustainable effluent pre-treatment strategies.
- 🧪 **SDG 3 (Good Health & Well-being):** Biocatalytic production of bioactive compounds and functional materials for pharmaceutical and biomedical applications.

This session invites attendees to explore how catalytic science is not only solving technical challenges but also shaping a more sustainable and equitable future. Engage with presenters to uncover the molecular mechanisms, process innovations, and interdisciplinary collaborations that are redefining the boundaries of catalysis.

Poster 2-1

Photocatalytic Butanol Reforming to Hydrogen Production Using Ag2O/TiO2 Composite Catalysts: Effects of Ag2O Loading, Calcination Temperature, and Reaction Parameters

Tumelo Seadira[1]*, Thabelo Nelushi[1]

[1]*Department of Chemical and Materials Engineering, University of South Africa, Johannesburg, South Africa*

Abstract

Photocatalytic biomass reforming for hydrogen production has gained attention over recent years as an alternative to an inefficient water-splitting reaction due to the required standard Gibbs free energy change of 237 kJ/mol. In this study, anatase-phase titanium dioxide (TiO2) particles were successfully synthesized by employing the sol-gel method, and the silver oxide (Ag2O) nanoparticles with varying weight percentages were loaded on the surface of the TiO2 via the incipient wet impregnation method to form composite photocatalysts. The structural and optical characteristics of the composite photocatalysts were investigated using various techniques such as Brunauer-Emmett-Tellet (BET), X-ray Diffraction (XRD), Scanning Electron Microscope (FESEM), and Diffuse Reflectance Spectroscopy (UV-vis DRS). The photocatalytic hydrogen activity of the prepared composite photocatalysts was studied under visible light irradiation, and it was found that varying the Ag2O loading influenced the photocatalytic activities of the prepared photocatalysts. Furthermore, it was found that the calcination temperature and the reaction parameters, such as pH and initial butanol concentration, also influenced the photocatalytic activity of the prepared photocatalysts for efficient hydrogen production. The highest photocatalytic hydrogen production efficiency was achieved with the 0.5wt%Ag2O/TiO2 composite photocatalyst (290 mmol/gcat). This activity was attributed to 100% anatase crystallite TiO2 particles that are highly active in terms of photogeneration of charge-carriers; the uniform distribution of Ag2O on the TiO2 surface, which facilitated improved retardation of the charge-carriers recombination rate. Lastly, the slightly acidic conditions of the butanol mixture facilitated efficient adsorption of butanol on the surface of the photoexcited photocatalysts, resulting in simultaneous rapid oxidation of butanol and efficient production of hydrogen molecules.

**Corresponding author: Tumelo Seadira*
Email address:tumelo.seadira@gmail.com (Tumelo Seadira)

Keywords: Photocatalytic Hydrogen Production, Butanol Reforming, TiO2 Composite Catalyst; Ag2O/TiO2

Notes

Poster 2-2

Combination of basic and amphoteric (Mg-Zn) catalysts for glycerol conversion to form glycidol and glycerol carbonate using transesterification.

Dube Sakhile[a,b], Qwabe Lindelani [b*], & Friedrich Holger [a],

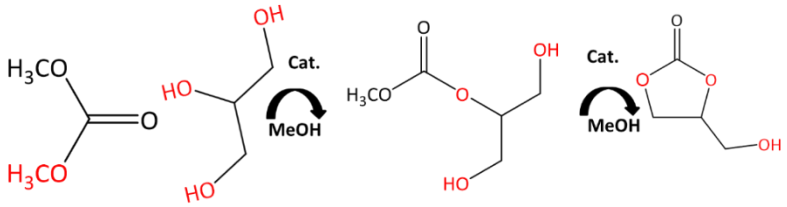
School of Chemistry and Physics, University of KwaZulu-Natal, Private Bag X 54001, Durban 4000, South Africa,

Faculty of Natural Science, Department of Chemistry, Mangosuthu University of Technology, 511 Mangosuthu Highway, Durban, 4000, South Africa

Keywords: Mg-Zn mixed oxides catalysts, basicity, transesterification, glycerol

Abstract

Biodiesel industry is booming attributing to the threat from petroleum depletion since the last decade [1,2]. Glycerol is generated at the proportion of 10% (w/w) of the total biodiesel production and the rapid growing industry has led to a surplus of glycerol. In this study, transesterification of glycerol with dimethyl carbonate was exploited to produce glycerol carbonate and glycidol under mild condition reaction over Mg-Zn mixed oxide catalysts aiming the route shown in **Scheme 1**. Prepared Mg-Zn oxide catalysts with different molar compositions were synthesized via co-precipitation method [3]. All prepared catalysts were characterized using N_2 physisorption, powder X-ray Diffraction (XRD), CO_2-Temperature-Programmed Desorption, X-ray Photoelectron Spectroscopy (XPS), Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM). Glycerol conversion was influenced by the molar ratios of Mg-Zn and catalyst basicity, which are responsible for the variation in amphoteric–base properties of the catalysts. The catalyst with a molar ratio of Mg-Zn 3:1 calcined at 550 °C exhibited superior activity with of glycerol carbonate and glycidol. Recyclability experiments proved that the catalyst was stable and produced conversions and selectivities that were very close to the fresh catalysts.



Scheme 1: Reaction route for producing glycerol carbonate

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Notes

Poster 2-3

Clean hydrogen production from ammonia decomposition reactions using metal-supported carbon-based materials as catalyst precursors.

Emile D Maggott[a], Filippo Bossola[a] and Vladimiro Dal Santo[a]

[a] *Consiglio Nazionale delle Ricerche - Istituto di Scienze e Tecnologie Chimiche 'Giulio Natta', Via Golgi 19, 20133 Milano, Italia.*
E-mail: emile.maggott@scitec.cnr.it

Keywords: Ammonia decomposition, hydrogen production, iron catalysts, carbon nitride materials, reaction optimization, stability testing.

Abstract

Given the rapid depletion of fossil fuels and the negative effect it has on the environment, there is a growing demand for clean energy vectors such as hydrogen and for sustainable industrial processes such as ammonia cracking.[1] Ammonia is considered as a promising hydrogen carrier and when decomposed, high purity hydrogen is released.[2] Generally, this process requires state-of-the-art ammonia cracking catalysts such as noble metals like ruthenium due to their high activity; however, their widespread application is limited by high cost, scarcity, and poor scalability, prompting a shift toward earth-abundant alternatives.[3,4] Therefore, the development of cost-effective catalysts for ammonia decomposition at low temperature is crucial for hydrogen economy applications.

In this paper, we present the synthesis, characterization, and catalytic evaluation of carbon nitride-based materials supported with an earth-abundant transition metal viz. Fe, as sustainable catalysts for ammonia decomposition under moderate reaction conditions. Various precursors and blends were employed to create nitrogen-rich environments that enhance metal-support interactions. Furthermore, a range of advanced solid-state analytical techniques were employed to evaluate structural and chemical properties of the catalysts.

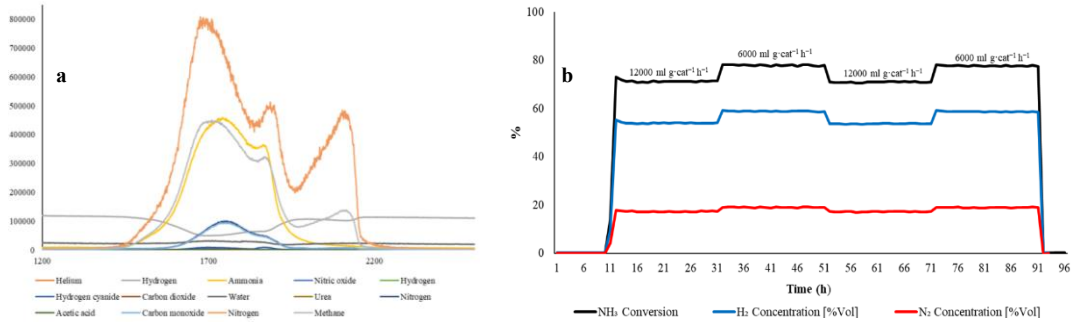

Figure 3: *H_2-TPD profile (a) Stability test (b)*

The materials were subsequently evaluated as catalyst precursors in the decomposition of ammonia to produce clean hydrogen. In addition, reaction parameters such as gas hourly space velocity (GHSV), catalyst loading, and temperature profiles to reach optimum reaction conditions are also discussed. Optimal conversion of pure ammonia was achieved >80% at 500°C and 6 000 $mL \cdot g^{-1} \cdot h^{-1}$. Stability tests at different GHSV were conducted over 90 hours and exhibited excellent catalyst durability with no loss in activity.

These findings illustrate that carbon-nitride materials as supports are promising for efficient hydrogen production from ammonia, offering a plethora of insights into next generation catalysts.

