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23–25 April 2025 | Online

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The 3rd International Electronic Conference on Catalysis Sciences

23–25 April 2025 | Online



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Welcome from the Chair

Welcome to the **3rd International Electronic Conference on Catalysis Sciences (ECCS 2025)**. It is my great honor and pleasure to extend a warm welcome to all participants joining us from around the globe. This conference serves as a premier platform for catalysis researchers and enthusiasts to share their latest findings, innovative ideas, and practical experiences. We are excited to announce a series of specialized sessions that will highlight cutting-edge research and developments in various areas of catalysis. These sessions include:

- A. Catalytic Materials;
- B. Environmental Catalysis;
- C. Photocatalysis;
- D. Electrocatalysis;
- E. Biocatalysis;
- F. Biomass Catalysis;
- G. Industrial Catalysis;
- H. Computational Catalysis.

We are confident that these sessions will provide an excellent opportunity to engage with distinguished experts, gain new insights, and establish valuable connections that will drive future research and innovation in the field of catalysis. We look forward to your active participation and contributions, which will undoubtedly enrich the scientific discourse and propel the field forward. Thank you for joining us at ECCS 2025. We hope that you have a productive and enjoyable conference experience.

Yours sincerely,



Prof. Dr. Evangelos Topakas
Conference Chair

School of Chemical Engineering,
National Technical University of
Athens, Athens, Greece



Prof. Dr. Keith Hohn
Conference Chair

Carl R. Ice College of Engineering,
Kansas State University,
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Keynote Speakers



**Prof. Dr. Detlef Werner
Bahnemann**

Institute of Technical Chemistry
Leibniz Universität, Hannover,
Germany



Prof. Dr. Juan M. Bolivar

Department of Chemical
Engineering, School of
chemical
Sciences, Complutense
University of Madrid, Madrid,
Spain



**Prof. Dr. Sambhaji S.
Shinde**

Department of Materials
Science and Chemical
Engineering, Hanyang
University, Ansan, Republic of
Korea



Prof. Dr. Gerhard Mestl

Clariant AG, Bruckmühl,
Germany



**Prof. Dr. Gregori Ujaque
Perez**

Departament de Química,
Universitat Autònoma de
Barcelona, Catalonia, Spain



Prof. Dr. Satu Ojala

Faculty of Technology,
University of Oulu, Oulu, Finland



Prof. Dr. Sónia Carabineiro

Department of Chemistry,
NOVA University Lisbon,
Lisbon, Portugal



Prof. Dr. Haoxiang Xu

College of Chemical
Engineering, Beijing University
of Chemical Technology,
Beijing, China

Invited Speakers



Prof. Dr. Zhiqi Cong

Qingdao Institute of Bioenergy and
Bioprocess Technology, Qingdao,
China



Dr. Sergio Nogales Delgado

Department of Chemical
Engineering and Physical
Chemistry, University of
Extremadura, Badajoz, Spain



Dr. Dominic Alfonso

Department of Energy, National
Energy Technology Laboratory,
Pittsburgh, PA, USA



Prof. Dr. Gabriella Garbarino

Department of Civil Engineering,
University of Genoa, Genoa, Italy



Prof. Dr. Haibo Ge

Department of Chemistry, Texas
Tech University, Lubbock, TX, USA

Program at a Glance

23 April-Morning	24 April-Morning	25 April-Morning
Session A. Catalytic Materials	Session F. Biomass Catalysis & Session D. Electrocatalysis	
23 April-Afternoon	24 April-Afternoon	25 April-Afternoon
Session C. Photocatalysis	Session B. Environmental Catalysis & Session G. Industrial Catalysis	Session E. Biocatalysis & Session H. Computational Catalysis

ECCS 2025 Program

A. Catalytic Materials

Date: 23 April 2025 (Wednesday)

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time in CEST	Speaker	Title
09:00-09:10	Prof. Dr. Evangelos Topakas & Prof. Dr. Keith Hohn Conference Chairs	<i>Welcome from the Conference Chair</i>
09:10-09:20	Prof. Dr. Narendra Kumar Session Chair	<i>Welcome from the Session Chair</i>
09:20-09:40	Prof. Dr. Narendra Kumar Keynote Speaker	Metal Modified Extrudate Shaped Catalytic Materials for Production of Fuel Components
09:40-10:10	Prof. Dr. Sónia Carabineiro Keynote Speaker	TBA
10:10-10:25	Pradeep R. Varadwaj Selected Oral Presenter	Ammonia Synthesis and the Role of Promoters in Designing Efficient Transition Metal Catalysts
10:25-10:40	Monica Pavel Selected Oral Presenter	Tailoring the structural and electronic properties of RbLaTa ₂ O ₇ double-layered perovskite by the rapid molten-flux synthesis route
10:40-10:55	Luca Calantropo Selected Oral Presenter	Synthesis of new LDH-derived composites with enhanced photo-thermal properties exploited in photo-thermocatalytic processes for CO ₂ conversion
10:55-11:10	Jędrzej Piątek Selected Oral Presenter	Catalytic hydrogen production from boranes on metal-based catalysts
11:10-11:25	Elena Spennati Selected Oral Presenter	Promotion of Ni/alumina catalysts for CO ₂ hydrogenation
11:25-11:40	Ruben Mas-Ballesté Selected Oral Presenter	Quinoline-based porous organic polymers with divergent photocatalytic properties
11:40-11:55	Oluchukwu Virginia Igboenyasi Selected Oral Presenter	Single-Step Oxidation of Methane to Methanol over Superhydrophobic Modified NiO-Ce/Al ₂ O ₃ Catalyst
11:55-12:10	Richard C. Holz Selected Oral Presenter	Degradation of Chlorothalonil by Catalytic Biomaterials
12:10-14:00	BREAK	

C. Photocatalysis

Date: 23 April 2025 (Wednesday)

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time in CEST	Speaker	Title
14:00-14:10	Prof. Dr. Jingrun Ran & Prof. Dr. Ioannis Konstantinou Session Chairs	<i>Welcome from the Session Chairs</i>
14:10-14:30	Halbo Ge Invited Speaker	TBA
14:30-14:45	Monir Uzzaman Selected Oral Presenter	Enhanced Photocatalytic Hydrogen production under Visible Light using Ammonia-Treated Graphene Oxide/ZnIn ₂ S ₄
14:45-15:00	Shoaib Mukhtar Selected Oral Presenter	Synthesis of metal sulfide/g-C ₃ N ₄ nanocomposite for photocatalytic degradation of organic pollutants under visible light
15:00-15:15	Christos Lykos Selected Oral Presenter	Thermally exfoliated urea-derived g-C ₃ N ₄ /Ti ₃ C ₂ TX MXene 2D/2D Schottky junctions as photocatalysts for the removal of pharmaceutical pollutants in aquatic matrices
15:15-15:30	Salah Eddine Stiriba Selected Oral Presenter	Merging decatungstate photocatalysis and a copper-catalyzed azide-alkyne cycloaddition reaction for the sustainable formation of 1,2,3-triazoles in water
15:30-15:45	Mst. Farhana Afrin Selected Oral Presenter	Enhanced Photocatalytic Cr(VI) Reduction in Aqueous Solution with Black TiO ₂ Under Visible Light Irradiation
15:45-16:00	Gregor Žerjav Selected Oral Presenter	Influence of Pt loading on the Schottky barrier height and the photothermal activity of TiO ₂ /Pt catalysts
16:00-16:15	Maria Teresa Armeli Iapichino Selected Oral Presenter	Sustainable carbon-based photocatalysts for solar H ₂ production by photoreforming of plastic materials
16:15-16:30	Yuri Okuno Selected Oral Presenter	Photocatalytic methane production from acetic acid solution with S-doped g-C ₃ N ₄ under visible light irradiation

Session F. Biomass Catalysis
Session D. Electrocatalysis

Date: 24 April 2025 (Thursday)

Time: 9:00 (CEST, Basel) | 03:00 (EDT, New York) | 15:00 (CST Asia, Beijing)

Time in CEST	Speaker	Title
09:00-09:10	Prof. Dr. Francesco Mauriello Session Chair	<i>Welcome from the Session Chair (Session F)</i>
09:10-09:40	Dr. Sergio Nogales Delgado Keynote Speaker	Catalytic conversion of biogas in a biorefinery context: perspectives and challenges
09:40-09:55	Dominique Agustin Selected Oral Presenter	Grafted polyoxometalates as recoverable catalysts for biomass valorisation
09:55-10:10	Haliru Abdullahi Selected Oral Presenter	Effects of Precipitation Variables on Phenolic Hydroxyl Group Content of Lignin Recovered from Black Liquor
10:10-10:25	Marco Chiocchini Selected Oral Presenter	Hydrothermal carbonization as a pre-treatment to selectively remove ashes from bamboo
10:25-10:40	Meghana H K Selected Oral Presenter	Strategic Design of Copper Nanoparticles on Modified Clay as Catalyst for Efficient Domino Synthesis of γ -Valerolactone from Furfural via Transfer Hydrogenation
10:40-10:50	Prof. Dr. Vincenzo Baglio & Prof. Dr. Donald Tryk Session Chairs	Welcome from the Session Chairs (Session D)
10:50-11:20	Dr. Sambhaji S. Shinde Keynote Speaker	Design strategies practical Zn-air batteries using advanced electrocatalysts
11:20-11:35	Antonella Castro Selected Oral Presenter	Development and Characterization of a Bismuth-based MOF Electrode for the Electrophotocatalytic Degradation of Rhodamine
11:35-11:50	Elmira Hadian Rasanani Selected Oral Presenter	CuCo ₂ O ₄ as Catalyst for Oxygen Evolution Reaction in Anion Exchange Membrane Water Electrolysis
11:50-12:05	Donald Tryk Selected Oral Presenter	Theoretical insights into how to inhibit an undesirable reaction while catalyzing a desirable reaction: hydrogen peroxide production during the hydrogen oxidation reaction in a proton-exchange membrane fuel cell

12:05-12:20	Sergey A. Grigoriev Selected Oral Presenter	Electrocatalytic layers for medium-temperature polymer membrane water electrolysis
12:20-12:35	Diana Fernandes Selected Oral Presenter	Juniperus brevifolia as a potential biomass source for the construction of efficient oxygen (electro)catalysts
12:35-12:50	Diego Ramón Lobato-Peralta Selected Oral Presenter	NiFe-LDH and Manganese-Based Catalysts for Advanced Metal-Air Battery Applications
12:50-13:10	Dr. Dominic R. Alfonso Invited Speaker	Optimization of Ag electrocatalyst performance for CO ₂ to CO conversion: Pairing Atomistic Simulations with Experiments
13:10-14:00	BREAK	

Session B. Environmental Catalysis
Session G. Industrial Catalysis

Date: 24 April 2025 (Thursday)

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time in CEST	Speaker	Title
14:00-14:10	Prof. Dr. Jean-François Lamonier & Prof. Dr. Albin Pintar Session Chairs	<i>Welcome from the Session Chairs (Session B)</i>
14:10-14:40	Prof. Dr. Satu Ojala Keynote Speaker	Alternative catalyst raw materials and environmental applications
14:40-14:55	Giusy Dativo Selected Oral Presenter	Photothermocatalytic valorization of CO ₂ using natural and artificial modified phyllosilicates
14:55-15:10	Chaitra N. Mallannavar Selected Oral Presenter	Enhancing activity of HAP catalyst by hydrothermal in situ Zn incorporation for transformation of CO ₂ to produce cyclic urea from diamine
15:10-15:25	Melissandre Richard Selected Oral Presenter	Impact of Periodic Rich/Lean Switching and Metal Zone-Coating on Three-Way Catalyst Performance
15:25-15:40	Eleonora La Greca Selected Oral Presenter	Hydrogen from Methane: new ground with Chemical Looping Technology
15:40-15:55	Bishal Hamal Selected Oral Presenter	Facile synthesis of Aluminum-doped Bi ₂ WO ₆ and enhanced remediation of aqueous Methylene Blue and Rhodamine B
15:55-16:10	Ana Júlia Briganti Bezerra Selected Oral Presenter	Oxidative denitrogenation of quinoline using cobalt ferrite catalysts
16:10-16:25	Souha Denguezli Selected Oral Presenter	The recycling of polyethylene by means of catalytic pyrolysis: The Effect of contaminants on the products from the catalytic pyrolysis of polyethylene

16:25-16:35	Prof. Dr. Guido Busca Session Chair	Welcome from the Session Chairs (Session G)
16:35-17:05	Dr. Gerhard Mestl Keynote Speaker	TBA
17:05-17:25	Professor Gabriella Garbarino Invited Speaker	Carbon as catalysts support: current opportunities and challenges
17:25-17:40	Chamssane Issouffou Selected Oral Presenter	Structural Insights and Bioactive Potential of Coconut Shell Lignin from acid-assisted Organosolv process
17:40-17:55	Kriti Mehta Selected Oral Presenter	Organocatalysis originating from 1,1-Diaminoazines

Session E. Biocatalysis
Session H. Computational Catalysis

Date: 25 April 2025 (Friday)

Time: 14:00 (CEST, Basel) | 08:00 (EDT, New York) | 20:00 (CST Asia, Beijing)

Time in CEST	Speaker	Title
13:00-13:10	Prof. Dr. Frank Hollmann Session Chair	<i>Welcome from the Session Chair</i>
13:10-13:40	Dr. Juan M. Bolivar Keynote Speaker	Biocatalytic reaction intensification in bioprocessing: from waste valorization to platform chemicals.
13:40-14:00	Professor Cong Zhiqi Invited Speaker	Engineering water tunnel to generate an efficient P450 peroxygenase biocatalyst
14:00-14:15	Omar Boualam Selected Oral Presenter	Oxidation of Malachite Green by Illite Impregnated with Iron/Indium
14:15-14:30	Leticia Lafuente Selected Oral Presenter	Use of DERA in Development of Novel N-heterocycle-based Statin Precursors
14:30-14:40	Dr. Dominic R. Alfonso Session Chair	Welcome from the Session Chair
14:40-15:10	Prof. Dr. Haoxiang Xu Keynote Speaker	Structural descriptor for rational design of transition metal catalysts
15:10-15:30	Prof. Dr. Sergio Nogales Delgado Invited Speaker	Catalytic conversion of biogas in a biorefinery context: perspectives and challenges
15:30-15:45	Poater Albert Selected Oral Presenter	From Predictive Chemistry to Machine Learning in Applied Chemistry
15:45-16:00	Basil Raju Selected Oral Presenter	A Novel Approach for First-principles Calculations of Charged Adsorbates in Periodic Metallic Systems
16:00-16:15	Pradeep R. Varadwaj Selected Oral Presenter	Dinitrogen Activation by Transition Metal Catalysts: Paving the Way for Future Energy and Sustainability
16:15-16:30	Manh Tien Nguyen Selected Oral Presenter	Theoretical study of CO ₂ capture mechanisms of SrO and Sr(OH) ₂ ·nH ₂ O (n=0,1,8)

Session A. Catalytic Materials

sciforum-111668: Copper Oxide Nanoparticles in Ligand-Free Conditions: A Path to Selective Ketone Hydrosilylation

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The hydrosilylation of ketones is an essential reaction in organic synthesis, with significant applications in the pharmaceutical and specialty chemical industries. This study explores the use of copper oxide (CuO) nanoparticles, synthesized via thermal decomposition in the absence of ligands, as catalysts for this reaction. ¹ CuO nanoparticles were characterized by X-ray diffraction (XRD), infrared spectroscopy (IR), and scanning electron microscopy (SEM), confirming their high purity and well-defined structural and morphological properties. ² Their catalytic activity was evaluated using dimethylphenylsilane as the hydrosilylation agent on various ketone substrates. The reaction products were analyzed by nuclear magnetic resonance (NMR) spectroscopy, including ¹H, ¹³C, and ²⁹Si NMR, to ensure precise structural identification. These results highlight the potential of CuO nanoparticles as efficient, durable, and cost-effective catalysts for hydrosilylation. Ongoing studies aim to optimize reaction conditions and evaluate the recyclability of the catalyst, underscoring its relevance for industrial applications and green chemistry practices.³

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- [2] Darezereshki / JMM 47 (1) B (2011) 73 – 78, DOI :10.2298/JMMB1101073D
- [3] Kantam, M. L., Laha, S., Yadav, J., Likhar, P. R., Sreedhar, B., & Choudary, B. M. (2007). Asymmetric Hydrosilylation of Prochiral Ketones Catalyzed by Nanocrystalline Copper (II) Oxide. Advanced Synthesis & Catalysis, 349(10), 1797-1802.



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sciforum-112499: Enhanced CoOOH-based catalysts for dye decolorization

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In recent years, water pollution has become one of the most predominant environmental problems. Organic refractory pollutants such as dyes and antibiotics are difficult to degrade in nature and thus cause water pollution. To solve this water pollution problem, the efficient removal of pollutants in wastewater is extremely important. Cobalt is the best metal element for activating peroxymonosulfate (PMS). In this study, we aimed to prepare transition metal-doped CoOOH catalysts to improve the activity of PMS.

The M-doped CoOOH catalyst was prepared as follows (M = Cu, Ni, Fe, Zn, and Mn). To 50 mL of 84 g/L of NaOH, 0.45 M Co(NO₃)₂·6H₂O and 0.05 M metal nitrates were added in a volume of 25 mL. The mixture was stirred for 30 min. Then, 60 mL of 30% H₂O₂ was added, and the mixture was stirred at 60 °C for 24 h with a hot stirrer. The product was washed with distilled water and vacuum-dried. Dye decolorization was performed in the presence of peroxymonosulfate using the prepared CoOOH catalyst.

XRD measurements confirmed that CoOOH was prepared, as the characteristic peaks of CoOOH were observed. Some peak positions were shifted to the lower angle side in CoOOH doped with Cu, Ni, Fe, and Zn compared to CoOOH. In the decolorization experiments, RhB was decolorized by 15.2% after 10 min of reaction, when PMS solution was added alone, and by 26.3% in the CoOOH/PMS system. The decolorization rate of the M-doped CoOOH/PMS system was faster than that of the CoOOH/PMS system. Especially in the Ni-doped CoOOH/PMS system, RhB was decolorized by 77.8%. Therefore, X% Ni-doped CoOOH with different Ni doping was prepared and decolorization experiments were performed (X = 5, 10, 20, and 30). As a result, 87.2% of RhB was decolorized in the 20% Ni-doped CoOOH/PMS system.



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sciforum-115730: Investigation of catalysts based on metal--organic frameworks (mof) of coordination compounds of Cu^{2+} and Gd^{3+} ions with benzene-1,3,5-tricarboxylic acid during propane dehydrogenation

Ksenia Seromlyanova *, Yulia Zaitseva, Ekaterina Markova, Anton Mushtakov and Alexander Cherednichenko

RUDN University

Introduction

Based on the structural--electronic structure of MOFs, it can be assumed that these materials can be unique macromolecular adsorbents that can form intermediates with organic reagents and then turn them into the final products of chemical transformations.

Methods

PXRD, IR-spectroscopy, thermogravimetric analysis, scanning electron microscopy, low-temperature nitrogen adsorption, and catalytic units were used in this study.

Results

The metal--organic framework structures of Cu-MOF and Gd-MOF were synthesized using nitrates of metals and benzene-1,3,5-tricarboxylic acid, an organic ligand. Replacing copper ions with gadolinium ions in MOFs increases the efficiency of the process. The conversion of propane at 400°C increases to 8.0 % for the Cu-MOF catalyst and to 20% for the Gd-MOF catalyst. At this temperature, there is no non-catalytic reaction. Synthesized metal--organic frameworks are porous materials with a specific surface area of 319 m^2/g for Cu-MOF and 551 m^2/g for Gd-MOF. The surface morphology of synthesized materials was studied using SEM. The resulting particles have the shape of an octahedron.

Conclusions

These materials have demonstrated high catalytic activity in the process of propane dehydrogenation at a temperature of 400°C. Propane conversion using Gd-MOF increased to 20.0 %, and selectivity for light olefins (ethylene and propylene) increased to 71.0 %, while when using Cu-MOF, propane conversion increased to 8.0 %, and light olefin selectivity by 69.0 %. For Gd-MOF, there was no decrease in the efficiency of its operation due to the deposition of amorphous carbon on the surface of the catalyst. This result allows us to predict the significant service life of this catalyst.



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sciforum-111306: Quinoline-based porous organic polymers with divergent photocatalytic properties

Ruben Mas-Ballesté *

Universidad Autónoma de Madrid

Introduction

The transition to a greener and more renewable productive model has been raised as a main challenge for science during recent decades. Reducing dependence on petrol fuels and finding new sources for industrial chemical precursors requires brand-new approaches with a lower or, ideally, no carbon footprint. In this context, photocatalysis has emerged as a greatly encouraging solution. Among the most promising heterogeneous photocatalysts, we can find reticular organic materials such as Covalent Organic Frameworks (COFs) and related amorphous materials, such as Covalent Triazine Frameworks (CTFs) or Conjugated Microporous Polymers (CMPs).

Results

A variety of conjugated microporous polymers (CMPs) and covalent triazine frameworks (CTFs) have been recently synthesized in our laboratory. A particular family of such materials is that containing quinoline fragments acting as photocatalytic moieties. Predetermined series of CMPs and CTFs with similar structural and photophysical properties show divergent photocatalytic activities for environmentally relevant reactions such as hydrogen evolution and the oxidation of furfural derivatives. Different catalytic behaviors arise from differences in their electronic structures, which were analyzed from both experimental and theoretical studies.

Conclusions

The results obtained suggest that nitrogen doping and electron-donating groups play a critical role in tuning the photocatalytic properties of organic materials, offering a powerful strategy for designing building blocks in heterogeneous organic photocatalysts. This underscores the versatility and broad applicability of nitrogen-enriched materials for various photocatalytic processes, from oxidation reactions to hydrogen generation.



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sciforum-115529: Ammonia Synthesis and the Role of Promoters in Designing Efficient Transition Metal Catalysts

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Ammonia synthesis is crucial for global fertilizer production, traditionally relying on iron-based catalysts in the Haber–Bosch process [1,2]. However, the limitations of iron catalysts—such as low reaction rates and susceptibility to deactivation—have driven interest in alternative catalysts, particularly Ru-, Co- and high-entropy-based transition metal systems. The use of promoters, both in single and double settings, has become key to enhancing the efficiency and stability of these transition metal catalysts [3]. This presentation focuses on the role of various promoters in optimizing Ru-, Co- and Fe-based catalysts, exploring their mechanisms and potential to advance ammonia synthesis.

Results:

The inclusion of promoters such as K_2O , Ba, Ce, or BaO, among others, significantly enhances the catalytic performance of Ru-, Co- and Fe-based catalysts. For iron, these promoters improve the adsorption of N_2 and its dissociation, leading to higher ammonia yields and longer catalyst lifespans. In cobalt-based systems, these promoters stabilize the active metal sites and promote efficient nitrogen dissociation within a temperature range of below 500 °C. The promoters modify the electronic properties of the catalysts, improving their overall efficiency. The nature of the rate-determining step cannot always be limited to N_2 decomposition; it can also involve other hydrogenation steps.

Conclusion:

Promoters are crucial in optimizing the performance of transition metal catalysts in ammonia synthesis. These promoters enhance catalyst stability, increase reaction rates, and suppress deactivation, offering a promising pathway for more efficient and sustainable ammonia production. Future research should focus on refining promoter–metal interactions to further improve catalyst performance and reduce energy consumption.

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sciforum-109310: An Innovative Method for Hydrogen Transfer Reactions Using Colloidal Mono- and Bimetallic Nanoparticles Anchored on Carboxymethyl Cellulose and Supported on Natural Phosphate

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In recent years, nanomaterials have grown in significance across a range of fields, such as electronics, biological sensors, catalysis, and energy. Rapid advancements have been made in the use of materials as heterogeneous catalysts, and characteristics like recyclability and low cost are essential for the circular economy and sustainable development. Thus, due to their durability and high surface area, nanocatalysts have become attractive substitutes for traditional materials.

Hydrogen transfer reactions play a crucial role in various chemical processes, including catalysis, organic synthesis, and energy conversion. Unlike conventional direct hydrogenation, catalytic transfer hydrogenation offers numerous advantages such as cost-effectiveness in hydrogen generation, hydrogenation selectivity, and catalyst recyclability.

Herein, we report the synthesis of various mono- and bimetallic Co_x-Ag_y NPs (Co, Ag, Co-Ag, and Co-Ag core shells) anchored in carboxymethyl cellulose and their deposition on mesoporous natural phosphate (m-NP). First, the colloidal NPs were prepared and then followed-up using spectroscopic methods such as UV-vis, IR, and XRD. Afterwards, the resulting colloids were supported on m-NP using a wetness impregnation method to obtain Co_x-Ag_y@NP nanocatalysts². The developed nanocatalysts were characterized using advanced analytical methods, i.e., XRD, XPS, FESEM-EDX, and TEM. Their ability to generate catalysis and transfer hydrogen were studied to assess the level of metal synergy in the prepared nanocatalysts³.



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sciforum-115712: Biodiesel production by transesterification using choline hydroxide as catalyst

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Biodiesel is a mixture of fatty acid methyl esters (FAMES) and is a biodegradable and renewable fuel, produced from fat sources mainly composed of triglycerides. The use of ionic liquids (ILs) in biodiesel catalytic production has been studied mainly in the ecological field, as it allows a high recycling efficiency. Choline (2-hydroxyethyl trimethylammonium)-based ILs have received attention due to their biocompatibility characteristics and potential for various industrial applications. Specifically, choline hydroxide (ChOH) represents a promising option. This work's objective is the optimization of the methyl transesterification reaction conditions using commercial and waste sunflower oil (WSO) as raw material and ChOH as a catalyst, assessing the possibility of recovering the catalyst between reaction cycles. Therefore, biodiesel production was carried out on heating plates with temperature control and with magnetic stirring, using methanol reflux. After phase separation, centrifugation was used to enhance biodiesel recovery. Reaction conversion was assessed by acidity drop determination, and the biodiesel FAME content was determined by GC-FID, through a procedure in accordance with EN 14103, using methyl heptadecanoate as the internal standard. IL recovery was carried out by solvent extraction with water-based binary systems, followed by an FTIR analysis of both phases for ChOH detection, and a comparison with initial IL samples. Optimal conversions, determined by acid value (AV) reduction or by biodiesel FAME mass content, were obtained using a 4%wt. catalyst load, oil/methanol molar ratio of 1:8, duration of 1 h, and temperature of 65 °C. The products' AV for WSO showed a significant reduction relating to the raw material AV (6.14 mgKOH/g). For the reactions with commercial sunflower oil (AV close to 0.20 mgKOH/g), the biodiesel phase AV remained low. ChOH recovery, performed with n-butanol/water and ethyl acetate/water systems, proved to be inefficient under the conditions tested. FTIR analysis showed the presence of ChOH in both liquid-liquid extraction phases.



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sciforum-112692: Catalytic Activity of Metal Oxide Nanoparticles Derived from Electronic Waste through Green Synthesis

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Electronic waste (e-waste) has emerged as a growing environmental concern due to inadequate recycling practices and mismanagement, leading to significant consequences. Repurposing e-waste as an efficient nanocatalyst can be a strategy to mitigate such waste with profound implications. Waste printed circuit boards (WPCBs) may be employed for the recovery of various commercial and precious metals due to the presence of rich elemental compositions. This study explores the potential of WPCBs as a source of metal precursor for the synthesis of nanoparticles (NPs) using a biological approach wherein cell-free culture supernatant (CFCS) is employed.

The main objective of this work was to biosynthesize metal NPs using WPCBs and to evaluate the catalytic activity of the NPs. The biosynthesized NPs were characterized by X-ray diffraction analysis, FESEM, FTIR, TEM, and SAED and fringe patterns, which suggested the formation of Cu_xO NPs. FESEM and TEM analyses revealed that the NPs are spherical in shape. FTIR analysis identified the presence of copper oxide and organic functional groups of biological origin, which indicated the action of metabolites present in the CFS as capping agents to stabilize the NPs. The catalytic activity of the Cu_xO NPs was evaluated using a model reaction involving the reduction of 4-nitrophenol (4-NP) to 4-aminophenol (4-AP) using sodium borohydride (NaBH_4) as a reducing agent. The synthesized NPs exhibited excellent catalytic activity, and the reduction reaction was found to follow the pseudo-first-order kinetics.



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sciforum-115502: Catalytic hydrogen production from boranes on metal-based catalysts

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Hydrogen fuel is a non-toxic and abundantly available energy source with a high potential in replacing traditional fossil fuels in the automotive sector. However, several challenges related to its storage need to be resolved for effective industrial applications. Compounds such as sodium borohydride (NaBH_4) present a promising option as hydrogen sources, capable of releasing hydrogen rapidly under controlled conditions when utilized with heterogeneous catalyst systems. The hydrolysis of NaBH_4 can be easily controlled by adding or removing a solid catalyst from its solutions. While numerous reports show many catalysts for this reaction, the main emphasis is on their efficiency. The ideal catalyst should not only demonstrate high performance, but also withstand operational temperatures of 60–80 °C, typical for hydrogen engines, and maintain its efficiency for as long as possible. These aspects are often neglected in other reports, while being crucial for their future applications.

In this presentation, I explore metal-based catalysts used for the hydrolysis of sodium borohydride, focusing on their efficiency, durability, and stability at elevated temperatures. We successfully synthesized a variety of cobalt catalysts from both primary and secondary sources and tested their long-term effectiveness in hydrogen production using a custom-built testing system. Our research highlights essential parameters that are crucial for the future industrial applications of hydrogen generation from borohydride hydrogen storage systems, offering valuable insights for advancements in energy production.



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sciforum-109475: Catalytic Oxidation of Phenol Using Iron-Supported Illite: Optimization of Parameters for Efficient Wastewater Treatment

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This study investigates the catalytic oxidation of phenol using an iron-supported natural illite clay catalyst, focusing on optimizing degradation efficiency and minimizing environmental impact. Phenol, a hazardous industrial pollutant, poses risks to ecosystems, particularly affecting plant germination and fish survival in contaminated waters. To address these concerns, an iron-impregnated natural illite clay catalyst was developed to enhance the stability and reactivity of iron sites, promoting effective phenol degradation in wastewater.

The optimal degradation conditions were achieved at pH 3 and 50°C, facilitating hydroxyl radical formation and accelerating the reaction kinetics. Under these conditions, the catalyst achieved a 99% degradation rate for phenol and an 83% reduction in chemical oxygen demand (COD), indicating significant pollutant mineralization. Minimal iron leaching was observed, ensuring catalyst stability. Additionally, the H₂O₂ concentration was optimized at 0.5 mM, balancing efficient degradation with reduced chemical use.

To understand the degradation mechanism, scavenger tests confirmed hydroxyl radicals (•OH) as the primary reactive species. The identification of intermediate by-products was performed using high-performance liquid chromatography (HPLC), revealing a stepwise oxidation pathway that demonstrated the effective breakdown of phenolic compounds into less harmful substances. The catalyst also showed excellent reusability over five cycles with minimal activity loss, highlighting its potential for sustainable application. This study demonstrates the potential of iron-supported natural clay catalysts as a cost-effective, environmentally friendly solution for treating phenolic pollutants, reducing toxicity and supporting healthier ecosystems in aquatic environments.



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sciforum-110601: Catalytic Oxidation of Phenol Using Iron-Supported Illite: Optimization of Parameters for Efficient Wastewater Treatment

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This study investigates the catalytic oxidation of phenol using an iron-supported purified natural illite clay catalyst, focusing on optimizing operational parameters and elucidating the degradation mechanism to achieve high efficiency and minimize environmental impact. The effects of pH (2–10), initial phenol concentration (20–100 mg/L), temperature (30–90°C), iron content (3–7%), catalyst dosage (0.5–1.5 g/L), and H₂O₂ concentration (4.75–12 mM) were systematically studied. Optimal conditions were determined at pH 3, a phenol concentration of 50 mg/L, 50°C, 5% iron content, a catalyst dosage of 1 g/L, and 8.7 mM H₂O₂, enhancing hydroxyl radical formation and reaction kinetics. Under these conditions, the catalyst achieved a 99% degradation rate for phenols and an 83% reduction in chemical oxygen demand (COD), with minimal iron leaching. The identification of intermediate by-products using HPLC enabled the construction of a detailed stepwise degradation mechanism, shedding light on the oxidative pathways and confirming the effectiveness of the process. The purified illite catalyst demonstrated excellent stability and reusability over multiple cycles, maintaining performance with minimal activity loss. Comprehensive material characterization (XRD, TGA, BET, SEM, FTIR, and laser granulometry) confirmed the structural and morphological integrity of the catalyst and provided insights into its active sites. This study underscores the potential of iron-impregnated purified natural clays as sustainable, cost-effective catalysts for treating phenolic pollutants in wastewater.



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sciforum-115397: Cellulose as a catalyst in water treatment

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Cellulose, the most abundant natural polymer, has garnered significant attention as a catalyst and a catalytic support in sustainable chemical processes. Its unique structure, high surface area, and tunable functional groups, such as hydroxyl moieties, make it an ideal candidate for facilitating various catalytic reactions. The functionalisation of cellulose enhances its catalytic properties, enabling acid-base, redox, and enzymatic reactions. Additionally, its biodegradability and renewability align with green chemistry principles, providing an eco-friendly alternative to traditional catalysts. Cellulose has emerged as a promising material for catalysis in water treatment. Its abundance, eco-friendliness, and ease of functionalisation make it an attractive alternative to conventional catalysts in addressing water pollution challenges. By incorporating functional groups or immobilising active species on its surface, cellulose can facilitate advanced oxidation processes, adsorption, and photocatalytic degradation of contaminants. Modified cellulose-based catalysts have demonstrated efficiency in removing organic pollutants, heavy metals, and microbial pathogens from water. Available as colloidal solutions, films, and hydrogels, nanocellulose is effective in removing contaminants like heavy metals, dyes, and pharmaceuticals. Cellulose-ZnO catalysts offer the dual advantage of high dye removal efficiency and environmental sustainability. Cellulose enhances the adsorption of the dye molecules, facilitating closer interaction with the reactive sites on ZnO. This study shows its successful photocatalyst degradation of Crystal Violet dye and reusability and the impact of factors like the pH and catalyst morphology. Cellulose-ZnO materials exhibit favourable structural properties, characterised using Fourier transform infrared and scanning electronic microscopy, for catalytic applications; these materials present a significant step toward achieving cleaner water and promoting environmental sustainability.



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sciforum-114794: Degradation of Chlorothalonil by Catalytic Biomaterials

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Introduction:

Chlorothalonil (2,4,5,6-tetrachloro-1,3-benzenedicarbonitrile, TPN, CAS: 1897-45-6) is a halogenated fungicide currently widely applied to a large variety of crops.¹ The Environmental Protection Agency has classified TPN as a likely human carcinogen, as has the International Agency for Research on Cancers. As of 2022, TPN has been banned in 34 countries around the world, but it is still widely applied in the United States.² Its carcinogenicity, embryo lethality, and high chronic oral toxicity in mammals, among other effects on a variety of organisms, have made its biodegradation of great interest. Chlorothalonil dehalogenase (Chd) from the bacterium *Pseudomonas* sp. CTN-3 offers a potential solution by catalyzing the first step in the degradation of chlorothalonil.³

Methods:

The Chd pET28a+ plasmid was transformed into competent BL21(DE3) *Escherichia coli* cells, expressed and purified as previously reported.⁴ Tetramethyl orthosilicate (TMOS) (Sigma-Aldrich) (813 μ L), 181.4 μ L of nanopure water, and 5.6 μ L of 0.04 M HCl were combined to make 1 mL of sol material as previously described. Alginate beads were prepared and coated in chitosan as previously described.⁵

Results:

Reported herein are the active biomaterials of Chd when encapsulated in tetramethylorthosilicate (TMOS) gels using the sol-gel method (Chd/sol), alginate beads (Chd/alginate), and chitosan-coated alginate beads (Chd/chitosan). Both Chd/sol and Chd/chitosan increased protection from the endopeptidase trypsin as well as imparted stability over a pH range from 5 to 9. Chd/sol outperformed Chd/alginate and Chd/chitosan in long-term storage and reuse experiments, retaining similar activity to soluble Chd stored under similar conditions.

Conclusions:

All three materials showed a level of increased thermostability, with Chd/sol retaining >60% activity up to 70 °C. All materials showed activity in 40% methanol, suggesting the possibility for organic solvents to improve TPN solubility. Overall, Chd/sol offers the best potential for the bioremediation of TPN using Chd.



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sciforum-111287: Development and Construction of a Laboratory-Scale Bubble Column Bioreactor for Immobilized Enzyme Fermentation Studies

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This study presents the design and fabrication of a laboratory-scale bubble column fermenter specifically developed for fermentation studies employing immobilized enzymes. Constructed from stainless steel for durability and sterility, the fermenter incorporates advanced features to ensure precision and reliability. An air supply system, powered by a compressor, ensures consistent aeration, while precise temperature control is achieved through a jacketed reactor connected to a circulating water bath. These features are critical for maintaining optimal conditions for enzymatic reactions. To optimize the fermenter's functionality, rate and design equations for bubble column fermenters were employed in calculating the operational parameters. The bioreactor boasts a working volume of 65 mL, a height of 80 mm, and an internal diameter of 10 mm, tailored for small-scale experimental setups. A custom-designed sparger with five evenly spaced 0.5 mm holes and a 0.2 mm spacing ensures uniform bubble formation. The generated bubble sizes, ranging from 0.5 mm to 3.93 mm, exhibited a controlled rise velocity of 0.1 cm/s, facilitating effective gas-liquid interactions critical for fermentation efficiency. Designed for a maximum operating temperature of 38°C, the system incorporates a compressor with a power rating of 0.152 kW, ensuring robust performance. Performance testing validated the fermenter's utility, achieving a maximum ethanol production efficiency of 50.58%. This result underscores the system's reliability for enzyme-mediated biochemical processes. The fabricated bubble column fermenter demonstrates significant potential as a versatile and efficient tool for both research and industrial applications in bioprocess engineering. By combining precision engineering with practical functionality, this study provides a valuable platform for advancing enzyme-based fermentation technologies, offering insights into scalable designs for broader biochemical and biotechnological applications.



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sciforum-115710: Dry reforming of methane with CO₂ over Gd (Co,Mn)O₃ perovskite-type oxides

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Current trends aimed at reducing the environmental impact of human activity have led to the need for the development of efficient and sustainable catalytic systems for the methane dry reforming process. Moreover, the by-products of the primary greenhouse gases represent valuable raw materials for the petrochemical industry. These materials, which meet the requirements for activity, selectivity, and thermal and chemical stability, are complex oxides with a perovskite structure.

Gd(Co,Mn)O₃ complex oxides were prepared by the sol-gel method with citric acid and characterized by X-ray diffraction and Fourier-transform IR spectroscopy. Their oxygen non-stoichiometry was also investigated by iodometric titration. The catalytic properties of the samples were studied in a flow reactor at atmospheric pressure with a volume flow rate of 0.9-1.0 L/h and a CO₂:CH₄ ratio of 1:1.

It has been shown that the addition of manganese to the anionic sublattice of a complex oxide inhibits the conversion of carbon dioxide into methane. In samples containing manganese, the reaction temperature is shifted towards lower values, with X_{50%} conversions of CH₄ and CO₂ occurring at almost 300 K lower than in unsubstituted samples of cobalt. The synthesis gas ratio does not reach stoichiometric levels, which may be due to an increased side reaction of CO₂ reduction. Despite the lower catalytic activity, less surface carbonization was observed in complex oxides containing manganese. The formation of trace amounts of hydrocarbons suggests that the adsorption of methane on manganese atoms occurs mainly through the formation of CH_x species. These results suggest that catalytic systems based on Gd(Co,Mn)O₃ have potential for the production of synthesis gas through the conversion of carbon dioxide into methane.



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sciforum-115695: High-Performance $\text{Gd}_{1-x}\text{A}_x\text{FeO}_3$ (A = Ca, Sr, Ba) perovskite catalysts produced via simulated bio-syngas hydrogenation

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The production of light olefins through carbon oxide hydrogenation represents a promising alternative to fine organic synthesis, where ethylene and propylene are crucial components of the synthesis chain for valuable products. This research focuses on iron-containing $\text{Gd}_{1-x}\text{A}_x\text{FeO}_3$ (A=Ca, Sr, Ba) complex oxides as catalysts for simulated bio-syngas hydrogenation. Ca/Sr/Ba-promoted GdFeO_3 catalysts were prepared by the sol-gel method and characterized by BET N_2 -physisorption, X-ray diffraction, and Fourier-transform IR spectroscopy. Their acid-base properties and oxygen non-stoichiometry were also investigated. Their catalytic performances were evaluated in a fixed bed reactor. Ca/Sr/Ba increase the CO conversion rate and ethylene-propylene selectivity, while they decrease the production of methane. A very small amount of A additive can help to enhance the performance of GdFeO_3 catalysts in the hydrogenation of carbon oxides. It is worth noting that Ca/Sr/Ba can promote the occurrence of oxygen vacancies and the growth of both acidic and basic centers, and this affects the catalytic properties. With the modification of the Sr promoter, CO conversion and light olefin selectivity both increase due to the increase in the number of catalytically active sites, and they reach their highest values at a silver content of 0.01 wt.%. As a result, Sr can be seen as an attractive candidate to replace more expensive noble metal promoters, such as Pt and Re, under industrial conditions.