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Notes

Poster 2-4

Photo-mediated catalytic degradation of antibiotics in water with Ag_3VO_4, $BiVO_4$ and TiO_2-based heterojunction photocatalysts

Kokoti Leshabane,[a] Mabuatsela Maphoru,[b] Benjamin Shotholo,[c] Themba Ntuli[d]

[a]*Department of Environmental, Water and Earth Sciences, Tshwane University of Technology, 175 Nelson Mandela Drive, Pretoria, 0007, South Africa,*

E-mail: kokotiriaan@gmail.com

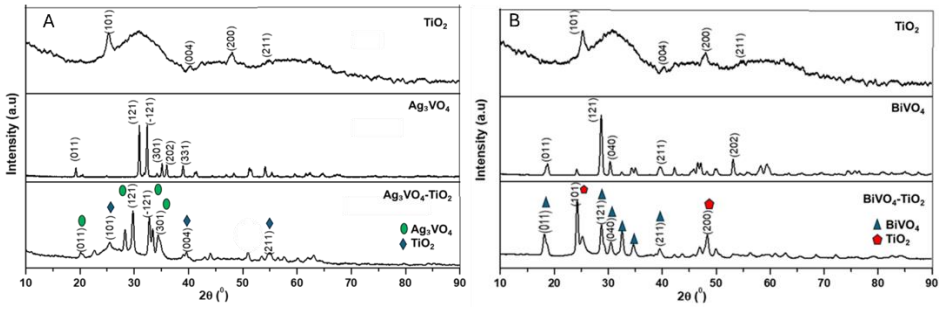
[b] *Department of Chemistry, Tshwane University of Technology, 175 Nelson Mandela Drive, Pretoria, 0007, South.* [c] *DSTI/Nanotechnology Innovation Center, Advanced Materials Division, Mintek, Randburg, 2125*

Keywords: heterojunction, semiconductor, band gap, antibiotics

Abstract

Over the years, there has been a growing attention towards emerging contaminants, notably antibiotics, within the realm of research. Many antibiotics are pervasive pollutants and have been detected in various sources such as wastewater effluent, groundwater, seawater, rivers, lakes, and even drinking water and Some of these substances pose a threat to human health due to their toxic nature [1]. Conventional wastewater treatment facilities are largely ineffective at breaking down these persistent pollutants, allowing them to remain in the environment [2]. Among emerging solutions, photocatalysis, has gained attention as an environmentally friendly technology that harnesses renewable energy to degrade resistant organic contaminants in wastewater. Titanium oxide (TiO_2) is frequently used in this context and is considered a highly promising photocatalyst due to its low cost, strong physicochemical stability, non-toxicity, and durable photoactivity [3,4]. However, TiO_2 has some limitations that includes a relatively low surface area and a wide band gap that restricts its absorption of visible light. This study propose that these limitations can be circumvented by the formation of heterojunction photocatalysts through the combination of TiO_2 with narrow band gap semiconductors like $AgVO_4$ and $BiVO_4$. In this study, synthesized Ag_3VO_4, $BiVO_4$ and TiO_2 based heterojunction photocatalysts were used in the degradation of antibiotics under UV and Visible light irradiation (120 minutes) using under standard ambient conditions. The structural properties of these photocatalysts were analyzed using X-ray diffraction (XRD) to identify their crystallographic features.

Figure 1: XRD patterns of (a) anatase TiO_2, monoclinic $BiVO_4$ and $BiVO_4$-TiO_2, (b) α- Ag_3VO_4, anatase TiO_2, Ag_3VO_4-TiO_2 photocatalysts.



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Notes

Poster 2-5

A Century of Fischer-Tropsch Chemistry: Evolving Applications in Aviation Fuel

Christina Kannigadu[a], Alexander Whaley[a]

[a]*LECO Africa, Gauteng, 1619, South Africa, E-mail: Christina@lecoafrica.co.za*

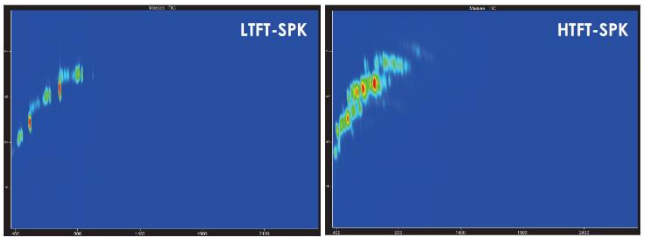
Keywords: Fischer-Tropsch, synthetic fuels, aviation, GCxGC-TOFMS, sustainability

Abstract

The Fischer-Tropsch (FT) process, first demonstrated in the 1920s, has undergone a remarkable transformation from a coal-to-liquids technology to a central pillar of sustainable fuel innovation. Over the past 100 years, FT synthesis has evolved into a highly tunable platform for the production of synthetic hydrocarbons, particularly synthetic paraffinic kerosenes (SPKs), now critical in sustainable aviation fuel (SAF) development. FT-derived fuels offer attractive physical properties, such as low sulfur content and reduced aromaticity, which contribute to cleaner combustion and improved environmental performance.

Modern advances in analytical science have played a pivotal role in this progression. Techniques such as comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GC×GC–TOFMS) now enable detailed chemical fingerprinting of complex FT-derived aviation fuels. These tools have helped differentiate between low- and high-temperature FT-SPK formulations and guided regulatory approvals such as ASTM D7566, which permits blending FT fuels with conventional jet fuels. Importantly, the ability to resolve thousands of individual hydrocarbon species has refined our understanding of critical fuel properties such as freeze point, viscosity, and seal compatibility—key factors in aviation safety and engine performance.

Figure 1 illustrates the GC×GC contour plot of a high-temperature FT-SPK (HTFT-SPK) sample, revealing the dominance of iso-paraffins and a reduced aromatic footprint compared to traditional Jet A-1. This high-resolution mapping is critical for understanding not only energy content but also combustion behaviour and material compatibility.



These analytical advancements not only streamline the certification process but also guide catalyst and process optimization, ensuring that FT fuels remain viable as renewable carbon feedstocks shift from coal to biomass and waste sources. As the aviation industry targets net-zero carbon emissions by 2050, the century-old FT process—reimagined through high-resolution analytics—continues to shape the future of flight.

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Notes

Poster 2-6

Hydroformylation of Internal Alkenes: Sensitivity to Reaction Conditions

Oluwasegun E Olaoye,[a] Jodi van der Merwe,[a] Daniel P Otto,[a] Hermanus CM Vosloo,[a] and Frans J Smit[a]

[a] *Research Focus Area for Chemical Resource Beneficiation, Catalysis and Synthesis Research Group, North-West University, 11 Hoffman Street, Potchefstroom, 2522, South Africa, E-mail: 55581293@mynwu.ac.za.*

Keywords: hydroformylation, internal alkenes, ruthenium catalyst, rhodium catalyst, selectivity.

Abstract

Hydroformylation is a key catalytic route for converting alkenes/olefins into aldehydes, valuable intermediates in the synthesis of alcohols, plasticisers, and fine chemicals (Figure 1). While terminal alkenes such as 1-octene are readily hydroformylated with high selectivity toward linear products, internal alkenes present greater challenges due to lower reactivity, competing isomerisation, and reduced regioselectivity. This study investigates the hydroformylation of trans-4-octene using Rh- and Ru-based catalysts, with direct comparison to 1-octene as a benchmark.

Catalytic activity and selectivity were examined under varying conditions of temperature, pressure, catalyst loading, and ligand environment. $Rh(acac)(CO)_2$ and Ru precursors were tested alongside different phosphorus ligands, with product distribution and conversion rates monitored to assess performance.

The catalyst $Rh(acac)(CO)_2$ efficiently hydroformylated trans-4-octene, strongly favouring branched aldehydes. Increasing catalyst concentration enhanced conversion (80–97%) and turnover frequency (200–242 h^{-1}) while limiting isomerisation. Temperature shifts altered regioselectivity, with branched aldehydes dominating at 70–80°C, whereas higher temperatures (90–100°C) promoted linear products. Pressure effects (30 bar and 50 bar) drove aldehyde formation (73% and 100% conversion), but 40 bar favoured isomerisation, cutting conversion to 33%. Rhodium and ruthenium showed similar activity (~72–73%), though ligand choice proved decisive. Triphenylphosphine offered modest results, while triphenylphosphite excelled, achieving 97% conversion, 243 h^{-1} TOF, and up to 75% selectivity for 2-propylhexanal. These findings highlight phosphite-modified Rh catalysts as highly effective, offering a pathway to extend hydroformylation to more challenging internal alkenes.

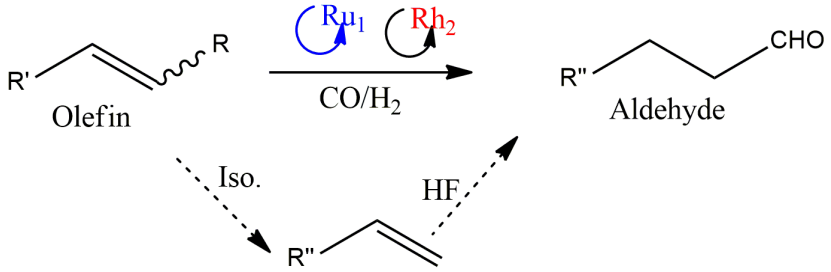

Figure 1: Rhodium–ruthenium catalyst systems for olefin hydroformylation.

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Notes

Poster 2-7

Nanostructured Cu-BDC MOFs for the detection of the antiretroviral drug Nevirapine in wastewater

Zondi Nate,[a] Thobane Godlo[a] and Philani Mpungose[a]

[a]*Department of Chemistry, Cape Peninsula University of Technology, Bellville, 7530, South Africa,*
E-mail: Natez@@cput.ac.za.

Keywords: copper metal organic framework, nevirapine, differential pulse voltammetry.

Abstract

According to the World Health Organization/UNAIDS 2023 estimate, approximately 39 million people are living with Human Immunodeficiency Virus (HIV). An estimated 25.6 million of this group are in Africa. South Africa is the country with the world's largest HIV epidemic, with 7.8 million people living with HIV in 2022. In 2022, the global estimated antiretroviral therapy (ART) coverage among this group was 76%. Several studies have reported the occurrence of antiretroviral drugs in wastewater. Antiretroviral drugs may have unpleasant effects even at low concentrations. This study reports the development of a highly sensitive and selective electrochemical sensor for detecting and quantifying nevirapine in wastewater. Cu-BDC MOFs were synthesized, and reaction parameters such as pH were optimized. The synthesized Cu-BDC MOFs were characterized using transmission electron microscopy, X-ray diffraction spectroscopy, Fourier transform infrared spectroscopy, and scanning electron microscopy. The electrochemical studies were conducted using cyclic voltammetry, differential pulse voltammetry, and electrochemical impedance spectroscopy. The fabricated sensor showed a good linear range and detection limit. Thus, the properties of copper metal organic frameworks improved the sensitivity and selectivity of the sensor for the detection of nevirapine.

Notes

Poster 2-8

Effects of La on the structure and activity of Co_3O_4 based catalysts in preferential oxidation (PROX) of carbon monoxide

R Mhlaba,[a]

[a]*Department of Chemistry, University of Limpopo, R71 and University Road, Sovenga, 0727, South Africa,*
E-mail: Reineck.mhlaba@ul.ac.za.

Keywords: Preferential oxidation, CO oxidation, metal oxide, catalyst, moisture.

Abstract

The interest in hydrogen production for fuel cells has increased the search for catalysts that produce hydrogen with minimal CO. CO poisons the Pt anode, reducing fuel cell efficiency [1, 2]. Preferential oxidation (PROX) is considered the most efficient method to remove CO and purify H2 [1, 3]. Noble metal catalysts perform well at low temperatures but are costly and have low selectivity at high temperatures [3-5]. Cobalt-based catalysts are reported to be good in converting CO to CO2 [1, 6]. In addition, hydrazine-treated cobalt oxides perform better in PROX but deactivates over time, especially in CO2 and moisture environments [1, 7]. Hydrogen reduces cobalt oxide to metallic cobalt, decreasing CO2 selectivity [1, 7]. It has been reported that La species improves CO chemisorption and reduces H2 and H2O effects, leading to better catalyst performance in a wide temperature range [2, 4]. La species on AlO3 boosts CO adsorption, decreasing H2 oxidation activity, benefiting PEM fuel cells [3, 8]. High CO conversion was observed across Au/LaAlO3 and Au/LaCeO2 catalysts, even with CO2 and H2O present [2, 8]. Recent studies have shown that hydrazine treated cobalt-based catalysts (such as CoO and Co3O4) perform better at lower temperature (80 to 120 oC) [1]. However, the catalysts deactivate in the presence of CO2 and H2O in the feed stream [1, 9]. Improving cobalt catalyst stability and selectivity could be economically beneficial.

Herein, the study investigated the effect of La on the structure and catalytic activity, selectivity and stability of cobalt-based catalysts in PROX of CO in dry, moisture and CO2 environment, respectively. Catalysts were prepared by precipitation coupled deposition method prior to hydrazine pretreatment and calcination at 350 oC. The structural composition of the catalysts was confirmed by XRD and HRTEM. An improvement in catalytic activity of Co3O4 was observed over an optimum load of 1 wt.% La/Co3O4. Increase in La load above 1 wt.% suppresses the catalytic activity of Co3O4. An improvement in catalytic stability in dry and moisture environments was observed over the 1wt.% La/Co3O4 catalyst (at 100 oC for 21 hours), though, its activity somehow decreases in the presence of CO2 species.

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Notes

Poster 2-9

A green pathway to 2,5-furandicarboxylic acid using whole-cell bioconversion and green chemistry.

N. Mosina,[a] C. van der Westhuysen[a] L. Steenkamp[a] and P. Steenkamp[b]

[a]Centre for Scientific and Industrial Research, Meiring Naudé Rd, Brummeria, Pretoria, 0184, South Africa.
E-mail: NMosina@csir.co.za.
[b]Department of Plant Metabolomics, University of Johannesburg, Corner Kingsway and University Road, Auckland Park, Johannesburg, 2092, South Africa

Keywords: biocatalysis, HMF, FDCA.

Abstract

A shift from conventional fossil-based polyethylene furanoate (PEF) and polyethylene terephthalate (PET) to renewable plastics is essential in reducing the carbon footprint of plastics [1]. 2,5-Furandicarboxylic acid (FDCA) is used as a renewable precursor for the synthesis of biobased PET, which is seen as an attractive substitute for conventional PET. In the conventional chemical process to produce FDCA, 5-hydroxymethyl furfuraldehyde (HMF) is 110ynthesi to FDCA under elevated oxygen pressure using precious metal catalysts in organic solvents [2]. This central role of HMF as a precursor makes this product a crucial feedstock for industry. In this study, the chemical synthesis of HMF from glucose, fructose or sucrose was achieved using green chemistry. Additionally, several manure samples were collected, and the isolated microorganisms were screened for their ability to convert the 110ynthesized HMF to FDCA. Among the eight isolates obtained, three isolates demonstrated the ability to convert HMF to FDCA. These findings further demonstrated the whole cell biocatalysis of HMF to FDCA by a Bacillus mobilis/Bacillus toyonesis (as identified by 16S rRNA sequencing) upon isolation from horse manure. Under optimal conditions, the strain tolerated up to 2 g/L HMF in mineral salt media and conversion to FDCA was achieved within 3 days of incubation at 30°C as determined by UPLC-MS. These findings demonstrate the potential to exploit industrial biocatalysis for the large scale-synthesis of FDCA. Although the production parameters have not been entirely optimized, more research may reveal the most favourable conditions for improved FDCA production, which will be assessed in future studies.

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Notes

Poster 2-10

Fe_3O_4 coupled to MIL-100(Fe)@PDA for the preparation of composites with enhanced photo-Fenton degradation of ciprofloxacin

Agnes Pholosi[a], Saheed Sanni[b] and Hua-Jun Shawn Fan[b]

[a]Department of Natural Sciences, Vaal University of Technology, Vanderbijlpark, South Africa
[b]College of Chemical Engineering, Sichuan University of Science & Engineering, Zigong 643000, China

Keywords: Iron-metal organic framework, sustainable, Photo-Fenton catalysis, ciprofloxacin

Abstract

Improving the rapid generation and conversion of Fe(II) to Fe(III) is crucial for addressing the challenging recycling and reuse of Iron-metal organic frameworks (Fe-MOFs) when applied to wastewater treatment, thereby enhancing their performance in photo-Fenton activities. The combined utilization of Magnetite (Fe3O4) and a sustainable polymer matrix, such as polydopamine (PDA), can effectively address these challenges. Here, Fe3O4-coupled MIL-100(Fe)@PDA composites were synthesized at different weight loadings, and their changes in physico-chemical structures and photo-electrochemical properties were investigated. As a photo-Fenton catalyst, the composites could efficiently activate H_2O_2 to degrade ciprofloxacin (CIP) in water, and achieved 81% degradation efficiency within 40 min. Notably, the Fe_3O^{4-} coupled MIL-100(Fe)@PDA composite evidenced broad pH applicability, good reusability, and the microstructure was maintained after five cycles, demonstrating excellent sustainability for applications in a practical aquatic environment. The active reactive oxidative species (ROS) involved in the removal of CIP in the photo-Fenton pathway were •OH, h^+, and $•O^{2-}$, which were confirmed through free radical quenching experiments and electron paramagnetic resonance analysis.

Notes

Poster 2-11

Catalyst design vs feedstock pre-treatment vs process conditions: towards sustainable fuels

Tendai O. Dembaremba[a], Adeniyi S. Ogunlaja[b] and Zenixole R. Tshentu[a]

[a]*Department of Chemistry, Nelson Mandela University, Gqeberha, Port Elizabeth, 6031, South Africa,*
E-mail: TendaiD@mandela.ac.za.

Keywords: Coordination polymers, metal organic frameworks, adsorptive denitrogenation, nano-architecture

Abstract

Pyrolysis coupled with carbon capture technologies is considered a techno-economically viable alternative to produce sustainable aviation fuels.1 The subject is gaining traction recently since it has been accepted that it will take time to replace certain petroleum derived transportation fuels such as aviation and shipping fuels by greener alternatives.1-3 However, alternative feeds such as biomass yield complex mixtures that have drained a lot of effort in optimizing reactor designs and operating conditions for their treatment to produce conventional products. As such, adsorptive denitrogenation (ADN) of liquid hydrocarbon fuels, especially bio-oils, has gained attention due to its importance in ridding nitrogen and oxygen containing compounds (NCCs) that have negative effects in the storage, processing and use of these fuels.2,3 This work investigated the benefits of developing advanced catalysts vs pre-treatment of feeds vs optimizing operating conditions in obtaining sustainable fuels. Strong emphasis was placed on the techno-economic and environmental impact of these processes. There is a strong indication that catalysis (reactor design and operating conditions) benefits a lot if coupled with feedstock pre-treatment technologies.

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Notes

Poster 2-12

Design and Synthesis of PdZnAl Hydrotalcite-like Catalyst for Efficient Sonogashira Cross-Coupling Reactions

Nokubonga Velaphi[a], Zondi Nate[a], Irene Mabuda[a], and Philani Mpungose[a]

[a]Cape Peninsula University of Technology, Cape Town, Western Cape, 800, South Africa,
E-mail: mpungosep@cput.ac.za.

Keywords: hydrotalcites, cross coupling reactions, Sonogashira coupling

Abstract

The Sonogashira cross-coupling reaction, which couples an aryl halide with a terminal alkyne, is widely applied in pharmaceutical chemistry and materials science. Conventional homogeneous palladium catalysts, however, face drawbacks related to recovery and reuse. In this work, a Pd-substituted ZnAl hydrotalcite (PdZnAl-HTIc) was synthesized via co-precipitation and investigated as a heterogeneous alternative.

Comprehensive characterization by XRD, FTIR, SEM, XRF, TGA, and NMR confirmed successful incorporation of Pd^{2+} into the hydrotalcite lattice. XRD indicated pure hydrotalcite structures with minor shifts after Pd substitution, while XRF showed a Pd content of 0.287 wt%. FTIR revealed characteristic Zn–O and Al–O vibrations with additional Pd–O bands, and SEM micrographs displayed spherical, aggregated particles. TGA analysis indicated typical hydrotalcite decomposition behavior, supporting the material's structural stability.

The effect of the reaction conditions on the catalytic properties of the PdZnAl-HTIc catalyst initially was studied in detail with the model Sonogashira reaction of iodobenzene and phenylacetylene to obtain optimum reaction conditions. The PdZnAl-HTIc catalyst then afforded substituted phenylacetylenes in good to excellent yields under these optimum reaction conditions. The catalyst was easily recovered by centrifuge and reused three times without significant loss of catalytic efficiency.

Notes

Poster 2-13

Hydrogenation of carbon oxides CO/CO_2 into long chain olefins

Seiso Seheri[a], Joshua Gorimbo[a], Yali Yao[a],

[a]*Institute for Catalysis and Energy Solutions, University of South Africa, c/o Pioneer Avenue and Christian De Wet, 1709, Florida, Private bag X6, South Africa,*
Email: Kenneth.seiso@gmail.com.