The results presented here offer a roadmap for tailoring the distribution of bio-syngas hydrogenation products to specific desired outcomes by adjusting the composition of the catalyst. To fully understand the active sites and phases and to unravel the underlying mechanisms, further in-depth investigations are required given the intricate nature of perovskite-based catalytic systems.

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sciforum-115754: METHOD FOR PRODUCING PROPYLENE AND "LIGHT" OLEFINS BY PROPANE CRACKING USING CATALYSTS BASED ON MODIFIED REE MOLYBDATES

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Introduction

Currently, much attention is paid to the development of new technologies and increasing the efficiency of existing processes for converting natural gas into "light" olefins, of which propylene is of greatest interest.

Methods

Synchrotron X-ray diffraction (s-XRD), Raman scattering, inductively coupled plasma atomic emission spectroscopy, low-temperature nitrogen adsorption, and a catalytic cracking unit were used.

Results

To obtain the catalyst, molybdates $\text{Ln}_2(\text{MoO}_4)_3$ were synthesized according to the developed method using rare earth nitrate and sodium molybdate dihydrate $\text{Na}_2\text{MoO}_4 \times 2\text{H}_2\text{O}$. Lanthanum, praseodymium, neodymium, and ytterbium molybdate catalysts for propane dehydrogenation increased feedstock conversion by 40.0% without recycling and the process yield of target propylene by 33.0% while maintaining high propylene selectivity (70.0%) and total selectivity for "light" olefins (83.0%). Over 8 hours of continuous operation, the catalyst activity decreased by less than 1.0%. The reaction activation energy decreased from 114 kJ/mol to 91.0 kJ/mol. A decrease in catalyst activity (about 15.0%) was observed after 200 hours of continuous operation. To regenerate the catalytic systems, it is proposed to treat their surface with an air flow at 573 K for 10 hours.

Conclusions

The formation of the mixed structure of $\text{Ln}_2(\text{MoO}_4)_3$ leads to a shift in the degree of conversion to the region of catalytic temperatures of 700-900 K with a predominance of the dehydrogenation reaction of 80%. It was revealed that the steric factor prevails over the energetic one in the process of propane destruction, making the reaction of ethylene formation stereospecific, with the achievement of a maximum in ethylene selectivity of 83%. It was determined that the non-isovalent substitution of K^+ leads to the deformation of the crystal structure and blocking of the most energetic Lewis centers, which leads to an insignificant decrease in propylene selectivity from 83% to 81% with a decrease in surface carbonization at high cracking temperatures.



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sciforum-112511: Molybdenum Schiff Base Complexes: Synthesis, Structural Analysis, and Catalytic Performance in Benzyl Alcohol Oxidation

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Molybdenum, a transition metal, is widely recognized for its ability to exhibit multiple oxidation states and form diverse complexes, including molybdenum Schiff base complexes. These complexes, formed by coordinating molybdenum with Schiff base ligands derived from primary amines and carbonyl compounds, possess unique properties and have garnered attention for their roles in biological and industrial applications. They are particularly important in catalytic processes, such as petroleum refining and chemical manufacturing. A key application of molybdenum Schiff base complexes is in the catalytic oxidation of benzyl alcohol to benzaldehyde, an essential industrial chemical. Benzaldehyde is valued for its almond-like aroma, making it a key ingredient in fragrances and cosmetics. It also serves as a precursor in the synthesis of pharmaceuticals, dyes, and agrochemicals, and its reactivity supports its role as an intermediate in organic synthesis. This highlights the industrial significance of molybdenum-based catalysts.

In this study, a Schiff base ligand was synthesized via the condensation of salicylaldehyde or 2-hydroxy-5-nitrobenzaldehyde with 2-furoic hydrazide and subsequently coordinated to the $[\text{MoO}_2]^{2+}$ core. Reactions in methanol yielded the complex $[\text{MoO}_2(\text{L}^{1\text{or}2})(\text{MeOH})]$, whereas reactions in acetonitrile produced $[\text{MoO}_2(\text{L}^{1\text{or}2})(\text{H}_2\text{O})]$. Characterization was performed using IR-ATR spectroscopy and thermogravimetric analysis, while molecular and crystal structures were determined by X-ray diffraction. These complexes were evaluated as catalysts for the oxidation of benzyl alcohol, demonstrating significant potential for catalytic applications, while the effect of varying oxidant quantities on selectivity and conversion was also investigated.



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sciforum-112673: Niobium-doped heteropolyacid included in silica--titania support as catalyst for selective sulfoxidation

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In the field of catalysis, the use of heteropolyacids is widespread, since they operate under mild conditions, favoring selectivity in reactions and reducing environmental pollution by not producing large volumes of waste. Heterogeneous catalysis is preferred because allows for easy recovery and re-use. This work shows the preparation of mixed silica--titania materials to immobilize a Keggin-type heteropolyacid doped with niobium and to use as a heterogeneous catalysts in sulfoxidation reactions under eco-friendly conditions.

Niobium-doped heteropolyacid (PMoNb) was synthesized by way of a hydrothermal synthesis method from orthophosphoric acid, molybdenum trioxide, and niobium pentoxide. Subsequently, PMoNb was included in different silica and titania supports using the sol--gel method from the precursors, i.e., tetraethyl orthosilicate and titanium isopropoxide. The prepared catalysts were characterized by XRD, FT-IR, Raman, and potentiometric titration, and tested in the selective oxidation of diphenyl sulfide to diphenyl sulfoxide.

The characteristic bands of both supports were found in the FT-IR and Raman spectra, with no appreciable differences due to the presence of PMoNb. Similar results were observed from XRD patterns. All the solids obtained present high acidity.

Regarding catalytic performance, bulk PMo and PMoNb catalysts were tested in the reaction, and it was observed that the incorporation of Nb improved the catalytic behaviour: 94% conversion and 94% selectivity (PMoNb) vs. 36% conversion and 100% selectivity (PMo) after 7 h. Moreover, the activity improved when the heteropolyacids were included in the support. However, the presence of Nb did not enhance the activity of the heterogeneous catalysts.

On the other hand, the high activity of TiO₂, undesired since it reduces selectivity, could be controlled when silica is incorporated into the structure. In this way, the best result was obtained using PMo, which was included in a support of silica--titania 1:1, with a conversion of 99% and a selectivity towards diphenyl sulfoxide of 88% after one hour of reaction.



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sciforum-114791: Polymer-inspired Ni-based catalysts for the dry reforming of methane

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The dry reforming of methane (DRM) is one method by which carbon dioxide and methane can be utilized for value-added products. DRM results in the formation of syngas, which is a combination of hydrogen and carbon monoxide. Syngas, in turn, can be used for energy or as a precursor for the production of liquid fuels, such as methanol. While the required energy input for the DRM reaction is quite high, the utilization of methane and carbon dioxide is enticing for environmental benefit.

Supported nickel (Ni)-based catalysts are often researched as DRM catalysts because they are active and less expensive than precious-metal-based catalysts. A major hurdle to DRM, however, is the deactivation of the catalysts due to carbon build-up during the reaction. The structure of the catalyst support material and its interaction with the active metal is thought to reduce coke deposition and catalyst deactivation during the DRM reaction.

In this study, novel polymer-inspired catalysts for DRM were prepared by pyrolyzing Ni-containing polydimethylsiloxane (PDMS). The pyrolyzed catalysts were found to be largely microporous Ni-based silica-supported catalysts, and the active nickel particles were nano-sized but did not disperse evenly in or on the catalysts. Even so, the catalysts demonstrated significant activity in the DRM reaction and had comparable performance to other catalysts reported in the published literature. The catalyst prepared with nominally 10 wt% Ni in PDMS (before calcination) displayed the highest methane conversion and lowest degradation of performance of the catalysts in this study. This research was successful in exploring polymer-inspired catalysts as novel catalysts for the DRM reaction.



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sciforum-115612: Polysiloxanes functionalized with platinum-group metal complexes

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Polymer-supported catalysts are versatile compounds for the synthesis of different molecules.¹ Among polymers, polysiloxanes possess good film-forming abilities, flexibility, a wide range of working temperatures (from -123 to +250 °C), and UV resistivity.² These properties make them desirable candidates for catalytic application in homogeneous and heterogeneous catalysis. The functionalization of polysiloxanes with platinum-group metal complexes opens up new opportunities for usage of the resulting metal-polymer compounds for catalytic hydrosilylation and dehydrocoupling reactions for platinum-containing complexes and for carbon-carbon cross-coupling reactions for palladium-containing polysiloxanes. Considering the nature of the catalytic reactions (homogeneous or heterogeneous), homogeneous catalysts usually demonstrate high catalyst activity and a short reaction time, but they contaminate the product of the reactions with metal and do not allow for the recovery and reuse of catalysts several times. This is crucial, taking into account the high price of platinum-group metals. Alternatively, heterogeneous catalysts can be used. Despite some of its limitations such as lower reaction rates and yields, heterogeneous catalysts are easier to recover and reuse several times.³

Thus, the aim of this study is to synthesize polysiloxanes that have functionalized using platinum and palladium complexes. We synthesized platinum-functionalized polysiloxane (Pt-PDMS) via Cu(I)-catalyzed azide-alkyne cycloaddition between a palladium *C,N*-cyclometalated complex and (3-azidopropyl)polysiloxane. Its activity was investigated in Si-O dehydrocoupling reactions⁴. Palladium-containing polysiloxane (Pd-PDMS) was synthesized in a similar way to the Pt-PDMS method. The catalytic activity of Pd-PDMS was examined in carbon-carbon cross-coupling reactions.³ The resulting catalysts demonstrated high catalytic activity in the performed reactions, without yield loss after several catalytic cycles. The usage of both Pt-PDMS and Pd-PDMS allows one to recover and reuse catalysts easily.

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sciforum-112684: Preparation and characterisation of diatomaceous earth/ $\text{MnMo}_9\text{O}_{32}$ system and its potential application in clean oxidation

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Heteropolyanions containing molybdenum and/or tungsten are an important class of compounds with properties such as high reactivity, selectivity, and structural diversity. In the present study, the heteropolymolybdate Waugh type containing Mn(II) as a heteroatom, $(\text{NH}_4)_6\text{MnMo}_9\text{O}_{32}$ (MnMo_9), was studied as a supported catalyst, using diatomaceous earth from northwestern Argentina as the support. The diatomaceous earths are highly adsorbent porous materials. Also, they are inexpensive and widely available in the pre-Cordillera region of Argentina. The HPOM and supported systems were characterised by DRX, FTIR, SEM-EDS, and RTP, among other physicochemical techniques. Given the chemical and structural properties of this phase, the clean oxidation of diphenyl sulfide (DFS) was chosen as the catalytic reaction for system evaluation. The reaction products, diphenyl sulfoxides (DPSOs) and diphenyl sulfones (DPSO_2), are of great interest as intermediates in the fine chemical and pharmaceutical industries. Diphenyl disulfide also acts as a test molecule for the study of processes to obtain ultra-low-sulphur fuels. The MnMo_9 system was evaluated as a bulk and a support in the oxidation of DPS with H_2O_2 , as a clean oxidant, at 80 °C. The results for the supported phase showed high reactivity, and a conversion of 100% of DPS was achieved at longer reaction times, with good selectivity for diphenyl sulfone at short reaction times.



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sciforum-115152: Preparation of metal oxides for effective catalysts

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Desired properties in catalysts include a nanosize and homogeneity of the particles that form the catalyst and/or its carrier. The creation of catalysts with the finest particles has been a hot topic of scientific research in recent decades. The particle sizes of catalytic oxides are set at the initial stage of forming; in wet-chemistry, this is a precursor to precipitation. It is possible to create optimal conditions by using homogeneous precipitation when the precipitant is formed in the solution itself due to a hydrolysis reaction. To solve this problem, urea was used in our work, and the hydrolysis products were ammonia and carbon dioxide. As a result of precipitation, hydroxides, carbonates, or hydroxy carbonates of metals can be obtained.

All precipitates were obtained from solutions of metal nitrates. The obtained hydroxides aluminum, indium, and iron, and the hydroxy carbonates nickel, cobalt, and zinc, were studied. The oxides obtained from these materials by calcination were also studied. They form the structure of the catalyst.

The following was found: metal hydroxides were obtained from aluminum, indium, and iron nitrate solutions. According to the XRD patterns, it was established that the crystallite sizes of the obtained hydroxides were, respectively, 1.5, 10, and 35 nm. The oxides obtained by the calcination of these hydroxides have similar sizes, from 0.6 to 15 nm.

Metal hydroxycarbonates were obtained from nickel, cobalt, and zinc nitrate solutions. The crystallite sizes of these compounds are quite large and exceed 100 nm. However, their thermal decomposition allows us to obtain oxides with crystallite sizes less than 15 nm.

The specific surface area and porosity of several of the obtained samples were also measured. It was found that the obtained oxides have a specific surface area that is significantly higher than similar samples obtained by other methods. Most of the porous volume and surface area is located in the mesopores.



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sciforum-112607: Promotion of Ni/alumina catalysts for CO₂ hydrogenation

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High levels of CO₂ emissions in the atmosphere cause global warming and an associated increase in Earth's temperature. To meet the target set by the United Nations for 2050, a new strategy must be found to reduce and reuse this CO₂¹. One promising strategy is CO₂ hydrogenation to methane using renewable hydrogen. This reaction is generally carried out with Ni/Al₂O₃ due to its low cost compared to noble metals and its natural abundance, but it has shown low catalytic performances at low temperatures and deactivation due to carbon deposition and particle sintering^{2,3}. A possible strategy to reduce these problems is the addition of lanthanides as promoters⁴. In fact, it is well known that lanthanum is a thermal stabilizer used for alumina support, and tailors acido-base properties as well. For these reasons, the aim of this work is to study the effect of preparation techniques and the lanthanide loading of Ni-based catalyst for CO₂ hydrogenation. Catalysts were prepared by co- or sequential incipient wetness impregnation, maintaining the Ni loading constant and varying the lanthanide one. Fresh and spent catalysts were characterized by BET, XRD, FE-SEM, IR, and UV-vis-NIR. The catalytic tests were carried out at atmospheric pressure and temperature range of 523–773 K in both ascending and descending mode to evaluate possible catalyst deactivation in line with our previous work [2,3]. In addition, kinetic, surface, and on-demand studies were performed on the most promising catalysts. The main finding of this work is related to the effect of catalyst preparation that strongly influences the obtained performances. All tested catalysts displayed remarkable activity in the CO₂ hydrogenation reaction, achieving high CO₂ conversion with high methane selectivity at low temperatures and approaching thermodynamic equilibrium at temperatures above 673 K. The best methane yield (92% at 623 K) was achieved in Ce-containing materials.



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sciforum-110686: Single-Step Oxidation of Methane to Methanol over Superhydrophobic Modified NiO-Ce/Al₂O₃ Catalyst

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Due to its acidity and high ionization energy and the strength of the C-H bond (439 kJmol⁻¹), there are challenges with the chemical utilization of CH₄. The low volumetric energy density of methane makes its transportation and storage difficult; this results in the flaring of methane. Instead of flaring, methane can be converted to a valuable product such as methanol, which is not only useful for transportation but can also be used as a valuable feedstock for other chemical syntheses.

In this study, we developed a gas phase reaction that involves passing CH₄, O₂ and H₂O over a superhydrophobic modified NiO-Ce/Al₂O₃ catalyst to selectively produce methanol. The catalyst was prepared by means of co-impregnation of nickel and cerium metal salts on Al₂O₃, followed by calcination at 450°C and superhydrophobic modification with perfluoro alkyl. Different reaction conditions such as hydrophobic modification, steam flow rate, time on stream and methane-to-oxygen ratio were explored to determine the optimum conditions for higher productivity. The modified catalyst has a methanol productivity of 298 μmol.g⁻¹_{Ni}.h⁻¹, while the hydrophilic unmodified NiO-Ce/Al₂O₃ has a lower productivity of 35 μmol.g⁻¹_{Ni}.h⁻¹ after a 10 hr run in a tubular fixed-bed reactor. Increasing the reaction temperature and lowering the gas flow rate while increasing the CH₄:O₂ ratio enhanced the productivity of CH₃OH.

NiO-Ce/Al₂O₃ shows good activity towards direct methane-to-methanol conversion. It is evident that hydrophobic modification improves the activity and stability of this catalyst.



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sciforum-109904: Solid-state synthesis and characterization of trirutile FeSb_2O_6

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The aim of this research is to synthesize and thoroughly characterize a ceramic material with the chemical formula FeSb_2O_6 . The iron antimony oxide, FeSb_2O_6 , crystallizes in a trirutile-type structure, classified under the tetragonal space group $P4_2/mnm$. Its crystal structure is composed of octahedral units, where FeO_6 and SbO_6 octahedra share edges in an alternating sequence of FeO_6 – SbO_6 – SbO_6 along the $[001]$ axis. Additionally, vertex-sharing octahedra are observed within the (001) planes, contributing to its distinct structural features.

FeSb_2O_6 is recognized as an n-type semiconductor. Recently, this compound has attracted significant interest due to its potential applications in photocatalysis, as well as in gas sensors, for detecting nitrogen oxides (NO_x) and hydrogen sulfide (H_2S). Furthermore, it shows promise as a dielectric material for microwave devices and is considered a viable alternative to commercial materials in lithium-ion batteries (LIBs) due to its advanced lithium storage properties and high specific capacity.

In this study, the sample was synthesized using the traditional ceramic method. Stoichiometric amounts of FeO and Sb_2O_3 were mixed and calcined at 950°C for 24 hours in an electric furnace under an air atmosphere. The synthesized material was characterized using various techniques, including powder X-ray diffraction (PXRD), scanning electron microscopy (SEM), and Fourier-transform infrared spectroscopy (FTIR).



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sciforum-111548: Synthesis of new LDH-derived composites with enhanced photo-thermal properties exploited in photo-thermocatalytic processes for CO₂ conversion

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The thermocatalytic CO₂ hydrogenation reaction is a high-energy-consuming process, and for this reason, it is important to develop new hybrid catalytic approaches, such as photo-thermocatalysis, in order to increase the efficiency of this process and overcome its main disadvantages. The aim of this research is to synthesize a set of new Layer Double Hydroxide-derived composite materials to be used as photo-thermocatalysts to perform in the CO₂ methanation reaction. LDHs are in fact an excellent candidate for the photo-thermocatalytic conversion of CO₂. This is due to their great adsorption properties, their surface basicity and the presence of optical band-gaps that can be modulated due to the possibility of interposing different metal ions within the LDH structure or on its surface. In this study, ternary LDHs were synthesized by co-precipitation and hydrothermal treatment, inserting different metal species such as Ni or Co as catalytic active species, Mg, Zn, or Zr as photocatalytic active species, and Al or Ce for the structural role. The LDHs were then modified with SiC or different phyllosilicates such as Halloysite, Bentonite, Sepiolite, and Montmorillonite to obtain new materials able to absorb a larger portion of the solar emission spectrum and to increase the conversion of solar radiation into thermal energy, favouring the methanation reaction through a photo-assisted thermocatalytic mechanism. Catalytic tests showed that SiC significantly increased the photo-thermocatalytic activity of LDHs, enhancing yield and selectivity in methane at lower temperatures compared to thermocatalytic tests, while the samples modified with phyllosilicate are currently under investigation. Future objectives of this work include exploring different compositions for the synthesis of LDH-phyllosilicates and the synthesis of LDH-MXene composites to take advantage of the LSPR effect of MXenes so as to improve the photo-driven thermocatalytic activity of the materials.