Keywords: Fischer-Tropsch synthesis, CO2 conversion, Hydrogenation, iron-based catalysts.

Abstract

Energy consumption and demand escalates with human population and industrial revolution, and it is responsible for the majority of climate change-causing greenhouse gas emissions, mostly from the burning of fossil fuels (coal, oil and natural gas) which is about 81% of the total energy supply globally, with oil comprising about 30%, followed by coal (28%) then natural gas (23%). Global emissions from fuel combustion were dominated by coal (45%), followed by oil (33%) and natural gas (22%). The International Energy Agency revealed that in 2022, the global carbon-dioxide (CO_2) emissions from fuel combustion increased by 1.3%, surpassing the levels preceding the COVID-19 pandemic [1]. Researchers has shown that it is not only important to link the chemical industry and energy sector with renewable resources nonetheless to carry out significant usage of carbon dioxide as a feedstock as to manage the anthropogenic carbon dioxide emissions globally [2]. The hydrogenative conversion of both CO and CO_2 into high-value multicarbon (C^{2+}) compounds, such as olefins, aromatic hydrocarbons, ethanol, and liquid fuels, has attracted much recent attention. The synthesis of carbon-dioxide hydrogenation catalysts to produce useful long chain olefins is currently one of the interesting and pivotal assignment related to resolve the problem of carbon-dioxide emission. Several researchers has used Iron-based catalysts doping with different metals as promotersfor hydrogenation of CO_2 into long chain olefins via Fischer-Tropsch process. For better catalyst stability and selectivity herein we will be focused on doping the Fe-based catalyst mainly by transition metals to produced long chain olefins from hydrogenation of carbon-dioxide via Fischer-Tropsch synthesis.

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Notes

Poster 2-14

Efficient Ruthenium(II) complexes as pre-catalysts for the dehydrogenation of formic acid: Insights into catalytic strategies and mechanistic insights

Pamela. S. Moyo[a], and Andrew. J Swart

[a]*School of Chemistry, University of Witwatersrand Johannesburg, Jorissen St, Braamfontein, Johannesburg, 2017, South Africa*
Email: pamela.moyo@wits.ac.za.

Keywords: Homogenous, ruthenium, hydrogen storage, formic acid dehydrogenation

Abstract

One of the most important societal concerns in light of the growing global population is the search for sustainable energy sources to meet our energy needs.1 Fossil fuels such as oil, gas and coal are depleting. A major breakthrough towards a hydrogen-based energy ecosystem is to adopt a proper hydrogen-carrier-material that can safely produce and store hydrogen (H2).2 Most popular hydrogen storage materials are organic compounds, so-called liquid hydrogen carriers (LOHCs). Formic acid (FA) is considered as a benign candidate for the reversible hydrogen storage which has a promising potential because of its favourable properties. FA contains 4.4 wt% of hydrogen, and it is liquid under ambient conditions, allowing it to be handled, stored, and transported easily and safely.3-4 It is one of the important liquid organic hydrogen carriers (LOHCs) due to its accessibility and comparatively low toxicity. Formic acid dehydrogenation offers a promising method for hydrogen production. FA can be selectively decomposed to pressurized H2/CO2 using an appropriate homogeneous or heterogeneous catalyst.5-6 This work focuses on the synthesize and characterization of ruthenium(II) complexes bearing amide-based ligands for the FA dehydrogenation. This could result in complexes with a variety of intriguing properties such as improved solubility, enhanced stability, and selective reactivity. The half sandwich ruthenium(II) complexes have been synthesized and characterized using various spectroscopic and analytical techniques.

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Notes

Poster 2-14

Hydrogenation of carbon dioxide to methanol over supported copper-based catalysts

Ndumiso Mkhonza[a], Lindelani Q. Qwabe[b], Masikana M. Mdleleni[c], Ebrahim. Mohiuddin[c], and Pinkie Ntola[a]

[a] *Department of Chemistry, Faculty of Applied Sciences, Durban University of Technology, P.O. Box 1334, Durban, 4000, South Africa.*

[b] *Department of Chemistry, Faculty of Natural Science, Mangosuthu University of Technology, Umlazi 4031, South Africa.*

[c] *Petro SA Synthetic Fuels Innovation Centre, South African Institute for Advanced Materials Chemistry, University of the Western Cape, Cape Town, Private Bag X17, Bellville, 7535, South Africa*

Keywords: copper-based catalysts, CO_2 hydrogenation, methanol, zinc-zirconia supports

Abstract

CO_2 emissions have become a challenging issue affecting not only humans but also climate change and global warming due to an intense increase in CO_2 concentration in the atmosphere. There are various technological approaches, such as Carbon Capture and Storage (CCS) and Carbon Capture and Utilization (CCU), as well as the catalytic conversion of CO_2 into value-added chemicals and fuels, that can mitigate the environmental problem by converting the large CO_2 emissions associated with the use of fossil fuels [1]. Methanol is one of the best products that can be synthesized by utilizing carbon dioxide as a starting material at a controlled temperature (°C) and pressure (Pa). Methanol is the primary feedstock for various industrial chemicals, including dimethyl ether, acetic acid, and biodiesel. Industrial syngas methanol synthesis has developed and improved over the years using copper-based catalysts [2]

In this study, we aimed to utilize copper-based catalysts to synthesize methanol using a fixed-bed continuous reactor under controlled conditions. The co-precipitation method was used for the preparation of mixed oxide catalysts, where a precipitation agent was used to facilitate the deposition of active metal onto the surface of the support through deposition precipitation.

Catalysts	$MeOH_{(aq)}$ (area %)
ZnZr	A= 61.34 %
10% Cu/ZnZr	A= 66.03 %
15% Cu/ZnZr	A= 68.64 %
20% Cu/ZnZr	A= 67.33 %
0.2% Ga/ZnZr	A= 65.37 %
0.2% Ga- 15% Cu/ZnZr	A= 66.67 %

Table 1. Obtained results on tested catalysts

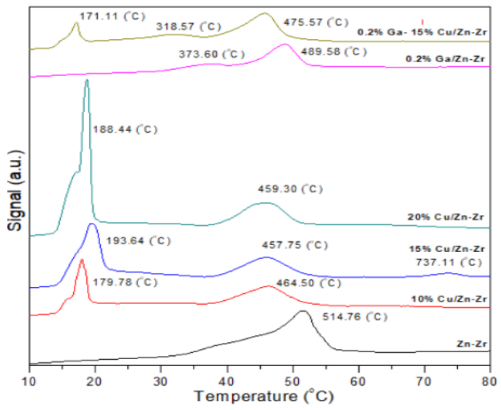

Figure 1. Stacked H_2-TPR of prepared copper-based catalysts.

Copper-based and gallium-promoted catalysts supported on Zn^{2+}: Zr^{4+} (1:2) were calcined in air at 350 °C for 3 hours. Copper-based and gallium-promoted catalysts were characterised (Figure 1) and investigated for conversion of CO_2/H_2 hydrogenation to methanol using a fixed-bed reactor (Table 1). The development of copper-based catalysts is expected to increase due to various advantages, such as easy preparation, low cost, and high ability to conduct the reaction, which impact the activity.

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Notes

Poster 2-16

Extraction of moringa extract from moringa powder using organic solvents for the synthesis of NZVI nanocomposite

Mookgo Mofokeng[a], Baraka Sempuga[a], Linda Jewell[b], Yali Yao[a*]

[a]*Institute for Catalysis and Energy Solutions (ICES), University of South Africa, Roodepoort, 1709, South Africa*

[b]*Civil and Chemical Engineering, University of South Africa, Roodepoort, 1709, South Africa*

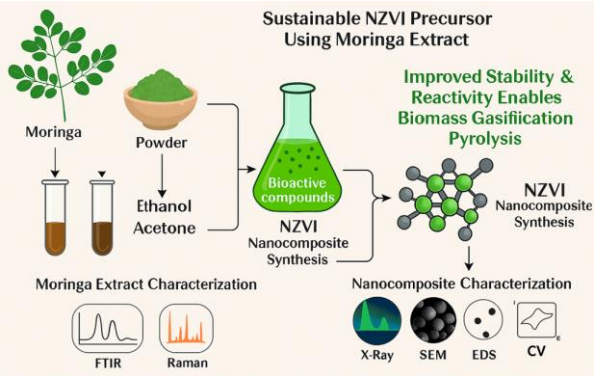
* Corresponding author: Yaoy@unisa.ac.za (Y Yao)

Keywords: Moringa oleifera, green synthesis, nanoscale zero valance iron, organic solvents, phytochemicals, nanocomposites, bioactive.

Abstract

This study presents a green and sustainable approach for synthesizing nanoscale zero-valent iron (NZVI) nanocomposites using *Moringa oleifera* extracts obtained through organic solvent extraction. Moringa powder was extracted using ethanol and acetone to isolate bioactive compounds predominantly polyphenols, flavonoids, and phenolics serving as natural reducing and stabilizing agents in NZVI formation [1-2]. The work emphasizes the role of advanced characterization techniques in elucidating the chemical, structural, morphological, and electrochemical properties of both the moringa extracts and the resulting NZVI composites. Fourier Transform Infrared (FTIR) confirmed polyphenol extraction (O–H at 3343 cm^{-1}, C=C at 1654 cm^{-1}) and Fe^0 formation (Fe–C at 630 cm^{-1}). Raman spectroscopy revealed selective flavonoid/phenolic solubilization and Fe–O bonding (~296 cm^{-1}) in hybrid architectures. X-ray diffraction (XRD) analysis revealed distinct diffraction peaks at $2\theta \approx 44.7°$, 65.0°, and 82.3°, corresponding to the (110), (200), and (211) planes of body-centered cubic α-iron, verifying the successful synthesis of crystalline NZVI superimposed on the amorphous moringa matrix, confirming structural transformation. SEM-EDS illustrated solvent-dependent morphology: acetone yielded needle-like Fe-rich domains, while ethanol produced layered, granular coatings with balanced C/O/Fe distribution. Cyclic voltammetry (CV) demonstrated amplified redox activity, with anodic peaks (~0.3–0.5 V) from flavonoids/phenolics and cathodic Fe^0 oxidation (~−0.5 V), highlighting synergistic electron transfer. Collectively, these techniques offered a comprehensive understanding of the composite's physicochemical profile, validating moringa's potential as a sustainable reducing and stabilizing agent for NZVI synthesis.

Graphic abstract



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Notes

Poster 2-17

Fabrication of ZnO and BiOCl heterojunction nanoparticles for the photodegradation of rhodamine B xanthene dye.

David. M Mabena,[a] Mabuatsela. V Maphoru,[a] Letlhogonolo. F Mabena,[a] and Lerato Hlekelele[b]

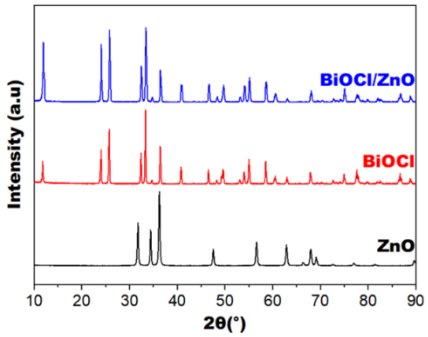
[a] Department of Chemistry, Tshwane University of Technology, 175 Nelson Mandela Drive, Pretoria, 0001, South Africa, E-mail:MabenaDM@tut.ac.za. [b] Centre for Nanostructures and Advanced Materials, DSI-CSIR Nanotechnology Innovation Centre, Council for Scientific and Industrial Research, Pretoria, South Africa.

Keywords: photocatalysis, semiconductors, metal oxide, rhodamine B, catalyst.

Abstract

Water is essential for human survival worldwide but its quality has deteriorated drastically over the years due to its contamination by various kinds of pollutants. These water pollutants originate from the chemical production, pharmaceutical, pesticide, herbicide and textile industries, whose contaminated effluents are discharged into various water bodies [1]. Organic contaminants such as Rhodamine B (RhB), a water-soluble dye that is commonly used as a dye in fabric industries, as well as a colourant in printing, leather, and plastic industries are amongst pollutants that can be found in water. Humans are susceptible to rhodamine B as studies in the medical field have confirmed that rhodamine B is mutagenic and carcinogenic, which results in developmental and simulation toxicity in animals and humans [2]. Semiconductors-based photocatalysts play a pivotal role in the development of green and sustainable processes for wastewater processing [3]. Photocatalysts are considered an eco-friendly technology due to their ability to degrade dyes into less harmful or non-toxic substances without undergoing degradation. ZnO and BiOCl are frequently used in photocatalysis due to their low cost, facile synthesis, and excellent stability [4]. The main drawbacks for ZnO and BiOCl is their large bandgaps of 3.4 eV and 3.3 eV, respectively, which limit them from harvesting light in the visible region [4]. Preparation of heterojunction structures from the two photocatalysts is expected to improve their performance by limiting electron-hole pair recombination. This study focuses on the performance of ZnO and BiOCl heterojunction structures created by varying the mass ratios of ZnO and BiOCl composites and using them to degrade RhB under UV light. The crystallographic structure was studied using XRD as illustrated in figure 1, while SEM and TEM will be used for microscopy studies.

Figure 1: XRD patterns of the photocatalysts.



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Notes

Poster 2-18

Cracking Heavy Waxes with Smart Pores: Hierarchical Pt/MOR for Fischer-Tropsch Wax Upgrading

Yuvna Nirel Bridglall, Patricia Jane Kooyman

Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Private Bag X3, Rondebosch, 7701, South Africa, E-mail: brdyuv001@myuct.ac.za.

Keywords: Pt/MOR, hydrocracking, bifunctional catalysts, hierarchical zeolites, dual templating

Abstract

The global transition towards sustainable energy requires the development of advanced catalytic processes able to upgrade Fischer–Tropsch (FT) waxes into high-quality liquid fuels and petrochemical feedstocks. FT waxes produced from biomass or syngas are typically long-chain paraffins that are challenging to convert selectively due to their size and chemical inertness. Conventional wax hydrocracking relies on the use of bifunctional catalysts, combining hydrogenation noble metals with zeolite supports. Among available zeolites, mordenite (MOR) is a particularly attractive support due to its strong Brønsted acidity and shape-selective channels which influence the product distribution. However, MOR is purely microporous resulting in diffusion limitations for the processing of long-chain paraffins. These limitations often reduce catalytic activity and promote undesired secondary cracking of primary hydrocracking products into C1-C4 gases, which decreases liquid fuel yields.

This study focuses on the synthesis and characterisation of hierarchical Pt/MOR of varying silica-to-alumina ratios, prepared via a dual templating method that is designed to introduce mesoporosity within the zeolite framework while maintaining the intrinsic acidity and crystallinity. The hierarchical structure aims to alleviate diffusion limitations by improving molecular transport and accessibility of reactants and reaction intermediates to the active sites and improving product removal, thereby reducing secondary cracking. Platinum nanoparticles are incorporated onto and within the MOR framework via wet impregnation to provide the metallic hydrogenation function. A C_{16} n-paraffin is employed as a model compound to simulate the hydrocracking of FT waxes under controlled experimental conditions, allowing for systematic evaluation of catalyst performance.

Comprehensive physicochemical characterisation will be employed to correlate catalyst structure with performance. Powder X-ray diffraction and nitrogen physisorption will be used to confirm crystallinity, surface area and the presence of mesoporosity. Transmission electron microscopy will provide insight into MOR morphology, Pt particle size and dispersion. Acid site density and strength of will be evaluated using NH_3-TPD. Pt loading will be quantified by ICP-OES. Temperature-programmed oxidation will be used to evaluate carbonaceous deposits and probe Pt oxidation behaviour. Catalytic evaluation in a fixed-bed reactor will focus on conversion, product selectivity, and cracking pathway analysis.
The anticipated outcomes of the study include improved accessibility of acid sites, enhanced Pt dispersion, and superior catalytic performance of hierarchical Pt/MOR relative to conventional microporous MOR. In particular, it is expected that these materials will demonstrate higher selectivity toward desirable distillate fractions while minimizing the formation of light gases. The findings will provide insights into the design of hierarchical bifunctional catalysts for FT wax upgrading and contribute to advancing sustainable liquid fuel production in South Africa, addressing both energy security and environmental goals.

Notes

Poster 2-19

Semi-rational design of an unspecific peroxygenase for the regioselective hydroxylation of fatty acids

Nita Olive van Wyk,[a] Ana Ebrecht,[a] Martha Sophia Smit,[a] and Diederik Johannes Opperman[a]

[a]*Department of Microbiology and Biochemistry, University of the Free State, 205 Nelson Mandela Drive, Park West, Bloemfontein, 9300, South Africa,*
E-mail: 2020228231@ufs4life.ac.za.

Keywords: oxyfunctionalisation, biocatalysis, lactones, regioselectivity

Abstract

The selective oxyfunctionalisation of un-activated C-H, C-C and C=C bonds remains a challenge in organic synthesis. Several oxidoreductase enzyme families, such as the P450s and unspecific peroxygenases (UPOs), are capable of these reactions under relatively mild conditions. Enzymatic catalysis is considered to be sustainable, as biocatalysts are not only produced from renewable resources, but are biodegradable and produce non-hazardous waste. Furthermore, biocatalysts can be engineered using mutagenesis techniques for improved activity, stability and selectivity. UPOs are a family of fungal-secreted heme thiolate enzymes that catalyse a broad range of reactions, including the oxyfunctionalisation of several substrates, ranging from aliphatic and aromatic hydrocarbons to other organic compounds containing heteroatoms such as nitrogen and sulfur. UPOs require only hydrogen peroxide for their activity and are therefore favoured over their P450 counterparts, as the latter require the supplementation molecular oxygen and expensive nicotinamide cofactors. This broad substrate scope and self-sufficiency has increased the interest of UPOs as an industrial biocatalyst for application in several industries, such as the pharmaceutical or flavour and fragrance industries.

The unspecific peroxygenase from Daldinia caldariorum (DcaUPO) has been shown to catalyse the in-chain aliphatic hydroxylation of several fatty acids, most notably octanoic acid, with ~90% conversion to produce C-4 and C-5 hydroxy fatty acids. These hydroxylated products undergo spontaneous cyclisation to form the γ-lactone and δ-lactone, respectively, which are cyclic esters that emanate pleasant aromas. The enzyme showed high regioselectivity, with ~95% of the products being oxidised at the C-4 and C-5 positions. However, the lactones did not encompass all of the products, as over-hydroxylation and keto-acid formation were also observed [1].

The aim of this study is therefore to engineer DcaUPO for improved regioselectivity toward the production of either the γ- or δ-lactone via structure-guided engineering techniques. As the three-dimensional crystal structure of DcaUPO has previously been solved, semi-rational design methods were used to produce a small mutant library via site-saturation mutagenesis of 13 amino acid residues in and near the catalytic active site. These mutants have been heterologously produced using Escherichia coli as an expression host and screened for altered regioselectivity using a high-throughput method for quick detection of base candidates. The optimization of this screening method will allow for the identification of amino acid sites responsible for the in-chain regioselectivity of the enzyme, and will serve as a basis for further mutagenesis via the generation of mutant libraries containing multiple mutations at several selected sites.

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Notes

Poster 2-20

Biocatalytic Production of Chiral Sulfoxides using Unspecific Peroxygenases

Sinèad Suter[a], Ana Ebrechta, Martie Smit[a] and Dirk Opperman[a]

[a]*Department of Microbiology and Biochemistry, University of the Free State, 205 Nelson Mandela Drive, Bloemfontein, 9300, South Africa,*
E-mail: sinead.suter.ss@gmail.com.

Keywords: Biocatalysis, Unspecific Peroxygenases, chiral sulfoxides.