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sciforum-112360: Tailoring the structural and electronic properties of $\text{RbLaTa}_2\text{O}_7$ double-layered perovskite by the rapid molten-flux synthesis route

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The development of simple and scalable synthesis methods that yield new materials or unique morphologies [1, 2] opens up new possibilities for customizing surface and bulk properties for energy storage and conversion applications. Layered perovskite tantalates are a particularly attractive group of oxide materials, exhibiting interesting optical, piezoelectric, and/or photocatalytic properties. Herein, a rapid molten salt synthesis route was used to synthesize $\text{RbLaTa}_2\text{O}_7$ layered perovskite with improved structural and electronic properties. Different samples were prepared by using a stoichiometric ratio of $\text{Rb}:\text{La}:\text{Ta} = 1:1:2$, a 10-fold molar excess of molten RbCl at 1200°C , and various reaction times (e.g., 4 h and 7 h). The effects of the flux-to-tantalate precursor ratio, the purity of the solids, and the synthesis duration on the particle growth of $\text{RbLaTa}_2\text{O}_7$ were examined and compared with the reference sample prepared through solid state reaction (SSR). XRD patterns revealed that the solid synthesized with molten RbCl in a short reaction time (4 h) primarily formed $\text{RbLaTa}_2\text{O}_7$, with only small amounts of LaTaO_4 impurities and unreacted RbCl . Increasing the reaction time to 7 h resulted in a pure $\text{RbLaTa}_2\text{O}_7$ phase with a tetragonal structure. The solid obtained by molten RbCl during 4 h led to well-defined platelet and rod morphologies, while a longer reaction time (7h) led to larger platelets with smooth surfaces. The molten salt approach led to products with larger specific surface areas and smaller band gaps than the reference. The CO_2 -TPD profiles of molten salt-based perovskites exhibited a prominent peak in the $550 - 650^\circ\text{C}$ range, attributed to the presence of strongly basic sites. This study emphasizes the benefits of the molten salt-assisted method, which not only shortens the synthesis duration but also yields high-purity layered materials with well-controlled structural and electronic properties.



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sciforum-111161: The Impact of Copper modification on the selectivity performances of Layered Double Hydroxide-Type materials

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Usually, in the presence of base active sites, the Claisen–Schmidt condensation reaction between benzaldehyde and cyclohexanone leads to the formation of a *di*-condensed compound, e.g. 2,6-dibenzylidene cyclohexanone^[1]. The optimization of layered double hydroxide-type (LDH) catalysts by means of the partial substitution of Mg with Cu(II) cations leads to a shift in the selectivity towards the *mono*-condensed product (e.g. 2-benzylidene cyclohexanone). Six $\text{Mg}_{0.375}\text{Cu}_{0.375}\text{Al}_{0.125}$ LDH materials were prepared from metal chlorides, nitrates and sulfate as precursors by applying two methods, co-precipitation and the mechano-chemical method, while using either the usual inorganic alkalis or a non-traditionally organic one for pH adjustment. The influence of the *memory effect* on the physico-structural properties of the considered materials was also investigated by hydrating them with *bi*-distilled water of the mixed oxides that were obtained by means of the calcination of the parent LDH at 460 °C for 18 h under an air atmosphere. The characterization of solids with different techniques (e.g. XRD, DRIFT, ATR, DR-UV-Vis, BET and basicity determination using irreversible adsorption organic molecules with different pK_a values) revealed that the pure layered structure was contaminated with different amounts of copper hydroxide depending on the metal salt precursors. The memory effect did not lead to a total reintegration of the Cu(II) in the octahedral positions of the layered structure, since part of it remained as stable CuO, obtained in the calcination step. The basicity and the catalytic activities for Claisen–Schmidt condensation showed similar variation trends, e.g., reconstructed LDH > parent LDH > mixed oxides. The copper's presence in the LDH structure decreased the basicity, leading to a higher selectivity to the *mono*-condensed product than the one that was obtained with unmodified MgAl-LDH. The copper-containing catalysts also promoted the transformation of benzaldehyde into benzoic acid as a side reaction.

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sciforum-112708: The Role of Catalytic Materials in the Development of Hyaluronic Acid-Based Hydrogels via Click Chemistry: US8512752 Patent Evaluation

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Hydrogels derived from hyaluronic acid (HA) are renowned for their biocompatibility, biodegradability, and extensive biomedical applications. However, conventional crosslinking methods often lack precision, resulting in limited control over the polymer's properties. This patent evaluation analyzes US8512752, which presents an innovative approach to synthesizing crosslinked derivatives of polycarboxylated polysaccharides, primarily HA, through "click chemistry". The process leverages copper-based catalytic materials, such as CuCl and CuSO₄·5H₂O, to enable efficient, regioselective Huisgen 1,3-dipolar cycloaddition reactions. These catalysts play a critical role in enhancing reaction yields, ensuring structural uniformity and avoiding undesirable side reactions.

The resulting hydrogels are distinguished by their modifiable viscoelastic properties, making them suitable for a variety of medical applications, including viscosupplementation, controlled drug delivery, and oncologic reconstruction. Notably, the incorporation of bioactive molecules during synthesis allows for the development of advanced drug release systems with improved efficacy.

The invention through the patent demonstrates the pivotal role of catalytic materials in enabling the efficient and regioselective crosslinking of HA derivatives. Copper catalysts not only accelerate the reaction but also preserve the functional integrity of incorporated bioactive molecules. The resulting hydrogels exhibit excellent mechanical properties and extended degradation times, making them suitable for advanced biomedical applications. Future studies may explore alternative catalysts to further enhance biocompatibility and reduce costs.

This analysis-based study highlights the patent's technical innovations and its significance in advancing hydrogel technology, addressing the limitations of traditional methods and opening pathways for further development in biomedical engineering and regenerative medicine.



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sciforum-112173: Unlocking the Heterogenization of Catalytic Chlorination: Iron-Based Waste Material as an Efficient Heterogeneous Catalyst for Allylic Functionalization

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Among sustainable alternative solutions, catalysis represents a keystone in chemical processes, offering numerous benefits, including energy and time management, resource management and environmental sustainability. Heterogeneous and homogeneous catalyses are widely used as sustainable alternatives for various processes in diverse fields of the chemical industry ¹. Among these processes, catalytic chlorination represents a convenient way to synthesize allylic and vinylic chloride derivatives ². These derivatives are highly valuable organic compounds that serve as building blocks in the synthesis of more complex atomic arrangements ³. The present work focuses on the valorization of industrial iron-based waste material via catalytic chlorination. First, a characterization study of the waste material was carried out using different advanced techniques. Thereafter, the catalytic activity was investigated, for the first time, using magnetically recoverable iron-based waste material as an efficient heterogeneous catalyst in a selective catalytic allylic chlorination reaction. The optimization of the catalytic reaction was carried out with carvone in the presence of sodium dichloroisocyanurate (NaDCC) as an eco-friendly, highly stable and freely available chlorine (FAC) agent. The optimized conditions were used to study other functionalized terpenic olefins to obtain high value-added allylic chlorides in good to excellent yields.

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sciforum-115646: Valorisation of waste cooking oils through [HMIM][HSO₄] ionic liquid-catalysed biodiesel conversion

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Biodiesel consists of a mixture of fatty acid methyl esters (FAMES) and is produced by processing vegetable oils or animal fats. Oil sources, not competing with the food market, such as waste cooking oils (WCOs), can be used, and ionic liquids (ILs) are promising catalysts, since they promote esterification/transesterification reactions to biodiesel. The objective was to study biodiesel production using 1-methylimidazolium hydrogen sulphate IL ([HMIM][HSO₄]) as a catalyst in esterification/transesterification reactions with methanol, for oleic acid (OA) and simulated high acidic oils, in mixtures of 40%(w/w) OA to 60%(w/w) WCO. The IL recovery procedure was also assessed using water as solvent. Biodiesel production was carried out on two heating plates with automatic temperature control and magnetic stirring (IKA, digital C-MAG HS4 model, and VWR, VMS-C4 model). A centrifuge (SIGMA, model 2-4) was used for phase separation. Samples were dried in an oven (CIENTIFIC, series 9000) and all masses were measured on an analytical balance (accuracy: ± 0.0002 g and maximum: 210g; AE, ADA 210/C). FAME content was determined by GC (SHIMADZU, Nexis GC 2030), with FID, an AOC-20i autoinjector and an Optima BioDiesel F capillary column (30mx0.25mm). Analyses were carried out by FTIR with a Perkin Elmer equipment, Spectrum Two, and an ATR universal accessory. Reaction conditions were as follows: 65°C, 4 hr, raw-material/methanol molar ratio 1:10, and 10%(w/w) IL load. Using OA as the raw material, an acidity drop conversion of 81.2% was obtained. After seven reaction cycles, the conversion dropped to 69.4%, while the FAME content decreased from 64.7% to 57.5%. For WCO, a conversion of 45.6% was obtained and after nine reaction cycles it decreased to 27.2%, while the biodiesel FAME content decreased from 24.1% to 14.0%. The FTIR correlation between initial and final IL samples was 99.3% for OA and 90.0% for WCO, showing that the recovery method is efficient. For these operating conditions, IL only promotes esterification reactions.



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Session B. Environmental Catalysis

sciforum-115483: *Croton Macrostachyus* Bark Extract-Assisted Sustainable Synthesis of CuO Nanomaterial for 4-nitrophenol Catalytic Reduction and Antibacterial Applications

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The eco-friendly synthesis of nanomaterials has emerged in modern science to resolve the increasing concerns of environmental pollution and sustainable development. Metal-oxide NPs, including TiO₂, ZnO, and CuO, are widely studied for their potential in facilitating a sustainable environment. Due to their ease of availability, low cost, chemical stability, and nontoxicity, they are considered the best candidates for environmental pollution control and bioremediation. Among these, CuO NPs have gained considerable focus for their antibacterial and catalytic properties. The green synthesis of nanomaterials using various plant parts promotes sustainable chemistry for the sustainability of the environmental and antibacterial applications. Thus, the plant-based biosynthesis of nanoparticles are highly necessary to achieve such environmental and health sustainability. In the present study, we prepared an eco-friendly, cheap, and straightforward sol-gel synthesis method of copper-oxide nanoparticles (CuO NPs) using the aqueous bark extract of *Croton macrostachyus*. At 200 mg/mL, the uncalcined CuO NPs demonstrated the highest inhibition diameter for *Staphylococcus aureus* (*S. aureus*), with 22±1.3 mm, and for *Escherichia coli* (*E. coli*), with 11±0.7 mm. Moreover, the calcined CuO NPs presented notable catalytic performance in reducing 4-nitrophenol to 4-aminophenol in 8 minutes with a removal of 98.79%. The kinetics of the process resulted in an apparent rate constant (K_{app}) of 0.507 min⁻¹ with a pseudo-first-order reaction. Therefore, this eco-friendly synthesis method not only eliminates the use of harmful reducing substances but also offers a hands-on solution to environmental pollution and disease-resistant bacteria problems.



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sciforum-110101: Bimetallic and trimetallic catalysts for methanol steam reforming

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The large amount of interest in methanol as a pioneering hydrogen source for fuel cell applications is related to its high energy density, easy storage/transportation and environmental safeguarding compared to conventional fuels. In fact, CH₃OH production from biomass and other renewable feedstocks benefits sustainable technologies available for its conversion to hydrogen¹. Methanol and steam, at moderate temperatures and under the assistance of a catalyst, can generate H₂ and CO₂. In particular, to enhance hydrogen selectivity and reduce CO formation, the identification of highly active, selective and stable catalysts is crucial. Sintering is one of the main drawbacks of Cu-based catalysts commonly selected for methanol steam reforming, and the addition of CeO₂ is expected to improve active-phase dispersion as well as metal-support interactions².

In this work, a series of non-noble (Ni, Cu and Zn) metal-based bimetallic and trimetallic catalysts were prepared by the sequential wet impregnation of the active species on the CeO₂-Al₂O₃ support (30 wt% of ceria) and tested for methanol steam reforming (MSR). After the catalysts' reduction in situ (at 800°C; heating rate of 10°C·min⁻¹), MSR was performed under a 10%CH₃OH-15%H₂O-75%Ar stream at atmospheric pressure from 600 to 200°C; the Weight Hourly Space Velocity was fixed at 2 h⁻¹. For the non-noble metal-based catalysts, methanol was completely converted up to 300°C. Moreover, the trimetallic Zn-Ni-Cu sample showed a methanol conversion rate of around 40% at 200°C. However, at low temperatures, CO formation became stable. The lowest carbon monoxide selectivity was recorded for the 20 wt%Cu/CeO₂-Al₂O₃ catalyst.



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sciforum-112339: Bioprocessing Strategies for Sustainable Nanocellulose Production from Lignocellulosic Residues

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Growing environmental concerns have increased the focus on sustainable, biodegradable alternatives to plastic-based materials [1]. Among these, nanocellulose (NC) is valued for its renewability, biocompatibility, and functional properties, making it a promising candidate for diverse applications. NC is classified into cellulose nanocrystals (CNCs), cellulose nanofibrils (CNFs), and bacterial nanocellulose (BNC), each derived through distinct processes [2]. Plant-based nanocellulose (CNCs and CNFs) is typically produced through the depolymerization of lignocellulosic biomass to remove hemicellulose and amorphous cellulose fractions, retaining nanoscale crystalline cellulose. This is achieved enzymatically, chemically, or mechanically [2]. In contrast, BNC is synthesized via a polymerization-based process, where bacteria convert sugars into cellulose [3].

Inspired by these pathways, we developed a dual bioprocess that integrates both approaches using lignocellulosic biomass to valorize the streams. Agricultural and forest residual feedstocks were subjected to a mild OxiOrganosolv pretreatment process [4], producing a cellulose-rich solid fraction and a hemicellulose-rich aqueous liquor. Both streams underwent enzymatic hydrolysis and saccharification, with sugar release quantified using spectrophotometry and other methods. The fermentable sugars were then used as a carbon source for the microbial production of BNC by *Komagataeibacter* sp., and the resulting nanocellulose was characterized to confirm its properties. Optimizing the process with various biomass sources, enzymatic treatments, and bacterial strains directed the system toward enhanced saccharification (maximizing sugar release for BNC synthesis) or higher cellulose integrity retention (enhancing CNF yield) [5]. Different enzyme combinations were tested to balance these outcomes, and various carbon sources were evaluated for their effectiveness in supporting bacterial strains to optimize nanocellulose production yield. This integrated process offers a sustainable, scalable approach to NC production, maximizing output with minimal input.



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sciforum-113290: Catalytic Applications of Terpenes and Resinous Compounds from Forest Trees: Advancing Green Chemistry and Pollution Mitigation

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The utilization of terpenes and resinous compounds derived from forest ecosystems presents a sustainable approach to developing catalytic materials for organic synthesis and environmental remediation. Terpenes, such as limonene and α -pinene, undergo various transformations—including oxidation, epoxidation, and isomerization—using heterogeneous catalysts like zeolites and acid resins. These processes facilitate the production of pharmaceuticals, fragrances, and biofuels, thereby enhancing both sustainability and economic viability. In the realm of environmental remediation, catalytic technologies play a pivotal role in converting pollutants into non-toxic substances. For instance, the epoxidation of terpenes has been explored for generating bio-based polymers, which can be utilized in applications like wastewater treatment and bioplastic production. Additionally, the conversion of terpenes to biofuels addresses environmental concerns by providing renewable energy sources and reducing greenhouse gas emissions, particularly in the aviation sector (Lapuert et al., 2023). Despite these advancements, challenges persist in optimizing the efficiency of catalysts and reducing associated costs. Recent studies have focused on developing both catalytic and non-catalytic processes for terpene epoxidation, employing various oxidizing agents and process intensification techniques. These efforts aim to improve the reaction selectivity, rates, and scalability, contributing to the commercial feasibility of terpene-derived products (Resul et al., 2023). This study delves into the catalytic capabilities of specific terpene compounds, emphasizing their effectiveness in pollutant removal and their roles in green chemical transformations. By examining their physicochemical properties and catalytic processes, the research underscores the potential of these compounds as environmentally benign alternatives to conventional catalysts. The findings highlight the significance of terpenes and resinous substances in advancing sustainable practices across various sectors, including pharmaceutical synthesis, wastewater treatment, and bioplastic production. In conclusion, harnessing terpenes and resinous compounds from forest ecosystems offers a promising pathway toward sustainable catalytic applications. Continuous research and innovation are crucial for optimizing processes and maximizing natural compounds' environmental and economic benefits.



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sciforum-112103: Catalytic conversion of biogas in a biorefinery context: perspectives and challenges

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The current energy scenario is changing and challenging, with a current trend focused on the search for alternative energy sources to reduce energy dependence due to different factors such as geopolitical aspects, among others. In this sense, apart from the obvious environmental advantages compared to refineries based on oil, biorefineries based on different wastes (with a difficult management approach) could be an interesting starting point to foster sustainable economic growth of different areas around the world. For instance, biogas is a promising energy source with endless opportunities, depending on its final use. In this sense, a gas with a relatively homogeneous gas composition can be obtained from variable wastes (agro-industrial, wastewater, manure, etc.), with a wide range of technologies related to energy production (upgrading, steam reforming, Fischer--Tropsch synthesis, etc.). However, high efficiency for these biorefineries is required in order to compete with traditional refineries. In this context, the role of catalysts is essential, which can have an influence on biorefinery processes (and, equally, these processes can influence their catalytic performance). Considering the above, the aim of this work was to assess, according to our own experience and resorting to the literature, different aspects related to catalytic conversion of biogas through different technologies (mainly steam reforming and Fischer--Tropsch synthesis). As a result, several recommendations like the use of high-quality biogas and purification technologies are offered in order to improve the efficiency of these processes.



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sciforum-112800: Chitosan/Carboxymethylcellulose/Vanillin@Graphene oxide nanocomposites for the removal of ketoprofen and naproxen from wastewater

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Introduction:

The COVID-19 pandemic has resulted in the increased use of non-steroidal anti-inflammatory drugs (NSAIDs), leading to their accumulation in wastewater, posing risks to human health and the balance of the ecosystem. Therefore, between 2019 and 2021, NSAIDs were detected in water sources at concentrations ranging from a few ng/L to hundreds of µg/L. The most commonly found drugs are diclofenac, ibuprofen, naproxen, acetaminophen, and ketoprofen. Though there are several techniques to reduce the emissions of environmentally unacceptable compounds from wastewater, such as Advanced Oxidation Processes (AOPs), adsorption, chemical precipitation, coagulation/flocculation, and flotation, adsorption is emerging as a simple, sustainable, cost-effective, and eco-friendly method for pharmaceutical contaminant removal.

Methods:

In this study, two nanocomposites, i.e., CS/CMC/VAN and the further modified CS/CMC/VAN@GO, were synthesized to remove ketoprofen and naproxen from aquatic solutions. Chitosan, a natural cationic polymer, is combined with vanillin via a Schiff base formation and offers effective and low-toxicity adsorption properties. Moreover, modified chitosan exhibits improved adsorption capacity when combined with carboxymethyl cellulose (CMC) and graphene oxide (GO), which are both known for their low toxicity and biocompatibility. In addition, graphene oxide is widely utilized in water treatment due to its high surface area, mechanical strength, and compatibility with various functional groups.

Results:

All the materials were characterized via FTIR and SEM techniques. Adsorption experimental results showed that the data fit better to the PSO model and the Langmuir isotherm model, providing adsorption capacities equal to 51.29 mg/g for ketoprofen and 46.30 mg/g for naproxen, with the optimum CS/CMC/VAN@GO at pH 5.

Conclusion:

This research contributes valuable knowledge to the field of water and wastewater treatment, providing a viable solution for controlling pharmaceuticals' environmental pollution.



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sciforum-112605: Development of a Solid Phase Extraction Method for Cadmium and Nickel Using Stearic Acid Modified Activated Carbon

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Heavy metals are essential raw materials for the manufacture of industrial products, but they are one of the causes of environmental pollution and are harmful to human health. Due to their toxicity, the presence of heavy metals in water and food is strictly regulated. Graphite furnace atomic absorption spectrophotometry (GFAAS) is a widely used technique for heavy metal analysis because of the small sample volume required and a simple operating procedure involved. However, sensitivity at trace concentrations of analyte in the matrix is limited by physical and chemical interferences. Overcoming this limitation requires the preconcentration and separation of analytes.

In this study, a solid-phase extraction (SPE) method using activated carbon modified with stearic acid (SA-CAA) as an adsorbent was developed to preconcentrate cadmium and nickel ions in water samples. Different characterization methods were employed to confirm the structural and surface modifications of the studied adsorbent. The results show that the stearic acid modification of activated carbon enhanced the interaction between the adsorbent and heavy metal ions, leading to an approximately twofold increase in recovery compared to unmodified activated carbon. The analytical parameters affecting recovery, including the adsorption time, amount of adsorbent, initial pH of the sample solution, desorbent conditions, and sample volume, were optimized. The analytical performance of the proposed method, such as the calibration curve, analytical precision, detection limit, and tolerance to interfering components, was evaluated.



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sciforum-112638: Enhancing activity of HAP catalyst by hydrothermal in situ Zn incorporation for transformation of CO₂ to produce cyclic urea from diamine

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The utilization of CO₂ for the synthesis of value-added chemicals can help to reduce its concentration in the atmosphere [1]. The synthesis of 2-imidazolidinone using a nontoxic CO₂ as carbonyl source has drawn greater attention as CO₂ is abundant, which can be used as C1 feedstock for chemical synthesis [2]. In this study, a ZnO-supported hydroxyapatite (HAP) catalyst was designed based on the active sites required for this reaction. The Zn-HAP catalyst was synthesized by the one-step hydrothermal method. This supported catalyst showed better activity than support HAP and unsupported ZnO. Higher yield could be achieved by tuning the acid-base sites by varying the ZnO loading and calcination temperature. The catalyst was characterized using different techniques such as XRD, N₂-sorption, SEM-EDS, TEM, XPS, CO₂ and NH₃-TPD to understand its structural and textural properties. It was found that the acidic and basic properties of the catalysts played vital roles in achieving better catalytic activity. The XPS analysis showed a decrease in the intensity of Ca 2p peaks of Zn-HAP as compared with HAP, indicating the replacement of Ca²⁺ by Zn²⁺ in the structure which results in generation of new active sites, leading to an enhanced catalytic activity. Design of experiment (DOE) was employed using response surface methodology (Central Composite Design) to optimize reaction conditions. The optimized catalyst was shown to be stable and reusable by achieving 81% of conversion for ethylene diamine and 97% selectivity for 2-imidazolidinone under moderate pressure and temperature in 10 hours. The catalyst also showed good versatility by giving good yield for the reaction between different types of amines and CO₂. The activity of the catalyst correlated well with its physicochemical properties.



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sciforum-115720: Fabrication of efficient and easily recyclable silver nanoparticle–anionic polymer hydrogel composite catalyst for rapid degradation of water pollutants

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In this study, a porous three-dimensional polymeric network of poly(3-sulfopropyl methacrylate) [p(SPMA)] is prepared and embedded with silver nanoparticles (Ag NPs) to design a nanocomposite catalyst. Analytical techniques including X-Ray Diffraction (XRD), Fourier-transform infrared spectroscopy (FT-IR), scanning electron microscopy coupled with energy-dispersive X-ray analysis (SEM-EDX), Rheology, and UV-visible spectroscopy are used to investigate the composition and morphology of the prepared nanocomposite catalyst. The fabricated p(SPMA) hydrogel exhibits a hydrophilic character, with a % swelling of 1974 in an aqueous medium. The porosity of the nanocomposite catalyst is corroborated using SEM, while the skeleton of p(SPMA) and the embedding of the AgNPs are affirmed using EDX. The catalytic performance of the synthesized nanocomposite catalyst is analyzed in the chemical reduction of two different dyes, methylene blue (MB) and methyl orange (MO), and two different nitroaromatic compounds, 4-nitrophenol (4-NP) and 4-nitroaniline (4-NA). The apparent rate constant (k_{app}) of the catalyst is found to be 0.365×10^{-2} , 1.059×10^{-2} , 0.159×10^{-2} , and $0.581 \times 10^{-2} \text{ sec}^{-1}$ for 4-NA, 4-NP, MO, and MB, respectively. The synthesized nanocomposite catalyst is recycled ten times in succession through the simple, quick, and effortless process of filtration via a plankton cloth filter, and it is found that the catalyst retains 70% of its activity in the tenth cycle.



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sciforum-108541: Facile synthesis of Aluminum-doped Bi₂WO₆ and enhanced remediation of aqueous Methylene Blue and Rhodamine B

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Pristine Bi₂WO₆ and different concentrations of aluminum-doped Bi₂WO₆ nanoparticles were synthesized using a simple hydrothermal method for a comparative study of the decolorization of aqueous organic pollutants. The synthesized nanoparticles were characterized using X-ray diffraction (XRD), UV-visible spectroscopy (UV-vis), Fourier transform infrared spectroscopy (FT-IR), Raman spectroscopy, Brunauer–Emmett–Teller (BET), Zeta potential, field-emission scanning electron microscopy (FE-SEM), selected area electron diffraction (SAED), high-resolution transmission electron microscopy (HR-TEM), and energy-dispersive X-ray spectroscopy (EDS). The XRD pattern revealed the formation of an orthorhombic structure for pure and Al-doped Bi₂WO₆. Aluminum doping decreased the crystallite size. The formation of 3D flower-like nanostructures that were composed of 2D nanosheets was observed through FE-SEM. The band gap increased because of the doping aluminum, which revealed the blue shift of the band gap. We performed both photocatalytic and adsorption experiments for 20 ppm aqueous Methylene Blue (MB) and Rhodamine B (RhB) for all synthesized catalysts. The aluminum-doped Bi₂WO₆ catalysts showed enhanced decolorizing efficiency, and 0.15Al-Bi₂WO₆ exhibited the best performance for adsorption. The results were analyzed using various models such as second-order kinetics, the BMG model, and the intraparticle Weber and Morris diffusion model. We found that 97.02% and 95.61% of MB and RhB dye solutions decolorized in 20 and 30 min using 0.15Al-Bi₂WO₆, with second-order rate constants of 0.566 Lmg⁻¹min⁻¹ and 0.225 Lmg⁻¹min⁻¹, respectively.



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sciforum-113753: GAS-PHASE SELECTIVE OXIDATION OF SOME PYRIDINE DERIVATIVES WITH A “GREEN OXIDIZER”—N₂O IN THE COHERENT SYNCHRONIZATION MODE

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Introduction

One of the practical applications of the principle of coherently synchronized oxidation could be the transformation of natural compounds for preparative purposes, and possibly on a larger scale. However, in order to move on to more complex nitrogen-containing heterocyclic compounds, similar in chemical structure to natural ones, it is necessary to study the corresponding reactions involving their individual fragments.

Methods

Oxidation reactions of nitrogen-containing heterocyclic compounds in the presence of N₂O were carried out in the gas phase, without the use of catalysts, at atmospheric pressure. Quantitative and qualitative determination of the resulting reaction products was carried out using “Agilent Technologies 7820A” gas chromatography–mass spectroscopy.

Results

The dehydrogenation reaction of piperidine was studied. As a result of our research (T = 200–400°C), optimal conditions for the dehydrogenation of piperidine were identified, under which a yield of 2,3,4,5-tetrahydropyridine (19.4 wt%) was achieved with a selectivity of at least 98%.

The oxidation of pyridine with N₂O was carried out in a wide range of varying process parameters: feed rate of pyridine and N₂O (T = 550–610°C). Under optimal conditions, the following were obtained: 2,2-dipyridyl with a yield of 23.0 wt.%, and 2,3-dipyridyl with a yield of 18.0 wt.%, selectivity not lower than 95 wt.%.

For the first time, 2,2-ethylenedipyridine was obtained by the oxidation of 2-picoline with N₂O. It has been experimentally shown that the yield of 2,2-ethylenedipyridine and 2,2-methylenedipyridine is 30.3 wt.% and 1.5 wt.%, respectively, where the selectivity is not lower than 96 wt.%.



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sciforum-112729: Green hydrogen production from catalytic ammonia decomposition

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Hydrogen is considered an efficient alternative fuel. Most of the hydrogen produced on a large scale mainly comes from the steam reforming of natural gas, which is considered the most established and least expensive method. Although water electrolysis is also a well-established technique used to produce hydrogen, it causes high energy losses. The generation, storage, and transportation of hydrogen as an alternative fuel have been extensively studied during the last few decades. Given the challenges in generating and storing hydrogen for portable applications, ammonia has been proposed as an alternative for on-site hydrogen production through its decomposition. In this study, the catalytic decomposition of ammonia was conducted to produce CO₂-free hydrogen. Ru-based catalysts have been recognized as efficient catalysts for ammonia decomposition under mild reaction conditions. For Ru-based catalysts, the supports were found to play a profound role in the ammonia decomposition process. CeO₂ is an efficient support for ammonia decomposition, but as it is expensive, CeO₂ cannot be used for large-scale industrial applications. Therefore, Ru-based catalysts were prepared using CeO₂-impregnated Al₂O₃ supports. CeO₂-impregnated Al₂O₃ supports were prepared in various Ce/Al molar ratios. The catalysts prepared from CeO₂-impregnated Al₂O₃ supports with molar ratios of 0.5 and 1.0 showed a comparative efficiency to those prepared from a pure CeO₂ support. The presence of less expensive Al₂O₃ in bulk while achieving comparable efficiency to that of a pure CeO₂-supported Ru catalyst resulted in cost-effective and efficient catalysts for ammonia decomposition.



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sciforum-114635: Heat-shedding TiO₂/VAE Nanocoating Formulation for Advanced self-cleaning and Coolant Fabrics

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High-temperature environments pose significant risks to human health and safety. That is why, these days, textile industries pay great attention to produce multifunctional fabrics. However, reports reveal that these fabrics are prepared with silane derivates, along with gold or silver, which makes them expensive with poor self-cleaning properties. Likely, organic--inorganic nanocomposites represent a new class of materials imparted due to their novel properties and low cost. Herein, we reported a commercially affordable SiO₂/TiO₂@Vinylacetate-ethylene (VAE) formulation for functionalizing fabric. The TiO₂-VAE hybrids were prepared by a ball milling-assisted sol--gel technique and imparted onto the bare fabrics via dip-coating. By taking a different amount of the polymer, the structural property and performance of the composite are optimized and characterized. XRD revealed the incorporation of rutile-TiO₂ on the fabric which has a cellulose I structure. In addition, ATR-FTIR confirmed the covalent interactions between the nano-SiO₂/TiO₂ and cellulose of the cloth without any chemical deterioration of the functional groups. In addition, SEM revealed that, unlike the bare cloth, it was composed of a plain surface with a woven network of cellulose fibrils with a thickness of 40 to 50µm, and TiO₂/VAE encompassed multi-thin layers where TiO₂ nanoparticles are immobilized on the surface of the functionalized cotton fibers. EDAX confirmed the presence of carbon, oxygen, titanium, and silicon, which are homogeneously distributed over the cloth surface. Interestingly, the hybrid coated fabric demonstrated a superior reflectance, at 91%, to the bare fabric, which recorded the least NIR reflectance at 73%. Furthermore, the imparted fabric displayed an excellent catalytic self-cleaning ability by the complete removal of methylene blue within 3 hours of sunlight illumination. Incorporating photocatalyst TiO₂ nanoparticles not only enhances UV shielding, but also offers a new self-cleaning character by absorbing sunlight. Thus, in fabric surface engineering, such a simple nanoformulation preparation technique paves the way for practical mitigation of global warming.



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sciforum-112062: Hydrogen from Methane: new ground with Chemical Looping Technology

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Methane decomposition through chemical looping reforming (CLR) is emerging as a promising and innovative approach for hydrogen production. This method efficiently transforms various feedstocks into high-purity hydrogen while drastically reducing greenhouse gas emissions. Hydrogen generated through CLR represents an environmentally friendly option, free from direct emissions of air pollutants or greenhouse gases. Additionally, it supports the use of a diverse range of low-carbon energy sources, contributing to its sustainability and versatility. In particular, supported nickel-based catalysts show promising features due to their strong catalytic activity and stability in reforming processes. The present study focuses on the performance of Ni and Ru-Ni catalysts supported on LaMnO₃, synthesized through precipitation assisted by microwave irradiation and sol-gel citrate methods. The redox stability was checked by performing multiple redox cycles during chemical looping experiments carried out isothermally, alternating the gas composition every 10 minutes from 15 vol% of CH₄ in N₂ (reduction) to 15 vol% of CO₂ in N₂ (oxidation). The CLR temperature was selected for each sample based on temperature-programmed reduction tests with methane, choosing for each one the temperature of maximum reduction. Through a comprehensive examination encompassing structural, morphological, and catalytic analyses, it was possible to study the impact of synthesis techniques on the performance of these catalysts in hydrogen production via chemical looping decomposition. These research efforts furnish valuable insights pivotal for the development of efficient and sustainable processes and crucial for meeting the escalating demand for clean energy solutions in the contemporary era.



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sciforum-115595: Impact of Periodic Rich/Lean Switching and Metal Zone-Coating on Three-Way Catalyst Performance

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The Three-Way Catalyst (TWC) plays a vital role in reducing engine exhaust gas emissions. However, steady-state exposure to exhaust gases can lead to catalyst deactivation via noble metal oxidation or active site poisoning. The periodic switching between rich and lean conditions has been shown to counteract deactivation, particularly enhancing methane oxidation.

This study explores the effect of periodic rich/lean switching ($\lambda = 1 \pm 0.02$ at 0.5 Hz) on pollutant conversion in a realistic car exhaust gas matrix containing NO, CO, H₂, and hydrocarbons (C1-C5) at 100–400 °C. Cordierite-based monoliths were prepared with alumina–ceria–zirconia washcoat layers loaded with Pd, Pt, and Rh. Two catalysts with identical total Pd contents were compared: one homogeneously coated and another zone-coated with Pd on one-third of the catalyst. Gas composition at the outlet was analyzed using infrared spectroscopy and μ -gas chromatography.

The results show that periodic switching enhanced the conversion of NO, CH₄, and C₅H₁₂ compared to steady-state regimes, attributed to the alternating active site poisoning and regeneration during the rich and lean phases. The zone-coated catalyst exhibited superior performance, likely due to its higher local Pd content, smaller particle size promoting effective Pd-support interactions, enhanced oxygen storage capacity (OSC), and exothermic effects during operation.

This work highlights the potential of periodic switching and zone-coating strategies to optimize catalyst performance while conserving scarce platinum group metals, offering insights into next-generation emission control technologies. Insights from this study have broader implications for catalysis, including gas-to-energy conversion applications.

[reference] Elgayyar, T. *et al.* Promotional Effect of the Periodic Rich and Lean Switching on the Performance of Three-Way Catalysts and Influence of Metal Zone-Coating. *Top Catal* (2024) doi:10.1007/s11244-024-02019-2



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sciforum-112604: Improved activation of peroxymonosulfate with NaBH₄-treated transition bi-metal oxide catalysts for Reactive Yellow 86 decolorization

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Dyes are persistent and toxic pollutants that significantly contribute to water pollution, particularly from the textile and dye industries. Advanced oxidation processes (AOPs) have attracted considerable interest as they are believed to be effective in removing persistent and toxic organic pollutants from water by generating reactive oxygen species. In addition, NaBH₄ treatment is believed to enhance catalyst reactivity by generating abundant oxygen vacancies. This study explored the activation of peroxymonosulfate (PMS) and the decolorization of Reactive Yellow 86 using MnCo₂O₄ catalysts treated with NaBH₄.

The MnCo₂O₄ (MCO) catalyst was synthesized by hydrothermal and calcination methods followed by NaBH₄ treatment, yielding the modified catalyst MCO-1.25. The catalytic performance of MCO and MCO-1.25 was compared in decolorizing Reactive Yellow 86 in the presence of PMS. Specifically, 1 mg of catalyst was added to a vessel containing 10 mL of 50 mg/L Reactive Yellow 86 and 10 mL buffer solution and stirred for 30 min. After adsorption equilibrium was reached, 0.48 mM PMS solution was added to initiate the decolorization reaction. The solution was aliquoted at regular intervals, and the reaction was quenched by the addition of methanol. After centrifugation, the supernatant was measured in a spectrophotometer and the decolorization rate was determined from the measured absorbance.

With MCO, approximately 90% of Reactive Yellow 86 was decolorized after 30 min. In contrast, with MCO-1.25, approximately 100% was decolorized after 20 min. The enhanced performance of MCO-1.25 was attributed to the increased oxygen vacancies induced by the NaBH₄ treatment, resulting in improved PMS activation. These modifications improved the generation and utilization of reactive oxygen species, leading to faster and more efficient decolorization.



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sciforum-109494: Optimized Catalytic Oxidation of Phenol Using Iron-Impregnated Illite Clay: Environmental Impact and Efficient Wastewater Treatment.

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This study explores the catalytic oxidation of phenol using an iron-supported natural illite clay catalyst, focusing on optimizing operational parameters to enhance degradation efficiency while minimizing environmental impact. The effects of pH, temperature, catalyst dosage, initial phenol concentration, and H_2O_2 concentration were systematically examined. Optimal conditions were found at pH 3 and 50°C , which promoted hydroxyl radical formation and improved reaction kinetics. Under these conditions, the catalyst achieved a 99% phenol degradation rate and an 83% reduction in chemical oxygen demand (COD), with no detectable metal leaching, ensuring catalyst stability. The catalyst's characterization was performed using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), BET surface area analysis, and laser granulometry, confirming its structural integrity and stability. Additionally, the H_2O_2 concentration was optimized at 8.7 mM to enhance the oxidation process while minimizing reagent excess. An analysis of intermediate by-products revealed stepwise degradation, highlighting efficient oxidation pathways. Environmental impact assessments demonstrated that the catalyst, with its low metal leaching and high stability, had minimal toxicity to aquatic life, particularly fish, confirming its safe use in wastewater treatment applications. This study underscores the potential of iron-impregnated natural clays as stable, non-leaching, cost-effective catalysts for the treatment of phenolic pollutants, with reduced environmental risks.



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sciforum-112347: Oxidative denitrogenation of quinoline using cobalt ferrite catalysts

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The presence of nitrogenated compounds in fossil fuels leads to NO_x formation during combustion; these are harmful pollutants that pose significant environmental and health challenges. Hydrotreatment, the conventional strategy for denitrogenation, requires severe conditions, which motivates the search for more environmentally friendly alternatives. Oxidative denitrogenation (ODN) requires milder operating conditions and explores the oxidative reactivity of nitrogen compounds. In this study, cobalt ferrite (CoFe₂O₄) catalysts were synthesized and coated with silica (SiO₂) or carbon (C), and applied for the ODN of quinoline, common in fuels, using hydrogen peroxide as the oxidant.

The superparamagnetic CoFe₂O₄(core) was synthesized using the sol-gel method and, using an adaptation of the Stöber method, further coated with SiO₂ or C (shell). Characterization techniques, such as XRD, FTIR, and contact angle measurements, confirmed the core-shell structure of the developed catalyst and showed a remarkable change in the ferrite's hydrophobic surface properties upon coating (a decrease from 130° to 40° with silica). Crystallite sizes in the range of 19-20 nm were obtained.

Quinoline adsorption tests showed the low adsorption capacity of the materials, in accordance with the low surface area and pore volume determined by N₂ adsorption isotherms at 77 K (S_{BET} = 9-10 m² g⁻¹). In oxidation reactions, CoFe₂O₄@SiO₂ showed the best catalytic performance (X_{QN} = 74%, 8 h), likely ascribed to its hydrophilic surface, favorable to the generation of oxygen reactive species through the decomposition of H₂O₂ and consequent higher quinoline removal. Quinoline degradation was verified by GC-MS, which indicated the opening of the pyridine ring.

The results highlight that cobalt ferrite-based catalysts employed in oxidative denitrogenation are capable of degrading and mineralizing quinoline under mild conditions, as confirmed by TOC analyses. The surface properties of the coatings significantly increased the catalytic efficiency, emphasizing their potential as environmentally friendly and efficient candidates for the removal of nitrogen compounds from fossil fuels.



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sciforum-112067: Photothermocatalytic valorization of CO₂ using natural and artificial modified phyllosilicates

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Currently, owing to the valorization of carbon dioxide through CCU (carbon capture and utilization) processes, it is possible to mitigate the impact of greenhouse gases and decrease the use of fossil fuels by reducing the amount of CO₂ through the use of solar fuels. In this work, the valorisation of CO₂ into CO and CH₄ was investigated using a hybrid catalytic approach as the photothermocatalysis and unconventional photocatalysts, i.e., modified commercial phyllosilicates, which was achieved using the montmorillonite K30. The modification of K30 with Ni and Ce was carried out using the hydrothermal method. The coatings with Mn and Cu oxides were created by means of the precipitation method. The catalytic tests were conducted in a cylindrical batch reactor at 120°C using a solar lamp for 5h of irradiation. The analysis of the reaction products was performed with GC-TCD/FID, and the samples were characterized by means of SEM, FT-IR, UV-DRS, Raman, CO₂-TPD, and N₂- physisorption. The best performance was obtained by K30-Ni/Ce@MnCuO_x, with 76.7% of the CO₂ being converted and 13.9 and 4.9 mmol/gcat•h CO and CH₄, respectively. With this latter sample, we also conducted stability tests using a treatment in a H₂ flow for the reactivation of the sample. The coating using noncritical mixed metal oxides improved the performance of the bare K30 and K30 that was modified with Ni and Ce. The photothermocatalysis also represents a greener strategy for mitigating the impact of CO₂. The performance of this catalyst was also compared to “artificial clays”, such as MXenes. These compounds were modified with the addition of CeO₂, TiO₂, and SiO₂ to further improve their photothermocatalytic activity due to their photothermal properties.