Abstract

Sulfoxides are an important class of organo-sulfur compounds in pharmaceutical ingredients and have found widespread applications in, amongst others, anti-microbial medication, proton pump inhibitors, blood pressure and narcolepsy medication [1]. Sulfoxides with the sulfur linked to two different substituents are stereogenic. These enantiomers show differences in their pharmacokinetics, duration of action, side effects and potency. Traditional chemical oxidative synthesis often yields racemic mixtures or overoxidation to the sulfone, necessitating downstream purification of the active enantiomer, which is difficult and expensive. In addition to these drawbacks, traditional synthesis is harsh on the environment; thus, biocatalysis has emerged as a promising alternative for the synthesis of chiral sulfoxides from their corresponding prochiral sulfides. Baeyer-Villiger monooxygenases and cytochrome P450 monooxygenases both use molecular oxygen and expensive nicotinamide cofactors for sulfoxidation reactions, whereas unspecific peroxygenases (UPOs) only require hydrogen peroxide. To date, most of these biocatalysts, however, have yielded (R)-sulfoxide enantiomers.

Here we have screened a small library of UPOs from various fungi for chiral sulfoxidation reactions. The UPOs were heterologously produced in Escherichia coli, purified and their activity evaluated using thioanisole as the model sulfide. Although all the UPOs showed activity towards thioanisole, only three produced the (S)-enantiomer. Of these, the UPO from Helicocarpus griseus (HgrUPO) showed high conversion (97% of 10 mM) of thioanisole, with the highest enantiomer excess. Unfortunately, the reaction also yielded the overoxidized sulfone. HgrUPO was subsequently screened against a panel of diverse sulfides. Sulfoxidation was observed with all the substrates tested; however, reduced activity and altered enantioselectivity were observed with substitutions on the aromatic ring. To determine the molecular determinants of enantioselectivity, HgrUPO was crystallised and the structure solved using X-ray crystallography. The 1.5 Å structure revealed an overall fold similar to other short UPOs, with a phenylalanine sidechain positioned in the active site that potentially directs the binding of thioanisole and controls enantioselectivity.

From the crystal structure of this enzyme, we have chosen key amino acid residues for site-directed mutagenesis to assess the changes in enantiospecificity and selectivity. Co-crystalisation studies are underway with thioether substrates, which will allow us to visualise the enzyme interaction with the substrate, further highlighting important residues in the active site that control activity and selectivity.

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Notes

Poster 2-21

Template free Synthesis and Characterization of ZSM-5 Zeolite

Mamaru Alem and Patricia J. Kooyman

Catalysis Institute, Department of Chemical Engineering, University of Cape Town, Rondebosch,7701, Cape Town, South Africa
E-mail: mamaru.alem@uct.ac.za.

Keywords: Catalyst, Si/Al ratio, Template free synthesis, ZSM-5

Abstract

Hydrocracking is an essential process used for the conversion of long hydrocarbons into high quality liquid fuels [1]. This process typically employs bifunctional catalysts that combine acidic supports with metallic components, which have gained significant attention due to their enhanced activity and selectivity [2]. ZSM-5 zeolite, with its unique microporous structure and strong acidity, serves as an excellent support for metal catalysts, facilitating efficient hydrocracking reactions [3]. Hence, there exist a huge research interest to Pt/ZSM-5 bifunctional catalyst in the hydrocracking reaction. However, ZSM-5 commonly suffers from diffusion limitations. Moreover, the Si/Al ratio ZSM-5 crucially determines its catalytic activity, yet the ratio in the zeolite has been found to deviate from that of the synthesis gel. Therefore, developing a reproducible synthesis method to obtain ZSM-5 with a tunable Si/Al ratio is essential to design a bifunctional catalyst.

The aim of this work is to synthesize ZSM-5 zeolite with the desired Si/Al ratio by proper optimization of Si/Al in the gel composition. Next to the synthesis gel composition, the crystallization temperature and time will be optimised.
The crystallinity and Si/Al ratio of the as-synthesized catalyst will be characterized using XRD and ICP-OES techniques, respectively. N2 sorption and NH3TPD will be employed to characterize surface area and acid site distribution. Finally, the catalytic performance will be determined for n-C16 hydrocracking using a plug flow reactor at mild reaction conditions [4].

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Notes

Poster 2-22

Co (II) complexes derived from phenoxyimine ligands as catalyst precursors for the coupling of carbon dioxide and propylene oxide.

Mihlali Fatyela[a] and Juanita van Wyk

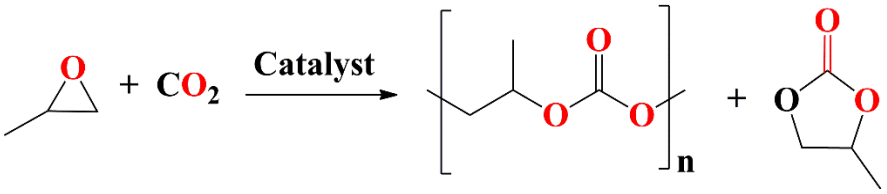
School of Chemistry, University of Witwatersrand, PO Wits, 2050,
2128646@students.wits.ac.za

Keywords: carbon dioxide, cobalt (II) complexes, epoxide.

Abstract

The rising carbon dioxide levels in the atmosphere have necessitated the need to develop chemical process that utilizes carbon dioxide as feedstock in order to move closer to a circular economy that is more sustainable. Utilizing carbon dioxide as a C1-feedsctock for chemical production is of particular interest due to its abundance, low-cost and non-toxicity. In recent years the coupling of carbon dioxide with epoxides have gain attention due to the atom economy of this reaction. In addition, this process produces biodegradable polycarbonates which could potentially be a replacement for nonbiodegradable polymers and cyclic carbonates which are also of commercial value (**Scheme 1**).[1] Due to the stability of carbon dioxide, a catalyst is required for this coupling reaction. Transition metal complexes derived from porphyrin and Salen ligands have been shown to be active catalysts producing either the polycarbonate or cyclic carbonates depending on the nature of the catalyst or the conditions used for the coupling reaction [2],[3],[4],[5]. In this study, Co (II) complexes derived from phenoxyimine ligands are prepared, characterized and investigated as catalyst precursors for the coupling of carbon dioxide with propylene oxide.

Scheme 1: *Coupling of propylene oxide and carbon dioxide*.



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Notes

Poster 2-23

Synergism between Ni-W in the hydrogenolysis of erythritol to value-added chemicals over zirconia-supported catalysts.

Wakhiwe M. Mthiyane[a,b] Alisa Govender[c] and Mzamo Shozi[a]

[a] School of Chemistry and Physics, University of Kwa-Zulu Natal, University Road, Westville, 3629, South Africa, Email: wmthiyane@wsu.ac.za. [b] Department of Chemical and Physical Sciences, Nelson Mandela Drive, Mthatha, 5099, South Africa. [c] Group Technology, Sasol R &T, Sasolburg, 1947, South Africa.

Keywords: structures, perspectives, reactions, metal, catalyst.

Abstract

Biomass-derived sugar alcohols, such as the polyol erythritol (C/O ratio = 1), are highly oxygenated platform compounds that present an opportunity for tailored and selective deoxygenation to useful chemicals, such as butanediols, through preferably C-O bond hydrogenolysis reactions. Previous studies have shown that the formation of butanediol isomers strongly depends on the reaction temperature. This is to say, 2,3-butanediol and 1,2-butanediol are mainly formed at 200 °C whereas 1,3-butanediol and 1,4-butanediol isomers are preferentially formed at 100 – 150 °C, independent of the catalyst used. Four catalysts comprising NiO and WOx supported on zirconia with 20 wt% total metal loadings (5Ni-15WOx/ZrO_2, 10Ni-10WOx/ZrO_2, 12.5Ni-7.5WOx/ZrO_2, 15Ni-5WOx/ZrO_2) were prepared via co-precipitation. The binding energy positions of the x-ray photoemission spectroscopy (XPS) spectra had doublet of peaks for Ni $2p_{3/2}$ which were indicative of Ni^0 and Ni^{2+} while that of W $4f_{5/2}$ and $4f_{7/2}$ showed W^{6+} species. These were corroborated by the H2-temperature-programmed reduction studies which indicated a possible interaction between both metallic species (Ni and W) and alumina support, forming the active Ni47W 3phase

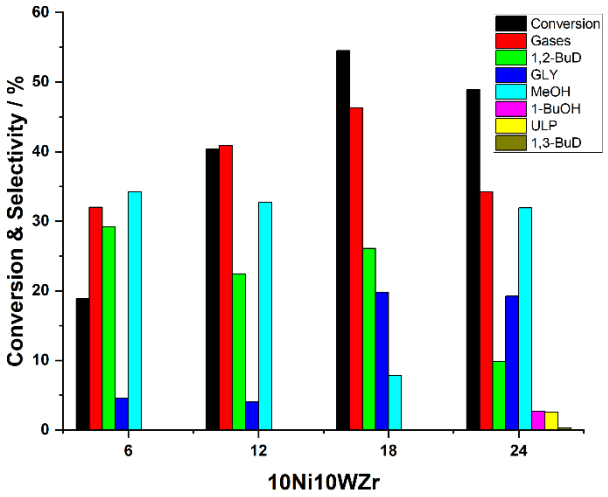

Figure 1: Catalytic performance of 10Ni10WZr over erythritol. Reaction conditions at 6 – 24 hr intervals: 25 mL of 15 wt% erythritol aqueous solution, T = 200 °C and $P(H_2)$ = 40 bar. Catalyst mass: 500 mg. C-based selectivity: GLY = glycerol, EG = ethylene glycol, BuD = butanediol. Gases: CO_2 (major) and CH_4 (minor).

Catalytic data showed a 19-54% conversion of erythritol over a 6-24h period over 10Ni10WZr catalyst. The selectivity to C-O hydrogenolysis products such as 1,2butanediol decreased from 28 to 12%, while that to 1,3-butanediol remained under 1% over a 6-24h period. Parallel reactions of unwanted C-C bond hydrogenolysis yielded glycerol and cracked products such as methanol and further to gaseous products.