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sciforum-112719: Synthesis and Photocatalytic Degradation of Tetracycline Using $\text{Ce}_x\text{-Mn-Ti}_\gamma\text{@Illite}$ Catalyst

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Introduction:

The contamination of water bodies by pharmaceutical pollutants, such as tetracycline, poses a significant environmental threat. Traditional water treatment methods often fall short in effectively removing these pollutants. This study investigates the synthesis of a novel $\text{Ce}_x\text{-Mn-Ti}_\gamma\text{@illite}$ catalyst, designed for the efficient photocatalytic degradation of tetracycline in aqueous solutions.

Methods:

The catalyst was synthesized by impregnating illite, a natural clay, with varying concentrations of cerium (Ce), manganese (Mn), and titanium (Ti) ions. The synthesis process was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy (EDX) to confirm the structural properties of the catalyst. Photocatalytic degradation experiments were carried out under UV light irradiation to evaluate the efficiency of tetracycline removal, with reaction parameters such as pH, catalyst dosage, and irradiation time varied to optimize performance.

Results:

The $\text{Ce}_x\text{-Mn-Ti}_\gamma\text{@illite}$ catalyst showed significant photocatalytic activity, achieving a high degradation rate of tetracycline under optimal conditions. The catalyst demonstrated excellent stability and reusability over multiple cycles, maintaining its efficiency in pollutant removal. The reaction kinetics were analyzed, revealing that the degradation followed pseudo-first-order kinetics. The catalyst's efficiency was further enhanced by the synergistic effect of the metal dopants, which facilitated charge separation and improved photocatalytic performance.

Conclusions:

The $\text{Ce}_x\text{-Mn-Ti}_\gamma\text{@illite}$ catalyst represents an effective and sustainable material for the removal of tetracycline from aqueous solutions. This study highlights the potential of clay-based catalysts in photocatalytic applications for environmental remediation. The results contribute to the development of cost-effective and eco-friendly materials for water treatment technologies, particularly for pharmaceutical pollutant degradation.



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sciforum-112698: The recycling of polyethylene by means of catalytic pyrolysis: The Effect of contaminants on the products from the catalytic pyrolysis of polyethylene

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This thesis investigates the catalytic pyrolysis of low-density polyethylene (LDPE) that has been contaminated with limonene, a terpene that is commonly found in orange juice and used as a model contaminant. The selection of limonene is based on its high prevalence in natural products and its strong affinity for polyethylene, as evidenced by several studies. The research aims to evaluate the influence of limonene on the thermal and catalytic degradation of LDPE and to explore how its presence alters the pyrolysis process. Additionally, the effect of ZSM-5 zeolite, a widely used catalyst that is known for enhancing LDPE conversion into valuable hydrocarbons, is assessed.

In this study, low-density polyethylene (LDPE, DOW 310E) and d-limonene (Alfa Aesar) were used to examine the limonene sorption by LDPE. For each experiment, 3 g of LDPE pellets was divided into three aluminum supports (1 g per support) and placed in an airtight desiccator containing 12 mL of limonene in a beaker. The setup was incubated at 40°C, and sorption was monitored by weighing the LDPE after 12 days to determine the absorbed limonene, which ranged between 150 and 160 mg per gram of LDPE. Pyrolysis experiments were conducted at 450°C with a nitrogen flow rate of 200 mL/min.

The results show that limonene influences the distribution of the pyrolysis phases (gas, liquid, and solid), with the liquid fraction being analyzed via Gas Chromatography–Mass Spectrometry (GC-MS). The chemical transformations of the pure and absorbed limonene were also characterized using Fourier Transform Infrared Spectroscopy (FTIR). These findings provide insights into the role of contaminants such as limonene in shaping the efficiency and product distribution of catalytic pyrolysis, contributing to a better understanding of how to valorize contaminated polyethylene waste.



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sciforum-115774: Tuning Perovskite Catalysts for Dry Reforming of Methane via Strontium Doping

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Dry reforming of methane (DRM) is a promising approach for syngas production, utilizing CO₂ as a reactant to mitigate greenhouse gas emissions and enhance sustainability. Despite its potential, DRM faces significant challenges, including the high temperatures required and catalyst deactivation due to coking and sintering. Perovskite-based catalysts, particularly those doped with transition metals and alkaline earth elements, have emerged as effective solutions due to their structural stability, tunable electronic properties, and ability to disperse active metals uniformly. In this study, the catalytic performance of La_ySr_{1-y}Ni_{0.5}Mg_{0.5}O₃ perovskites with varying Sr substitution levels (y = 0.2, 0.4, 0.5, 0.6, 0.8) was investigated for DRM. The catalysts were synthesized via solution combustion synthesis (SCS) and characterized by their ability to enhance CO₂ and CH₄ conversions. The results demonstrated that Sr substitution significantly influenced catalyst performance by altering structural properties, oxygen mobility, and basicity. Catalysts with higher Sr content exhibited improved CO₂ adsorption and activation at lower temperatures, while La-rich samples showed enhanced stability and activity at elevated temperatures. Notably, the y = 0.8 sample achieved the highest CO₂ and CH₄ conversions (80% and 70%, respectively) at 750 °C. These findings underline the synergistic roles of Sr and La in optimizing the catalytic behavior for DRM, providing insights into the design of efficient and stable catalysts. By advancing our understanding of perovskite modifications, this work contributes to the development of sustainable technologies for CO₂ utilization and greenhouse gas reduction.



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sciforum-112573: Utilizing Highly Reactive Lewis Pairs Generated by Enabling Oxygen Vacancies in Cu-Mo Oxide Catalyst for Cycloaddition of CO₂ to 1,2-Propanediol

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This work describes the generation of highly reactive Lewis pair sites on CuMo-oxides for CO₂ activation and utilization over the cyclization reaction to produce propylene carbonate from 1,2-propanediol. The CuMo-oxides were synthesized by enabling the oxygen vacancies that enhance the catalytically active sites, resulting in the formation of metastable cations (Mo⁵⁺ and Cu⁺) and oxygen vacancies. Under ethanol-PEG-400 medium, the pure phase of Cu₃Mo₂O₉ obtained at 500 °C exposed maximum defects without any secondary phase compared to the other screened catalysts. The experimental and theoretical investigations provided evidence for determining and correlating the characteristics of active sites with catalytic performance. The catalysts were extensively characterized along with DFT studies, which revealed the presence of defect centers as one of the key factors in the enhanced activity. From the chemical bonding analysis, i.e., the Crystal Orbital Hamiltonian Population (COHP) and Electron Localization Function (ELF), the CO₂ molecule is known to form a strong chemisorption interaction with the catalyst surface that is facilitated by the oxygen vacancy/Lewis pairs. The Cu-Mo oxide catalyst exhibited a better performance under optimal reaction conditions with a 1,2-propanediol conversion of 99% and propylene carbonate yield of 97% compared to the reported catalysts due to its inherent physicochemical properties. Thus, Cu-Mo oxides were shown to be highly efficient catalysts with good recyclability for the 1,2-propanediol and CO₂ reaction.



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Session C. Photocatalysis

sciforum-112682: Chemo-green synthesis of ZnO nanoparticles via sol--gel method and its application for photocatalytic degradation of toxic malachite green dyes

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Background:

Acacia arabica tree is a moderate-sized, short-trunked, and almost evergreen tree mostly found in drier areas. The aqueous stem bark extract of this plant contains phenolic, condensed tannin which acts as a reducing and capping agent in green synthesized ZnO NPs, making it the least toxic semiconductor photocatalyst for the treatments of wastewater containing dye effluents, with moderate bandgap energy.

Methodology:

At the initial stage, a 40 mL aqueous leaf extract of *Acacia arabica* was combined with 460 mL of 4.36M $(\text{CH}_3\text{COO})_2\text{Zn} \cdot 2\text{H}_2\text{O}$ and heated at 60°C while stirring, after which the obtained precipitate was filtered. Next, 30 mL of NH_4OH solution was added dropwise to 500 mL of the filtrate obtained from the initial reaction stage with constant stirring for 20 minutes at room temperature, and then stirred at 60°C for 4 h. The resulting chemo-green ZnO NPs were filtered and washed with ethyl alcohol, followed by calcination at 450°C for 2.5 h, then again washed with ethyl alcohol and dried in an oven at 100°C. XRD, zeta potential, and FTIR and DRS, measurements were carried out to examine the crystallinity, surface charge, and optical properties of chemo-green synthesized ZnO NPs. For photocatalytic testing, a 10 mg/L aqueous solution of malachite green dyes and 1 g/L ZnO NPs was stirred in the dark, followed by irradiation in sunlight.

Results and Discussion:

Here, chemo-green synthesized ZnO NPs have direct band gap energies equivalent to ZnO NPs from the chemical and green method; they had negatively charged surfaces and good dye degradation in 160 minutes, which suggests the reutilization of unused filtrate obtained from the green method for further high-yield synthesis of ZnO NPs with scant use of ammonium hydroxide, stimulating sustainability and lightening the economic burden; they can be used for the demineralization of dyes coming from wastewater from the textile industry.



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sciforum-112723: Novel Strategy to Evaluate Platinum Photocatalysts for Hydrosilation-Curable Silicones

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Hydrosilation, a reaction between silane (Si-H) and vinyl groups, is leveraged in the manufacture of release coatings. However, cross-linking requires high temperatures, leading to this process being generally regarded as time- and energy-intensive. In recent decades, photopolymerization has emerged as an environmentally conscious alternative and is actively being explored due to the advantage that it is a low-temperature cross-linking process. The performance of UV-activated Pt hydrosilation catalysts can be assessed relative to industry-standard MeCpPtMe₃ (Pt-99) by monitoring the cross-linking of model silanes as ultra-thin (2-3 μm thick) films via an industrially relevant novel ATR-FTIR strategy. This strategy improves upon previous methods, in which ≥100 μm thick films are monitored via transmission mode FTIR. The percentage of the hydride consumed after the initial LED excitation (λ = 365, 400 nm) was determined by monitoring the bending mode of the Si-H bond relative to an unchanging Si-C stretching mode present in both silicone fluids. This allowed for the generation of percent conversion versus dark cure reaction time plots, as well as the calculation of kinetic parameters including the initial rate, rate constant, and final percent conversion. Eco-inspired innovations in the curing process will produce novel Pt(IV) photocatalysts that can be evaluated against the current benchmark, with the potential to create UV-cured release coatings on a cost-competitive scale to those cured thermally.



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sciforum-115220: An Overview of the Photocatalytic Performance of TiO₂ Nanoparticles for Dye Degradation

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Titanium dioxide (TiO₂) nanoparticles have become an exceptionally effective photocatalyst for the degradation of organic dyes in wastewater treatment. This breakthrough has been related to the distinctive physicochemical features inherent to these nanoparticles. These characteristics include a substantial surface area, remarkable chemical stability, and a potent oxidative capacity upon exposure to ultraviolet (UV) radiation, making TiO₂ a great photocatalyst. This work examines processes involving photocatalytic activity in TiO₂, focusing on the production of reactive oxygen species (ROS) via the formation of electron-hole pairs via photoinduced reactions. This research focuses on significant parameters that affect photocatalytic performance. These factors include particle size, crystal phase (anatase, rutile, or brookite), surface changes, and doping with metals or non-metals to enhance visible light absorption. This paper examines current improvements in TiO₂ nanoparticle production methods and their effects on the effectiveness of photocatalytic processes. An examination of the applications of TiO₂ for the degradation of synthetic dyes, including methylene blue, rhodamine B, and azo dyes, is conducted to highlight its potential to mitigate environmental issues caused by industrial dye pollution. Ultimately, challenges such as the fast recombination of charge carriers and the diminished efficacy of visible light are acknowledged, with several solutions suggested to mitigate these issues. This study seeks to elucidate the function of TiO₂ nanoparticles in dye degradation and to provide a foundation for future research aimed at producing more efficient and ecologically sustainable photocatalytic systems.



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sciforum-112375: Assessment of the photocatalytic efficiency of Pd-M (M=Cu, Ag) nanoparticles supported on TiO₂

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The effect of modifying TiO₂ with Pd, as well as of Cu and Ag co-catalysts on TiO₂, on the photocatalytic efficiency exhibited by these catalysts in the photocatalytic water splitting and nitrate reduction reaction was studied. Mono- (Pd, Cu, and Ag) and bimetallic (Pd-Cu and Pd-Ag) nanoparticles were prepared by a modified protocol of the alkaline polyol method [1]. The size, shape and specific morphologies of nanoparticles can be controlled from the preparation method [2, 3]. The physical and chemical properties of the Pd-M (M=Cu, Ag) catalysts supported on TiO₂ were investigated using different methods such as TEM, XRD, XPS, H₂-TPR, UV-Vis, CO chemisorption and fractal analysis. The photocatalytic activity of the prepared catalysts was tested by evaluating the generation of hydrogen from water under UV light (150 W high-pressure lamp with inner irradiation). The catalytic and photocatalytic removal of nitrates from aqueous solutions was examined using TiO₂-based materials containing bimetallic nanoparticles.

TEM and CO chemisorption measurements confirmed that the particle size is in the nanometric range. TEM images were examined in detail using the "box-counting method" to determine the fractal dimension [4]. The studied catalysts showed fractal behavior. H₂-TPR and XPS analyses provided information about the metal-support interaction and oxidation states of metallic components. Bimetallic Pd-Cu nanoparticles dispersed on TiO₂ with various molar ratios showed better activity for photocatalytic water splitting and nitrate reduction reaction compared to the Pd-Ag/TiO₂ sample. Depending on the surface atomic composition of the co-catalyst, an estimation of the optimal Pd-M (M=Cu, Ag) molar ratio was made to improve the photocatalytic performance in the H₂ generation reaction. A better understanding of the role of bimetallic nanoparticles is of the utmost importance for the design of efficient photocatalysts.



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sciforum-111326: Copper-based quantum dots for efficient photodegradation of methyl orange dye

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In recent years, there has been a consensus in the scientific community to seek more sustainable technologies that minimize environmental impact while providing social benefits. Among the most common pollutants being addressed in natural and wastewater, dyes stand out as a significant concern. Advanced Oxidative Processes (AOPs) stand out as one of the most widely used methodologies for environmental remediation. These methods employ catalysts to generate reactive oxidative species, such as hydrogen peroxide (H₂O₂), which produces hydroxyl radicals and water as products after a catalytic reaction [1]. However, controlling the amount of peroxide involved in the reaction, as well as the excess released into the environment, is essential. Thus, photocatalysis has emerged as a more efficient strategy and as an alternative to commonly used AOPs. This approach requires only a semiconductor material and sunlight as an energy source to drive the reduction reactions. Among semiconductor materials, Quantum Dots (QDs) are particularly notable due their unique optical properties, which arise from quantum confinement, as well as their low production costs. Additionally, these nanocrystals can catalyze the decomposition of H₂O₂, leading to the generation of anionic radicals [2]. In this study, copper-based QDs were prepared by colloidal synthesis in an aqueous medium. A 10 ppm solution of methyl orange (MO) dye was brought into contact with the QD suspension, both in the presence and absence of H₂O₂, and exposed to a full-spectrum solar lamp, simulating sunlight. The photodegradation process of the dye was characterized using UV/Vis spectroscopy. The preliminary results showed a significant decrease in MO concentration in the presence of QDs and light irradiation. These results represent a promising advancement in photodegradation technology while reinforcing a commitment to environmental sustainability.

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sciforum-112568: Cu-modified $\text{Zn}_6\text{In}_2\text{S}_9$ photocatalyst for hydrogen production under visible-light irradiation

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As energy and environmental problems caused by economic development become more serious, hydrogen is attracting attention as the next generation of clean energy. Photocatalytic hydrogen generation is a method with low environmental impact because it uses natural energy sources such as water and sunlight. Indium zinc sulfide is a photocatalyst with visible light response and chemical stability. The aim of this study was to improve the photocatalytic activity of indium zinc sulfide while reducing the use of expensive indium.

Copper-modified zinc indium sulfide was synthesized by heating and stirring zinc chloride, indium chloride tetrahydrate, copper(I) chloride, and thioacetamide in an autoclave at 180 °C for 18 h. Six types of catalysts were prepared by varying the amount of copper added. To evaluate the photocatalytic activity, 40 mg of catalyst was added in 40 mL of an aqueous solution containing 20 mL of 0.25 M Na_2SO_3 /0.35M Na_2S (sacrificial agent) and 1.2 mL of hexachloroplatinic acid solution (co-catalyst). The solution was purged with nitrogen for 30 min, with stirring, followed by irradiation with visible light ($\lambda \geq 420$ nm) for 6 h. Hydrogen production was measured using gas chromatography every 3 h. Catalyst characterization was also performed.

Compared to the hydrogen production rate of $\text{Zn}_6\text{In}_2\text{S}_9$, the hydrogen production rate of $\text{Zn}_{5.7}\text{Cu}_{0.3}\text{In}_2\text{S}_9$ was about five times higher. Therefore, the catalysts were characterized, and the characterization showed that the addition of copper suppressed the recombination of electron-hole pairs, increased the optical absorption in the visible light region and narrowed the band gap. The results indicate that the addition of copper to indium zinc sulfide improves the photocatalytic activity. The quantum yields for $\text{Zn}_{5.7}\text{Cu}_{0.3}\text{In}_2\text{S}_9$ were found to be consistent with the DRS trend, indicating that hydrogen production occurs from the photocatalyst.



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sciforum-115951: Development of a ZnO–Graphene Oxide Composite for Enhanced Photodegradation of Sandalfix Orange P3R and Sandalfix Turquoise Blue PG Dyes Under Sunlight Irradiation

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Rapid industrial growth has led to a serious pollution problem, primarily due to the discharge of wastewater containing significant amounts of organic pollutants, such as dyes, oils, and solvents. Among these, water pollution caused by dye-contaminated wastewater is particularly concerning. Conventional treatment methods have proven inadequate for the effective removal of dyes from wastewater. Sunlight-assisted photocatalysis has emerged as a promising approach for eliminating toxic organic substances from aqueous media. In this study, we report the development of ZnO-decorated graphene oxide (ZnO-GO) as a photocatalyst for the degradation of Sandalfix Orange P3R and Sandalfix Turquoise Blue PG dyes under sunlight irradiation. Graphene oxide was synthesized using the Hammer and Offeman method, and ZnO-GO composites were prepared via chemical reduction in a 1:1 ratio. The synthesized ZnO-GO was characterized using XRD, TEM, DR-UV-Vis, FTIR, and surface area analysis. Its photocatalytic performance was evaluated for the degradation of the two dyes. More than 95% of 100 mg/L (50 mL) of each dye was successfully degraded within 120 minutes of reaction time. ZnO-GO exhibited 2.2- and 1.9-fold higher catalytic activity in degrading Sandalfix Orange P3R and Sandalfix Turquoise Blue PG dyes, respectively, compared to graphene oxide and ZnO alone. This enhanced activity is attributed to the efficient transfer of photo-induced electrons through the graphene sheets, which play a crucial role in preventing the recombination of positive holes and electrons, thereby significantly improving photocatalytic performance.



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sciforum-112643: Development of photocatalytic reduction system for Cr(VI) in solution with modified g-C₃N₄

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Heavy metal pollution, particularly Cr(VI) contamination, has recently garnered significant attention. Cr(VI), which is commonly discharged in industrial wastewater, is a serious environmental and health threat due to its carcinogenic and mutagenic properties. Developing effective methods to reduce Cr(VI) to Cr(III)—a less toxic form—is therefore highly desirable. In this study, we developed an environmentally friendly and highly efficient photocatalytic method for Cr(VI) reduction. The reduction efficiency was enhanced by using modified carbon nitride under visible-light irradiation. For catalyst preparation, urea was dissolved in pure water and heated in an electric furnace at a rate of 2 °C/min to 600 °C, and this temperature was held for 2 hours. A modified version, g-C₃N₄ (HB), was synthesized by adding 5 mg of 1,3,5-HB before calcination. For the reduction experiments, the reaction solution was prepared with 30 ppm of Cr(VI), 100 ppm of EDTA, and 15 mg of photocatalyst. The mixture was stirred in the dark for 30 minutes to achieve adsorption/desorption equilibrium, followed by 90 minutes of irradiation with blue light (450 nm). The Cr(VI) concentration was analyzed using the diphenylcarbazide method, with the absorbance measured by a UV-visible spectrophotometer. The incorporation of 1,3,5-HB into carbon nitride increased the reduction rate by 40%, likely due to the introduction of hydroxyl groups into the carbon nitride framework. Additionally, calcination at 550 °C yielded higher reduction rates after 90 minutes compared to 600 °C, possibly because the lower temperature minimized catalyst loss during calcination. In future studies, we plan to confirm the structural changes using techniques such as SEM and TEM and evaluate the catalytic performance through electrochemical measurements.



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sciforum-112671: Dye decolorization under visible light irradiation using bismuth subcarbonate

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The photocatalytic decolorization of organic dyes is considered one of the most efficient and promising methods. Bismuth Subcarbonate ($\text{Bi}_2\text{O}_2\text{CO}_3$) exhibits photocatalytic activity, although its wide bandgap limits its ability to absorb visible light. Therefore, it is important to extend the light-responsive range. In this work, $\text{Bi}_2\text{O}_2\text{CO}_3$ photocatalysts were prepared by adding bromide (Br) sources and subjecting them to nitric acid treatment under various conditions. The photocatalytic activity of the prepared $\text{Bi}_2\text{O}_2\text{CO}_3$ was evaluated by decolorization experiments using Rhodamine B (RhB) as a representative dye.

To provide pretreatment $\text{Bi}_2\text{O}_2\text{CO}_3$, Br sources were dissolved in nitric acid solutions of different concentrations. Then, $\text{Bi}_2\text{O}_2\text{CO}_3$ was added to the resulting solution, and the mixture was stirred for 2 hours. Finally, the products were washed with water and ethanol and vacuum-dried at 60°C for 12 hours.

The photocatalytic activity was assessed by the decolorization of RhB. In particular, 20 mg of the synthesized photocatalyst was dispersed within the RhB solution (10 ppm, 35 mL) and stirred in the dark for 60 min to achieve adsorption/desorption equilibrium. The solution was then irradiated with a 500 W Xe lamp ($\lambda \geq 420$ nm). At regular intervals, the aliquots of the solution were collected and centrifuged. The decolorization rate of RhB was analyzed using a UV-visible spectrophotometer by measuring the absorbance at 554 nm.

Pure $\text{Bi}_2\text{O}_2\text{CO}_3$, as well as catalysts treated only with acid or only with a Br source, exhibited almost no photocatalytic activity under visible-light irradiation. Acid-treated $\text{Bi}_2\text{O}_2\text{CO}_3$ with cetrimonium bromide (CTAB) as the Br source enhanced RhB decolorization performance. The results showed that the combined effects of these modifications are essential.



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sciforum-112365: Efficient photocatalytic degradation of nadolol using silver-modified PMMA/TiO₂

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The commonly used β -blocker nadolol is regularly detected in wastewater and purified wastewater, representing a serious environmental problem. Photocatalysis has emerged as an innovative strategy to address such pollutants, with TiO₂ being a widely studied photocatalyst due to its potential in water treatment. However, its practical application is hindered by the high recombination rate of photo-generated electron-hole pairs. Therefore, the modification of TiO₂ to increase photocatalytic performance is one of the most important objectives in photocatalyst studies. For the modification of catalysts, various polymers can be used, such as polyvinylidene fluoride, hydroquinone superlattice, polypropylene, and poly(methyl methacrylate) (PMMA). Among these, PMMA stands out as a low-cost, non-toxic, water-insoluble polymer. In this study, powder PMMA was modified with silver, combined with TiO₂ nanopowder, and applied for the degradation of nadolol under UV-LED radiation. The degradation kinetics were monitored using high-performance liquid chromatography, and pH changes were observed using a pH meter. After 120 min of UV-LED irradiation, the materials demonstrated a significantly higher removal efficiency of nadolol compared to direct photolysis, specifically a 94 % removal efficiency of nadolol, significantly outperforming direct photolysis. The photocatalytic activity results demonstrated the practical applicability of the novel materials. The degradation followed pseudo-first-order kinetics, as evidenced by the calculated rate constant.



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sciforum-112685: Enhanced Photocatalytic Cr(VI) Reduction in Aqueous Solution with Black TiO₂ Under Visible Light Irradiation

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The photocatalytic reduction of hexavalent chromium (Cr(VI)) is an advanced method for remediating toxic chromium pollution in water. Cr(VI) is highly poisonous, carcinogenic, and water-soluble, making it a significant environmental and health concern. Photocatalysis offers a sustainable approach to reducing Cr(VI) to its less toxic and insoluble trivalent state (Cr(III)) using light energy and a photocatalyst. Titanium dioxide (TiO₂) is one of the most widely used photocatalysts due to its high catalytic efficiency, non-toxicity, chemical stability, resistance to photo corrosion, abundance, and cost-effectiveness properties. However, due to its wide bandgap (~3.2 eV), it can adequately work under UV light only and exhibit relatively less quantum efficiency. To overcome these limitations, black TiO₂ (BT) with oxygen vacancies, Ti³⁺ sites, enlarged surface area, and active sites may be considered as potential alternatives. Herein, BT was synthesized via chemical reduction using NaBH₄ as a reducing agent. In total, 40 mg photocatalytic efficiently reduced 60 ppm of Cr(VI) within 60 min of visible light (450 nm) illumination at room temperature using EDTA-2Na (500 ppm) as a hole scavenger. The 1,5-Diphenylcarbazide (DPC) colorimetric method was utilized to detect the reduction of Cr(VI) to Cr(III). From UV-vis DRS spectra, a clear red shift was observed for BT compared to TiO₂, suggesting the improved light absorption capability and Tauc plot disclosed reduced energy bandgap (~1.5–2.5 eV), which further accelerated the transition of photo-generated electrons from the valance band to the conduction band.



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sciforum-112655: Enhanced Photocatalytic Hydrogen production under Visible Light using Ammonia-Treated Graphene Oxide/ ZnIn_2S_4

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Photocatalysis is considered an ideal energy conversion technology that can convert solar energy into clean hydrogen energy through water splitting. Hydrogen can be used directly as a source of energy rather than fossil fuels due to its higher energy yield and eco-friendly attributes. However, most photocatalysts exhibit low photocatalytic performance due to their lower light absorption capability, higher energy bandgap, poor charge separation and migration capability, and rapid electron-hole pair recombination properties. To overcome the above-mentioned problems, in this study, we performed the in situ simultaneous photodeposition of ammonia-treated graphene oxide (NGO) on CTAB-assisted ZnIn_2S_4 (ZIS) for photocatalytic hydrogen evolution from splitting under visible light irradiation (450 nm). Amounts of 1 wt% of both Pt and triethanolamine were used as the co-catalyst and hole-scavengers, respectively. The reaction conditions (catalyst and co-catalyst loading, ammonia concentration and mixing, and reaction temperature and pH) were optimized. The NGO/ZIS composite increased H_2 production by 3.25-fold and 67-fold compared to pure ZIS and NGO, respectively, indicating the achievement of a synergetic effect. Synthesized photocatalysts were characterized by XRD, XPS, FTIR, SEM, TEM, BET, TRPL, DRS, PL, and EIS analysis. Density functional theory indicated that the free energy, dipole moment, HOMO-LUMO bandgap, chemical reactivity, and surface charge were significantly increased in NGO compared to pure graphene oxide. Due to the NGO/ZIS composite formation, the light-harvesting capability, energy bandgap, charge separation and migration, surface area and morphology, and electron-hole pair recombination properties were significantly improved.



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sciforum-112649: Enhancement of Hydrogen Production Activity by Constructing Heterojunction of TpTSN-COF and Cu-doped ZIS

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Introduction

Covalent organic frameworks (COFs) are promising photocatalysts due to their excellent visible light absorption, large surface area, and high chemical stability. However, their photocatalytic activity is often limited by the rapid recombination of photogenerated electron-hole pairs. In this study, we aimed to enhance hydrogen production activity by constructing a heterojunction between TpTSN-COF and Copper-doped ZnIn₂S₄.

Methods

Synthesis of TpTSN-COF/Cu-doped ZIS: The prepared Cu-doped ZIS was added to a mixture of dioxane, mesitylene, and acetic acid and then sonicated. Tp (1,3,5-triformylphloroglucinol) and TSN (o-Tolidine Sulfone) were subsequently added, and hydrothermal synthesis was performed. The resulting product was designated x%-TpTSN-COF/ Cu-doped ZIS, where x% indicates the weight ratio of TpTSN-COF to Cu-doped ZIS.

Hydrogen production test: A Pyrex reactor was charged with a photocatalyst, distilled water, sodium ascorbate (as a sacrificial agent), HCl (for pH adjustment), and H₂PtCl₆ (as a co-catalyst). Before light irradiation, the reaction system was purged with N₂ gas to remove any dissolved oxygen. An LED lamp (450 nm) was used as the light source, and the hydrogen production rate was calculated based on the amount of hydrogen production after 3 hours.

Results

The hydrogen production experiments were conducted with different ratios of TpTSN-COF and Cu-doped ZIS. As a result, 5%-TpTSN-COF/Cu-doped ZIS exhibited the highest hydrogen production rate of 40,000 μmol/g·h, which was approximately 1.5 times higher than that of TpTSN-COF and Cu-doped ZIS individually. The characterization revealed that the increased activity was attributed to improvements in light absorption, charge transfer properties, and an increase in the surface area.

Conclusions

The novel hybridized photocatalyst, TpTSN-COF/ Cu-doped ZIS, was successfully synthesized. The optimal photocatalyst (5%-TpTSN-COF/Cu-doped ZIS) showed approximately 1.5 times higher activity than that of TpTSN-COF and Cu-doped ZIS individually, and this increased activity was attributed to improvements in light absorption, charge transfer properties, and an increase in the surface area.



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sciforum-112612: Graphitic Carbon Nitride Modified with 1,3-Benzothiazole-2-carbaldehyde for Enhancement of Visible Light Hydrogen Production Activity

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The utilization of clean energy is being explored to address energy and environmental challenges, with hydrogen emerging as a promising next-generation energy source. Research efforts are focused on hydrogen production through water splitting using graphitic carbon nitride (g-C₃N₄), a polymer semiconductor photocatalyst. In this process, a photocatalyst-dispersed aqueous solution is irradiated with light to generate hydrogen. g-C₃N₄ is characterized by its non-toxic nature, thermal and physical stability, and favorable bandgap [1]. However, its low specific surface area, limited light absorption range, and high photogenerated electron--hole recombination rate hinder its photocatalytic efficiency [2]. In this study, 1,3-benzothiazole-2-carbaldehyde is introduced into g-C₃N₄ to enhance the intramolecular charge transfer, thereby improving hydrogen production activity.

The photocatalyst was synthesized by the triple calcination of dicyanodiamide and 1,3-benzothiazole-2-carbaldehyde. Photocatalytic activity was evaluated by adding triethanolamine (sacrificial agent) and hexachloroplatinic acid to the catalyst in an aqueous solution, purging with nitrogen, and irradiating with visible light ($\lambda \geq 420$ nm) for 6 h. Hydrogen production was quantified by gas chromatography (GC/TCD). The crystal structure, morphology, surface state, and optical properties of the photocatalysts were also characterized.

The optimized g-C₃N₄ modified with 1,3-benzothiazole-2-carbaldehyde demonstrated a hydrogen generation rate of 690 $\mu\text{mol h}^{-1} \text{g}^{-1}$ through photocatalysis. This rate was roughly 14 times higher than that observed for unmodified g-C₃N₄. The characterization results showed that the benzothiazole-doped g-C₃N₄ exhibited exfoliation of the nanosheets and changes in surface structure. Additionally, a low fluorescence intensity and an extended visible light absorption range were observed. These effects were attributed to the introduction of 1,3-benzothiazole-2-carbaldehyde, which formed a donor--acceptor structure, enhancing the separation and transfer of photogenerated carriers. Consequently, the number of reactive electrons increased, leading to improved hydrogen production activity.

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sciforum-112628: Improvement in hydrogen production activity under visible-light irradiation using Tp-Pa-COF photocatalyst

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To achieve a sustainable society, it is essential to have a clean energy system that does not rely on depletable resources. Hydrogen production through water splitting using photocatalysts driven by sunlight is attracting attention as a promising solution. Covalent organic frameworks (COFs) are ideal for this application, as they have a high density of surface-active sites and are water-dispersible, thermally durable, and metal-free. However, current synthesis methods have industrial disadvantages due to the complex and harsh synthesis conditions, such as temperature and atmosphere. In this study, we attempted to synthesize a highly active photocatalyst under simple and mild conditions in order to introduce chlorine substituents into the imine-bonded COF, Tp-Pa-COF.

1,3,5-Trifluoromethyl fluoroglucinol (Tp) and 1,4-phenylenediamine (Pa) or 2,5-dichloro-1,4-phenylenediamine (Pa-Cl₂) were reacted to synthesize Tp-Pa-X-COF (X = H₂ or Cl₂). After 30 minutes of ultrasonic treatment, the mixture was stirred at different temperatures (room temperature to 120 °C) and times (6 to 24 hours) under air atmosphere. Photocatalytic hydrogen evolution was performed using hexachloroplatinic acid as a co-catalyst, sodium ascorbate as a sacrificial agent, and an LED lamp ($\lambda=450$ nm, 17.5 mW/cm²) as a light source. UV-vis DRS was used to measure visible-light absorption capacity, and gas chromatography (TCD) was used to quantify hydrogen.

As a result, it was found that even at room temperature and atmospheric pressure, chlorine substitution improved photocatalytic hydrogen production activity, improved visible-light absorption, and suppressed the recombination of electrons and holes. It was revealed that factors such as reaction time, temperature, and solvent affect the crystallization and photocatalytic activity of Tp-Pa-COF.



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sciforum-112059: Influence of Pt loading on the Schottky barrier height and the photothermal activity of TiO₂/Pt catalysts

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This study investigates the influence of platinum (Pt) loading on the photothermal NO₂ reduction activity of TiO₂/Pt catalysts, focussing on the relationship between Schottky barrier height (SBH) and catalytic performance. Noble metals such as Pt generate “hot electrons” under visible light due to their localised surface plasmon resonance (LSPR) properties. These electrons are injected into the TiO₂ conduction band, and the efficiency depends on the SBH at the TiO₂/Pt interface. Catalysts with different Pt loadings (0.5-2 wt%) were synthesised by wet impregnation and then extensively characterised using techniques such as XRD, TEM, SEM-EDS, XPS and UV-vis DR spectroscopy to evaluate their optical, electronic and structural properties. The results showed that higher Pt loading reduced the SBH from 0.42 eV for TiO₂/0.5%Pt to 0.16 eV for TiO₂/2%Pt. This reduction facilitates faster electron injection and minimises recombination, which increases the photothermal NO₂ reduction performance. The average size of Pt nanoparticles increased from 1.1 nm to 1.5 nm with increasing Pt content, but the morphology and crystallinity of TiO₂ remained stable. Catalytic tests showed that TiO₂ was inactive below 100 °C, while TiO₂/Pt catalysts enabled NO₂ reduction at temperatures as low as 30 °C under visible light. However, a higher SBH value reduced the activity due to increased electron-hole recombination at the TiO₂/Pt interface. The results confirm the multifunctionality of TiO₂/Pt catalysts and demonstrate their suitability for hybrid photothermal reaction systems for NO_x reduction at low temperatures. These results underline the crucial role of optimising Pt loading to balance SBH and improve catalytic performance in photothermal applications.



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sciforum-114537: Merging decatungstate photocatalysis and a copper-catalyzed azide-alkyne cycloaddition reaction for the sustainable formation of 1,2,3-triazoles in water

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Merging photoredox and catalysis by transition metals, coined as metallaphotoredox catalysis, has proven to be an excellent new platform for the development of new synthetic strategies for the formation of carbon-carbon and carbon-heteroatom bonds [1]. In this presentation, we will present a dual catalytic system that has been successfully developed for the ligation of azides with alkynes to yield 1,4-disubstituted-1,2,3-triazoles in a regioselective manner. Our strategy consists of merging decatungstate anion $[W_{10}O_{32}]^{4-}$ photocatalysis in the presence of a hydrogen donor solvent to reduce the Cu(II) precursor into the catalytically active species Cu(I), consequently starting a copper-catalyzed azide-alkyne cycloaddition reaction (CuAAC).

The resulting bifunctional $H^+[W_{10}O_{32}]^{5-}/Cu(I)$ catalytic system operates efficiently in an environmentally benign water-ethanol solvent mixture as a reaction medium, producing only 1,4-disubstituted-1,2,3-triazole derivatives with high yields of up to 99% under mild conditions. This metallaphotoredox approach can be applied to a large range of substrates and large-scale reactions. To prove the sustainability of this dual catalytic process, CuAAC was performed under sunlight exposure too [2].

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sciforum-114403: Noble metal-modified TiO₂ obtained by the sol--gel method: Ethanol photodegradation

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Introduction:

Nanopowders with different compositions, purities, sizes, and dimensional distributions can be created using the sol--gel method [1,2]. The metal precursors were added either during synthesis (in a single step) or by post-synthesis impregnation to the sol--gel method used for obtaining the powder photocatalysts.

Methods:

The materials used include ethanol, TiO₂, and Pt/TiO₂ powders (obtained by the sol--gel method). Characterization methods such as thermal analysis (DTA), infrared spectroscopy (IR), X-ray diffraction (XRD), and X-ray fluorescence (XRF), and the determination of the specific BET surface area and pore distribution, are complementary and necessary.

Results:

As a result of the post-synthesis heat treatment, oxide compounds were obtained in the form of white (TiO₂) and gray (Pt-modified TiO₂) crystallized powder. The photocatalytic activity of titanium dioxide synthesized by the sol--gel route was compared to that of pristine and platinum doped photocatalysts, both during synthesis and by post-synthesis impregnation. As a result of the post-synthesis heat treatment, oxide compounds were obtained in the form of white (TiO₂) and gray (Pt-modified TiO₂) crystallized powder. The photocatalytic activity of titanium dioxide synthesized by the sol-gel route was compared to that of pristine and platinum-doped photocatalysts, both during synthesis and by post-synthesis impregnation. The samples were tested as photocatalysts in the oxidative degradation of ethanol in the gaseous phase and under solar simulated light irradiation. The following is an increasing order of powder reactivity in the photocatalytic tests: TiO₂, TiO₂-Pt in-situ, and TiO₂-Pt by post-synthesis impregnation (with the highest conversion being 72,24%).

Conclusions:

The topic of this paper focuses on the development of the photocatalytic activity of simple and noble metal-modified TiO₂ used for the degradation of contaminants in the gas phase and ambient conditions.

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sciforum-112533: Photocatalytic Behaviour of Powdered Manganese (Mn)- and Iron (Fe)-doped Tin Oxide nanomaterials

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Semiconductor metal-substituted tin oxide (SnO₂) has drawn a great deal of attention due to its excellent properties. This study focuses on the photocatalytic properties of 3d transition metals, specifically manganese (Mn) and iron (Fe), emphasizing the role of unpaired electrons in enhancing photocatalytic activity. A Sn_{0.99}-Mn_{0.05}-Fe_{0.05}O₂ sample was synthesized by the sol-gel wet chemical precipitation method. The crystallite size and structure of doped SnO₂ were determined using a modified Debye Scherer's formula. Lattice constants were evaluated from peaks obtained by the X-ray diffraction (XRD) technique. The value of crystallite size estimated by Debye Scherer's formula lies in the range 3–5 nm, indicating the nano-crystalline nature of the sample. Using transmission electron microscopy (TEM), the obtained average diameter was 3.75 nm, calculated with the help of ImageJ, which is in good agreement with the crystallite size obtained via XRD. The irregular morphology of the sample was analyzed by field emission scanning electron microscopy (FESEM). An energy dispersive X-ray (EDX) analysis confirmed the presence of elements such as tin, oxygen, manganese and iron. Fourier transform infrared (FT-IR) spectrum displayed Sn-O characteristic bands as well as inculcated metal elements. The optical and photocatalytic results were characterized using UV-Visible spectroscopy. The absorbance for pristine and intercalated samples was observed at 217 nm and 218 nm, respectively. Their optical band gaps were 3.10 eV and 2.69 eV, respectively, indicating that the band gaps narrow upon intercalation. Photoluminescence spectra were obtained in the visible spectrum range (300–600 nm) and confirmed the defects and impurity states formed due to the intercalation of Mn and Fe transition elements. The photocatalytic activity results revealed that Mn-Fe/SnO₂ has a better photocatalytic performance of methylene blue (MB) dye solution compared to pristine SnO₂.