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Notes

Poster 2-24

Influence of Water Vapor Treatment for NH3-TPD on Solid Acid Catalysts

J. Adolphs[a]*, Y. Konishi[b]

[a]*Microtrac Retsch GmbH, Retsch-Allee 1-5, 42781 Haan, Germany,*
E-mail: j.adolphs@microtrac.com
[b]*MicrotracBEL Corp., 8-2-52, Nanko-higashi, Suminoe-ku, Osaka 559-0031 Japan*

Keywords: Ammonia TPD, solid acid catalysts, zeolites

Abstract

Introduction

Temperature programmed desorption of ammonia (NH3-TPD) is commonly used to evaluate the acidity (acid amount, acid strength) of solid acid catalysts such as zeolites. In many cases, there are two peaks, *l*-peak (low temperature) and *h*-peak (high temperature) in the TPD spectrum.

Experimental/methodology

The *l*-peak is derived from ammonia molecules which are adsorbed by hydrogen bonding on NH4+ cation on acid sites and is not considered to indicate the acidity. However, in the case of zeolites with weak acidity, such as Y-type zeolites, the *l*-peak and *h*-peak overlap, making it difficult to evaluate acidity. NH3 TPD measurement with steam treatment is considered being effective to eliminate the *l*-peaks. In this contribution the procedure, and precautions are described. Ammonia as probe molecule is adsorbed onto the zeolite sample until it reaches equilibrium. Then the temperature of the sample is continuously increased, causing an enrichment with the desorbed molecules in the inert carrier gas (Helium). The standard TCD (Thermal Conductivity Detector) measures the total adsorbed amount and not the specific desorbed constituents. However, since zeolite adsorbs water in its pores, it is necessary to use a detector that can detect water and ammonia separately when measuring TPD. Also, since water vapor is introduced at high temperature, this method is not applicable to samples whose properties are changed by water vapor. Therefore, a quadrupole mass spectrometer is used to detect the desorbing ammonia at mass number 16. Mass number 17 was not used because the peak at 17 can be affected by the desorbed water.

NH3-TPD measurements were performed under the following conditions.

Measuring equipment	: BELCAT II + BELMASS
Sample	: MFI, 50 mg
Temperature ramp rate and target temperature	: 10°C/min, 610°C
Adsorption gas	: NH3/He 5%

According to Igi et al [1], in their experiments the steam treatment was performed by repeating the evacuation of the sample cell with following steam introduction. Differently, the catalyst analyzer BELCAT II is a dynamic flow type equipment operating permanent at atmospheric pressure. Fully saturated water vapor is generated by an advanced bubbling method with inert gas at room temperature under atmospheric pressure.

Results and discussion

The experimental results show that steam treatment eliminates the *l*-peak and leaves the *h*-peak shape almost unchanged, indicating that steam treatment in NH3-TPD measurement is very effective for eliminating the *l*-peak and examining the *h*-peak in detail. To perform NH3-TPD measurement with BELCAT II, the vapor option and a quadrupole mass spectrometer BELMASS is necessary.

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Notes

Poster 2-25

The hydrolysis approach towards the pre-treatment and biodegradability of red meat abattoir effluent

Dimakatso Makwakwa, [a] Makgatho Seshibe and Mabatho Moreroa [a]

[a]Department of Chemical Engineering, College of Science, Engineering & Technology, Institute for Catalysis and Energy Solutions, University of South Africa, Florida Park, 1709 Johannesburg, South Africa
Email:18211291@mylife.unisa.ac.za.

Keywords: pre-treatment, abattoir wastewater, hydrolysis, anaerobic digestion.

Abstract

Abattoir effluent is one of the reasons that contributes to water pollution when it gets released into bodies of water without sufficient treatment. Water pollution is a global concern characterised by the introduction of harmful compounds into aquatic environments, leading to severe changes in water quality, which adversely affect both ecosystems and human health [1]. Abattoir effluent contains a high amount of organic waste with a high chemical oxygen demand (COD) concentration, which, when released into the environment, may harm aquatic life by reducing oxygen levels in the water body. Furthermore, the effluent contains significant amounts of fats, oils, and grease (FOG), total suspended particles (TSS), nitrates, and other contaminant parameters, necessitating effluent treatment before the release. There are various treatment methods previously studied to pre-treat abattoir effluent, such as chemical, biological, physical and thermal, etc [2], [3], [4], [5]. However, some methods, such as physical and chemical pre-treatments, are often expensive because of their high energy demands and operating costs as compared to biological pre-treatment, which has low energy requirements, eliminates the need for chemicals, and operates under mild environmental conditions by utilising microorganisms to treat lignocellulosic materials and enhance enzymatic hydrolysis [6]. As a result, this research aims to investigate the viability of using a novel hydrolysis agent to pre-treat and eventually biodegrade red meat abattoir effluent. The red meat abattoir effluent will be biodegraded using anaerobic digestion to produce biogas. The raw abattoir effluent will be characterised into the following parameters: COD, FOG, TSS, pH and dissolved oxygen, to name a few, and the results will be compared with the pre-treated effluent to measure the effectiveness of the hydrolysis agent in reducing the organic content from the raw effluent. The pre-treated effluent will then be digested in an anaerobic digester to measure the biodegradability of the effluent to produce biogas. The biogas produced in this study could be used to assist SA in dealing with the crisis of loadshedding.

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Notes

Poster 2-26

Suppressing zinc dendrite formation using a conductive polymer as capping agent in zinc-air batteries

Sabelo C. Xaba[a], Touhami Mokrani[a], Phumlani F. Msomi[a*]

[a]*Institute for Catalysis and Energy Solutions, College of Science, Engineering and Technology, University of South Africa, South Africa, 28 Pioneer Ave, Florida Park, Roodepoort, 1709,*

21822468@mylife.unisa.ac.za

Keywords: Rechargeable Zinc-air batteries, Zinc dendrites, Artificial layer

Abstract

Zin-air batteries (ZABs) have attracted a lot of interest due to their high energy density and high-power density compared to traditional battery systems. Rechargeable Zinc-air batteries (RZABs) are viewed as promising prospects for the future generation of portable and stationary energy storage systems due to the shift towards green energy. However, they still face several challenges that limit the performance delivered by the battery and prevent them from being commercially available. RZABs suffers from dendritic growth during the cycling and recycling of the battery. The formation of Zinc dendrites impacts the performance of the battery by short circuiting, shortening the cycle life, reduce the capacity leading to low coulombic efficiency therefore resulting to overall low battery performance. Different strategies have been reported in mitigating the detrimental effects associated with the growth of zinc dendrites. This work discusses one of the strategies, which is the application of artificial layer made of PVB polymer modified with encapsulated TiO_2 nanoparticles to coat the Zinc anode, promoting homogenous stripping and platting of Zinc, inhibiting the occurrence of unwanted reactions thus leading to an improved performance of the battery. The synthesized TiO_2 nanoparticles were confirmed by FTIR which showed a strong band for Ti-O-Ti stretch between 400 cm^{-1} - 700 cm^{-1}, Ti-OH bending vibration at around 1500 cm^{-1}. SEM-EDS confirmed the presence of titanium and oxygen with titanium having 55.8 wt% and oxygen having 40.0 wt%. XRD analysis of the synthesized nanoparticles confirmed the crystallite nature of the nanoparticles, and the average crystallite size was calculated to 25.9 nm. Figure 1 represent the overall objective of this work, using PVB composite as an artificial layer to prevent Zinc dendrites formation.

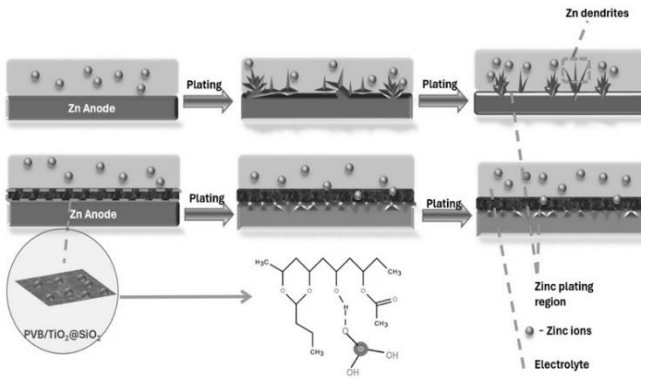

Figure 1. Depicting the application of PVB artificial layer to suppress dendrite formation

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Notes

Poster 2-27

Nitrogen functionalized carbon nanotubes/ quaternized poly (p-phenylene oxide) composite anion exchange membrane for fuel cell application

Nobuhle B. Mthethwa[a], Nozipho Gumbi[b], Phumlani F. Msomi[a]

[a] *Institute for Catalysis and Energy Solutions, College of Science, Engineering and Technology, University of South Africa, South Africa*

[b] *Institute for Nanotechnology and Water Sustainability, College of Science, Engineering and Technology*

Presenting Author: nobuhle021@gmail.com

Keywords: fuel cell, anion exchange membrane, polymer.

Abstract

The growing demand for clean and sustainable energy has highlighted fuel cells as a promising alternative to fossil fuels. A key challenge in anion exchange membrane fuel cell technology lies in developing the anion exchange membranes (AEMs) with high ionic conductivity, chemical stability, and mechanical strength. Traditional AEMs often degrade in alkaline environments, limiting their performance and long-term use, thereby reducing overall energy output. This work focuses on the fabrication of a novel composite AEM using nitrogen-doped carbon nanotubes (N-CNTs) and quaternized poly (p-phenylene oxide) (QPPO) as base composites. Nitrogen doping enhances the conductivity and stability of carbon nanotubes, while QPPO provides a thermally and mechanically stable polymer backbone that can act as a solid electrolyte. The integration of these materials is expected to create a membrane composite with improved hydroxide ion conductivity, reduced degradation, and enhanced durability. This work aims to advance the development of efficient, durable, and cost-effective membranes for alkaline fuel cells, contributing to the wider adoption of renewable and sustainable energy technologies. Chlorination of PPO was confirmed through FTIR, peak around 726,54 cm^{-1}. Synthesis of NCNTs was explored through TGA, showing decomposition and evaporation of the samples around 100°C to 400°C.

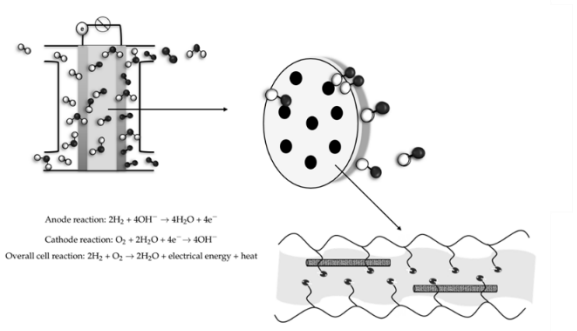

Figure 1. Schematic of an anion exchange membrane fuel cell.

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Notes

Poster 2-28

Fabrication of Composite Nanofiber Anion Exchange Membrane for Application in Zinc-Air Batteries.

Amogelang G. Metseeme,[a] Shidong Song,[b] Phumlani F. Msomi[a]

[a]college of Science, Engineering and Technology, Institute of Catalysis and Energy Solutions, University of South Africa,28 Pioneer Ave, Florida Park, Roodepoort 1709,
E-mail: 20920075@mylife.unisa.ac.za.
[b]School of Material Science and Engineering, Tiangong University, Tianjin 300387, China

Keywords: Rechargeable zinc-air battery, Anion exchange membrane, and Application.

Abstract

Rechargeable Zinc-Air batteries (RZABs) meet the three main goals of sustainable technology: ensuring safety during use while promoting a healthy environment; maximizing energy efficiency and conserving natural resources; and supporting the shift to renewable energy sources. RZABs find application in portable electronics, electric vehicles and have the proven potential to be used as stationary energy storage systems. Rechargeable zinc-air batteries (RZABs) face significant challenges related to short-circuiting, which greatly limit their overall performance and slow down large-scale commercialization. A key factor influencing the performance, lifespan, and power output of RZABs is the anion exchange membrane (AEM), located at the core of these batteries. The AEM enables the transport of hydroxide ions (OH^-) and helps prevent the migration of unwanted species, such as zincate ions. However, AEMs used in metal-air batteries and other energy storage systems are prone to accelerated degradation. While some degradation over the membrane's operational life is inevitable, its rate can be reduced through various interventions. This work aims to develop novel anion exchange membranes (AEMs) based on polyaniline (PANI) functionalized with quaternary ammonium groups, co-polymerised with fluorene-based polymer. Functionalization of PANI with Br_2 was characterized using FTIR, which showed a C-Br peak around 668 ppm, and EDX indicated 40.1% weight of Br_2, confirming bromination of PANI. NMR confirmed the shift of protons in the benzene ring toward the downfield, confirming bromination. Borylation of fluorene polymer was confirmed using NMR, which showed methyl group peaks at around 1.24 ppm–1.64 ppm (s, 24H). The successful coupling of PANI ES-DBHF was confirmed with NMR (1–1.5 ppm(m, 24H); 1.5–1.8 ppm(m, 16H); 3–3.5 ppm(t, 8H)) and FTIR (C-H stretch 2933–2854 ppm; C-H bending 1464–135 ppm; B-O/C-O 1133 ppm; C-H 779 ppm; & C-Br 620–513 ppm). Figure 1 shows the synthesis of AEM for this project.

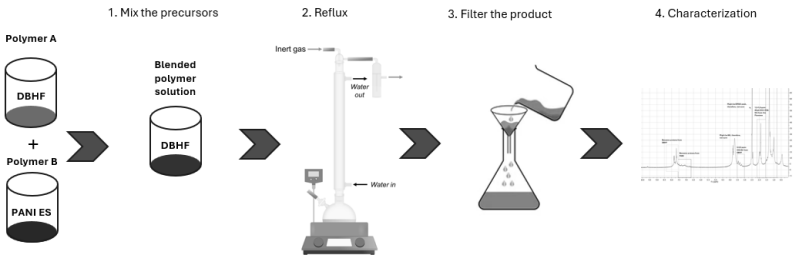

Figure 1: Schematic showing the preparation of the AEM polymer solution.

Notes

Poster 2-29

Engineering of *Komagataella phaffii* for the production of δ-dodecalactone

Rosshique Farmer[a], Martha Sophia Smit[a], Diederik Johannes Opperman[a], Ana Ebrecht[a]

[a] Department of Microbiology and Biochemistry, University of the Free State, E-mail: 2019255898@ufs4life.ac.za. [a] Faculty of Natural and Agricultural Sciences, 205 Nelson Mandela Drive, Bloemfontein, 9300, South Africa.

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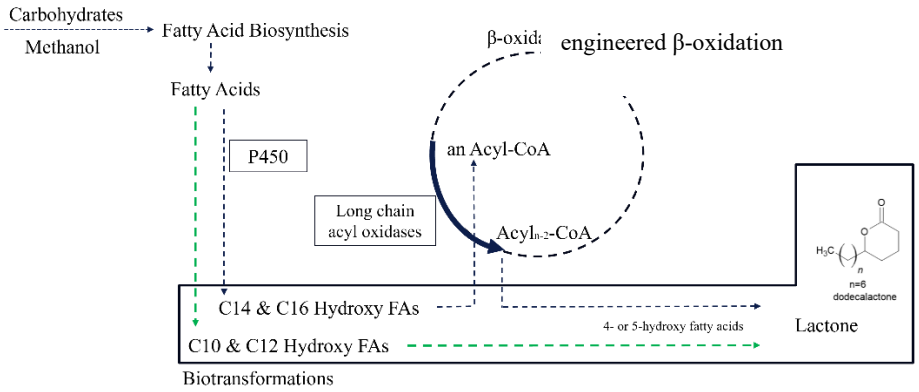
Abstract

Metabolic engineering has enabled the development of highly efficient cell factories capable of producing a diverse array of chemicals, which range from flavours and fragrances to active pharmaceutical ingredients. Among the leading platform organisms used in this field are *Escherichia coli* and *Saccharomyces cerevisiae*. However, when these organisms struggle to express certain proteins effectively, *Komagataella phaffii* (also known as *Pichia pastoris*) presents an alternative yeast host for heterologous protein production. *K. phaffii* is a methylotrophic yeast which can utilise methanol as a sole carbon source. Previously in our lab, *K. phaffii* strains were successfully engineered to produce δ-dodecalactone, a valuable flavour and fragrance compound, by expressing in-chain hydroxylating cytochrome P450 monooxygenases [1]. *K. phaffii* is an ideal host to express these in-chain hydroxylating cytochrome P450s since it does not contain any other cytochrome P450s that could interfere with the production of δ-dodecalactone. This lactone was synthesised from fatty acids and fatty alcohols such as dodecanoic acid and 1-dodecanol, but its production was hindered by the consumption of substrates and product through β-oxidation [1]. To address this challenge, we are exploring δ-dodecalactone production by *K. phaffii* strains with limited β-oxidation, created by German collaborators using CRISPR/Cas technology. We are evaluating the effects of limited β-oxidation on the growth of *K. phaffii*, the degradation of dodecanoic acid and δ-dodecalactone, and finally the production of δ-dodecalactone when the genes encoding in-chain hydroxylating cytochrome P450s are introduced.

Scheme 1: Overview of *de novo* biosynthesis of δ-dodelactone using engineered *Komagataella phaffii* as cell factory host.



[1] Smit MS; Mpeyake JM; Jacqueline van M; Aschenbrenner JC; Opperman DJ. *Applied Microbiology and Biotechnology* 2023.

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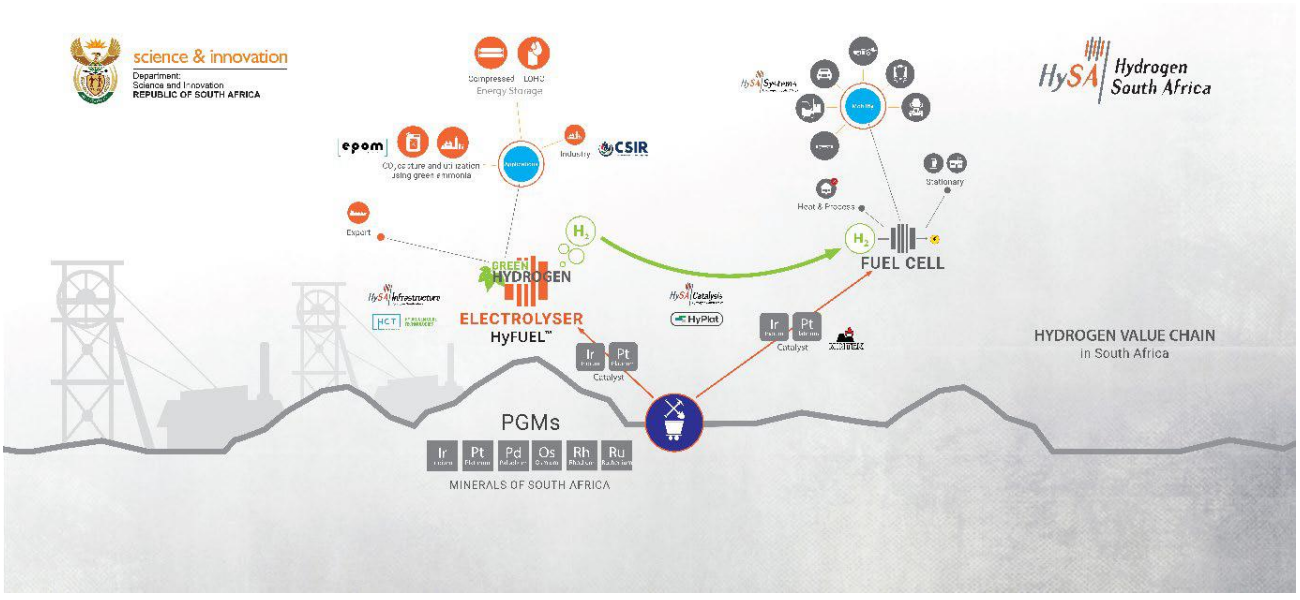

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