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sciforum-112630: Photocatalytic degradation of dyes using TpPa-COF-Cl₂ membrane

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The degradation of organic pollutants using photocatalysis is a more environmentally friendly method because it uses solar energy. Covalent organic frameworks (COFs) are photocatalysts that are composed of covalent bonds of light elements and do not contain harmful metals. COFs have been studied in various fields, but their use in removing organic pollutants has not been fully investigated. In this study, the photocatalyst TpPa-COF-Cl₂ was made into a membrane and its activity against dyes was examined. TpPa-COF-Cl₂ slightly decolorized methyl orange.

-Synthesis of catalyst

① Mesitylene (4.5 mL), 1,4-dioxane (4.5 mL), acetic acid (3M, 1.5 mL), 1,3,5-triformylphloroglucinol (Tp), and 2,5-dichloro-p-phenylenediamine (Pa) (molar ratio Tp:Pa=1:1.5) were added, heated, and stirred to obtain TpPa-COF-Cl₂ powder.

② A mixture of 20 mg of TpPa-COF-Cl₂ powder, sodium alginate, and 1.7 mL of water was heated and stirred, spread on a glass plate, and immersed in a CaCl₂ solution (3 wt%) for 24 hours to synthesize 5 to 6 TpPa-COF-Cl₂ films.

-Dye degradation

One membrane was placed in 5 ppm methyl orange (MO) and left in the dark for 30 minutes to reach adsorption equilibrium, after which it was irradiated with a 450 nm LED lamp for 60 minutes and its absorbance was measured every 10 minutes.

-Result, Conclusion

SEM and TEM revealed that the powdered TpPa-COF-Cl₂ had a layered structure. In addition, an absorption edge at 600 nm was confirmed by DRS.

The TpPa-COF-Cl₂ membrane formed by the cross-linking reaction of alginic acid and calcium ions maintained its structure even after the photocatalytic reaction. The TpPa-COF-Cl₂ membrane decolorized approximately 5% of MO. Although the decolorization efficiency was inferior to that of the powder form, it was easier to remove the catalyst.



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sciforum-112613: Photocatalytic dye degradation using modified g-C₃N₄

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Dye wastewater is a highly toxic organic pollutant that is not easily degraded. For that reason, it causes serious environmental damage to nature and ecosystems. Therefore, the degradation research of organic matter by using photocatalysts is attracting attention because of their low cost and environmental friendliness. Graphitic carbon nitride (g-C₃N₄), a photocatalyst, has the advantages of being inexpensive, chemically and thermally stable, and easy to prepare. On the other hand, g-C₃N₄ possesses a small surface area, narrow visible light absorption, and a quick-recombination photogenerated electron-hole pair. Photocatalysts are also known to incorporate heteroatoms within their structures and to develop various characteristics depending on the atoms incorporated. In this research, we aim to enhance the dye degradation performance by synthesizing g-C₃N₄, incorporating heteroatoms.

The photocatalyst was obtained by mixing urea, a carbon nitride source, and a heteroatom source, followed by thermal treatment. Bulk g-C₃N₄ (CN-U), N-deficient g-C₃N₄ (CN-N), Br-doped g-C₃N₄ (CN-Br), S-doped g-C₃N₄ (CN-S), and O-doped g-C₃N₄ (CN-O) were prepared. Photocatalytic degradation was carried out under visible light irradiation using a Xenon lamp equipped with a cutoff filter. Methyl orange (MO) and methylene blue (MB) were selected as decolorizing targets. They were characterized in a variety of ways to clarify their photocatalytic properties.

A series of characterization results showed that the typical structure of g-C₃N₄ was maintained. It has been shown that doping carbon nitride with heteroatoms changes the optical properties of carbon nitride. Furthermore, we confirmed that doping carbon nitride with heteroatoms prevents the recombination of photogenerated electron-hole pairs. From the results of the dye degradation experiment, for MO, CN-N degraded the most. For MB, CN-U and CN-N degraded the most. We think this is due to the improved optical properties resulting from the incorporation of heteroatoms.



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sciforum-112591: Photocatalytic methane production from acetic acid solution with S-doped g-C₃N₄ under visible light irradiation

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Graphitic carbon nitride (g-C₃N₄) is one photocatalyst that has garnered attention due to its good visible-light responsivity, chemical stability, and synthesis from low-cost materials. However, single g-C₃N₄ suffers from a high recombination rate of electrons and holes. To overcome this limitation, the hybridization of g-C₃N₄ with other materials has been studied. In this work, S-doped g-C₃N₄ photocatalysts were synthesized from urea and thiourea by calcination in an electric furnace. Photocatalytic methane production was conducted from an acetic acid solution with S-doped g-C₃N₄ photocatalyst under visible light irradiation (450 nm) for 6 hours. Cu was applied as a co-catalyst to enhance performance, and the evolved gas was analyzed using a GC-FID system. Optimal conditions for methane production were investigated, including the weight ratio of urea to thiourea, and the proportion of the Cu co-catalyst. S-doped g-C₃N₄ was synthesized by the calcination of a mixture of urea and thiourea. The characterization of S-doped g-C₃N₄ was performed by SEM, TEM, DRS, PL, XRD, and XPS. The S-doping could be confirmed by the color of photocatalyst materials and XPS analysis.

The photocatalyst synthesized with 30 wt% thiourea showed the best activity, with a production rate approximately 3.3 times higher compared with that of g-C₃N₄ synthesized from urea alone. The production rate with 1.0 wt% co-catalyst was about 2.3 times greater than that without the co-catalyst. The structural, morphological, and optical properties were analyzed through various characterizations. The analysis results showed the formation of g-C₃N₄ with characteristic peaks and structures, a redshift due to sulfur doping, a low recombination rate of electron-hole pairs, and improved charge separation. The enhanced photocatalytic activity was attributed to increased visible-light absorption induced by sulfur doping. These findings suggest that Cu-modified S-doped g-C₃N₄ can serve as a highly promising photocatalyst for methane production under visible light.



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sciforum-114509: Photocatalytic Performance of Composites of Prussian Blue and Its Analogues with Anatase for UV-Driven Degradation of Aqueous Methylene Blue Solutions: Chemical and Ecotoxicological Evaluation

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This study explores the development of cost-effective photocatalysts based on Prussian Blue (Iron(III) Hexacyanoferrate(II)) and its analogues (Cobalt(II) Hexacyanoferrate(II), Iron(III) Hexacyanocobaltate(III), and Cobalt(II) Hexacyanocobaltate(III)) combined with commercial anatase nanoparticles (particle size 25 nm, purity 99.7%) for UV-driven degradation of aqueous methylene blue (MB) solutions. The materials were characterized using XRF, FTIR, SEM, and XRD, confirming the successful formation of side-by-side composites without core@shell morphology. The formation of heterojunctions remains inconclusive.

Photocatalytic experiments demonstrated that the composites achieved high decolorization efficiencies (80–90%), significantly outperforming pure anatase (25%). However, total organic carbon (TOC) analysis revealed only partial mineralization, with MB content reducing minimally (64.5 mg/L to 62.12 mg/L) under irradiation with a xenon and mercury UV lamp. Importantly, no bleaching of MB solutions occurred with pure Prussian Blue or its analogues alone.

Ecotoxicological assays using *Scaptotrigona postica* bees revealed that the photodegraded dye solution exhibited reduced toxicity compared to untreated MB, as evidenced by lower mortality risks (HR = 0.8973) and longer median lethal times (TL50 = 12 days vs. 11 days for untreated dye). Stingless bees exposed to untreated MB faced higher mortality risks (HR = 0.6161), emphasizing the ecological risks of untreated dyes.

Therefore, it is imperative to continue studying the development of innovative and sustainable photocatalytic systems, focusing on Prussian Blue composites, their efficient reuse, and their coupling with hydrogen peroxide and/or persulfate, to advance water treatment and the remediation of dyes in an economically viable and environmentally friendly manner.



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sciforum-112264: Photocatalytic Performance of Iron-Modified Carbon Nitride Using Uv-A Irradiation

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To address environmental concerns, solar-driven photocatalytic processes are proposed for the removal of anthropogenic pollutants. The textile industry's wastewater, rich in emerging organic pollutants, including dyes, is a primary target for this approach.

Carbon nitride (C_3N_4) is a low-cost semiconductor material that can absorb light in the visible solar spectrum, in addition to being easy to manufacture, non-toxic, and biodegradable. The nanoparticles of this material possess optical and electronic properties associated with their nanoscale structure. To overcome its own limitations, strategies have been designed that consider modification with metals, such as iron. In this context, carbon nitride particles (CN) were synthesized from the calcination of urea. Then, the CN were modified by applying the calcination and impregnation methods with the Fe (II) salt (CNFe (II)c and CNFe (II)i, respectively).

The synthesized catalysts were characterized by IR-ATR. UV-vis absorption spectra and the zeta potential of the aqueous suspensions were determined. Time-resolved as well as steady-state photoluminescence measurements were measured. Total organic carbon (TOC) and some other characterization techniques were applied to obtain more information on the material.

The photocatalytic properties of each material were evaluated using methyl orange (MO) as a model contaminant and 350 nm monochromatic light. In all cases, samples were taken periodically, and UV-visible spectroscopy was used to monitor the concentration of MO. The MO removal percentages indicate that CNFe (II)i exhibits a significantly higher MO removal efficiency compared to unmodified CN and CNFe (II)c under identical experimental conditions.

Based on the obtained results, a future study is proposed to investigate the mechanisms involved in MO degradation. This will provide a deeper understanding of the results and lay the groundwork for future studies related to the toxicity of the reaction mixture after each treatment of the treated samples, as well as the implementation of other contaminants.



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sciforum-112572: Photocatalytic Study of Rose Bengal Dye using Sol–Gel-Synthesized Titanium dioxide incorporated with Transition metal elements (Manganese and Cobalt)

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This study is concerned with the photocatalytic degradation of rose bengal dye using modified titanium dioxide, specifically using different metal ions, like manganese (Mn) and cobalt (Co). The TiO₂/Mn/Co composites were prepared via a sol–gel route since it favors the homogenous introduction of metal ions into the TiO₂ matrix. For the preparation of the composites, titanium dioxide (0.89 mol) was mixed with manganese (II) chloride (0.05 mol) and cobalt chloride hexahydrate (0.06 mol). The structural and morphological properties of the synthesized photocatalysts were assessed by characterization techniques such as X-ray diffraction (XRD) and transmission electron microscopy (TEM), Fourier-Transform Infrared (FT-IR) and UV-VIS spectroscopy. The average particle size was found to be 74.8 nm, which was calculated using image J software, and the interplanar d-spacing was 0.3567 nm, as calculated from HR-TEM images. The TEM images also revealed the spherical morphology of the composite. Optical studies have revealed the narrowed band gap of the TiO₂/Mn/Co nanocomposite. Photocatalytic performance under sunlight was evaluated, indicating enhancement in the efficiency of rose bengal degradation compared to pure TiO₂ through the incorporation of manganese and cobalt. The degradation efficiency was 92% in the case of TiO₂ and increased to 94% with the TiO₂/Mn/Co nanocomposite. The suggested mechanism for the degradation process, through the generation of reactive oxygen species during sunlight irradiation, elucidates an essential role of the latter in breaking down the molecular structure of the dye. Overall, these results prove that TiO₂/Mn/Co composites may have the potential to offer an effective solution for dye removal from wastewater, thereby making a positive contribution towards environmental sustainability.



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sciforum-115107: Robust mesoporous N-doped TiO₂ nanoparticles for wastewater treatment under sunlight

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Photocatalysts are vital for tackling environmental crises; however, their poor solar-energy utilization is a bottleneck. Herein, N-doped titania (N/TiO₂) nanomaterials were successfully synthesized using a facile sol–gel technique. The importance of the annealing gases' environment on physicochemical properties and photocatalytic efficiency under sunlight was examined. Spectroscopy data revealed that the spheroidal N/TiO₂ crystals were transformed from monophasic anatase with less crystallinity to dual-phase anatase/rutile (A/R) with higher crystallinity in argon/nitrogen and air, respectively. Moreover, XPS confirmed the incorporation of interstitial nitrogen in the bare titania structure; this introduction not only led to a red shift towards visible light but also lowered the bandgap energy (2.35 eV) and suppressed charge-carrier recombination according to DRS and PL results. Furthermore, they showed a typical IV isotherm of mesoporous nanomaterials with a high surface area, up to 103 m²/g. Particularly, their rhodamine B photodegradation and thermal stability were dictated by the annealing gas type. Notably, the N/TiO₂ prepared in air demonstrated the highest degradation performance of 99% with the fastest rate of 0.0158 min⁻¹, which is twice faster than the control TiO₂. This improved performance is mostly attributed to its higher crystallinity, A/R mixed phase, aqueous-dispersion character, and lower charge recombination. Such a gas-driven synthesis of catalysts has practical applications in designing other solar-energy conversion systems.



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sciforum-112599: Surfactant-assisted synthesis of bismuth tungstate for dye decolorization under visible light irradiation

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Dyes are highly toxic organic pollutants that are difficult to decompose, causing significant environmental damage. In recent years, research has been conducted on dye degradation using photocatalysis, an environmentally friendly, efficient, and clean pollutant degradation technology. Among photocatalysts, bismuth tungstate (Bi_2WO_6) has been reported to possess photocatalytic activity under visible light irradiation due to its stable physicochemical properties and suitable band gap. However, the narrow light absorption region and high recombination rate of electron-hole pairs require further studies to improve their photocatalytic performance. In this work, the effect of surfactants in synthetic systems on the morphology and photocatalytic activity of Bi_2WO_6 is investigated.

Bi_2WO_6 was synthesized by a simple one-pot solvothermal method using ethylene glycol. Various surfactants, including cationic, anionic, and nonionic types, were introduced during catalyst preparation, respectively. The photocatalytic efficiency was evaluated through the decolorization of Rhodamine B as a model dye.

The decolorization rate of RhB after 120 minutes of light irradiation confirmed that adding surfactants to the synthetic system improved the photocatalytic activity. In particular, high decolorization rates were achieved when cationic (benzalkonium chloride, hexadecyl trimethylammonium bromide) and anionic (sodium oleate) surfactants were used. Various characterizations suggest that the enhanced photocatalytic activity could be attributed to the improved ability to separate and transfer photogenerated carriers.



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sciforum-111960: Sustainable carbon-based photocatalysts for solar H₂ production by photoreforming of plastic materials

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Photocatalytic hydrogen production is among the top ten emerging technologies in chemistry. In particular, the photoreforming (PR) of organic substrates is an attractive way to obtain green H₂ together with the valorisation of waste or biomass. This reaction combines water reduction with the oxidation of a sacrificial agent using a semiconductor. In this context, it is possible to use, as sacrificial agents, new emerging water pollutants as plastic materials like polystyrene (PS) and polyethylene (PE) to obtain H₂ with a contextual water purification. Furthermore, an important point is the choice of photocatalysts. Carbon-based materials are prospective candidates for their remarkable electrical, thermal, and mechanical properties. For this reason, the focus of this work was to study the performance of composites based on metal carbides (MCs) (SiC, MoC, TiC) with different amounts of graphitic carbon nitride (g-C₃N₄). For the preparation of these catalysts, thermal polymerization was used, whereas for increasing the production of H₂, Pt (1 wt%) was added with wetness impregnation. The photocatalytic tests were performed with 50 mg of the photocatalyst, homogeneously suspended in an aqueous solution containing previously pre-treated PS or PE, with the photoreactor irradiated for 5 h using a solar lamp. A good production of H₂ was verified from all the investigated sacrificial agents. PE PR using the TiC1%g-C₃N₄-Pt sample allowed more H₂ (750 $\mu\text{mol H}_2/(\text{gcat}\cdot\text{h})$) to be produced compared to PS PR (170 $\mu\text{mol H}_2/(\text{gcat}\cdot\text{h})$). This can be due to the easier C-C bond cleavage and C-C bond coupling of PE with respect to PS during the pre-treatment and the photoreforming reaction. The results obtained in this work pave the way for future environmental perspectives in which the pollutants can be considered new raw materials to obtain H₂, contextually preserving the water by the emerging contaminants.



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sciforum-112411: Synthesis of metal sulfide/g-C₃N₄ nanocomposite for photocatalytic degradation of organic pollutants under visible light

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Graphitic carbon nitride (g-C₃N₄) is an intriguing two-dimensional (2D) material characterized by remarkable features, such as visible light absorption, superior thermal stability, and a large abundance of its components in the Earth's crust. In contrast to conventional photocatalysts like titanium dioxide (TiO₂), g-C₃N₄ may function well in visible light, which constitutes a substantial segment of the solar spectrum. This makes it a more sustainable alternative for environmental cleanup. Nonetheless, the efficacy of pure g-C₃N₄ in photocatalysis is impeded by challenges such as the rapid recombination of electron-hole pairs and a very limited surface area. To tackle these issues, g-C₃N₄ is modified with metal sulfides such as zinc sulfide (ZnS) and bismuth sulfide (Bi₂S₃) by a simple, sustainable process employing starch. These adjustments boost charge carrier separation and improve light absorption, leading to a significant increase in photocatalytic efficiency.

These composite materials have shown remarkable efficacy in effectively degrading coumarin and para-nitrophenol upon exposure to visible light. The amalgamation of g-C₃N₄ and metal sulfides markedly enhances degradation rates, making them very useful for environmental remediation applications. This advancement offers an effective and eco-friendly method for degrading organic contaminants present in wastewater and industrial discharges.

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sciforum-115150: Synthesis of n-type Zinc-doped metal dichalcogenide for efficient visible light photocatalytic degradation of Antibiotic and photo-electrochemical study

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In recent decades, the release of drugs into aquatic ecosystems has heightened human apprehension. The literature includes multiple studies that have recorded Ciprofloxacin (CIP) levels in diverse sources, such as wastewater treatment facilities, untreated drinking water, hospital effluent, lakes, and discharge from pharmaceutical manufacturers. This literature review indicates that semiconductor-based AOPs can be used to effectively remove pharmaceuticals from wastewater. In order to facilitate the water splitting reaction, it is necessary to use catalysts that are highly active, stable, low-cost, and abundant.

The synthesis of molybdenum diselenide and the doping of zinc metal (X= weight percentages, 2.5%,5%, 7.5%,10%) into it have been conducted in this study. Using techniques such as FESEM, EDX, XRD, Raman, FTIR, and XPS, extensive investigations have been conducted which indicate the catalyst's efficient production. FESEM confirms the nanoflower structure with a size range of 30-50 nm. UV-VIS DRS analysis has been carried out to assess the synthesized sample's optical characteristics; it also helps to identify the band gap that promotes effective visible light absorption. The semiconductor type, charge transfer kinetics, and charge separation and transfer inside the on and off zones have been investigated using the Mott--Schottky plot, an Electrochemical Impedance Spectroscopy (EIS) study, and photocurrent investigation, respectively. An appropriate photochemical reactor was used to break down ciprofloxacin (CIP), and the reaction rate constant was measured. Under optimal conditions, the residual concentration of the antibiotic decreased to a point where it was no longer detectable after 45 minutes.

Further, the 5% doping of Zinc metal over molybdenum diselenide allowed for maximum photocatalytic efficiency due to the Se vacancy creation in the MoSe_2 structure under visible light illumination. Also, Zinc doping reduces the residence time to achieve faster reaction rates.



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sciforum-112703: The degradation of endocrine disruptors via photocatalysis in a continuous-flow microreactor: a proposal for numbering-up

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Numbering-up is a strategy used to scale up microchemical processes by distributing fluids in microchannels, used as microreactors, which allows efficient mass transport under laminar flow conditions. Due to the reduced diffusion path from the aqueous solution of the contaminant to the catalyst layer, mass transport limitations are reduced, which easuky overcomes one of the main drawbacks of catalyst immobilization.

In this work, the efficiency of a continuous-flow photo-microreactor with TiO₂ supported on a silicone column and irradiated by UVA-LED was evaluated, considering the effects of its operating conditions on the degradation of two endocrine disruptors, BPA and DBP.

The experimental design was 2k and considered pH, temperature, H₂O₂ concentration, and volumetric flow rate as the process variables. The controlled reaction included equipment, such as injection pumps, peltier, pressure control, and online sensors (pH, ORP, NMR 1H). The output variables were the photocatalytic efficiency of the reactor, assessed through reaction monitoring by NMR-1H, IR, UV-Vis, and TOC. Variations in Reynolds numbers were measured from the viscosity of the solutions at the set up and end of the reactions.

The optimal operational parameters for BPA degradation were pH = 4, T = 20 ° C, Q = 1 mL/min, and [H₂O₂] = 2 ppm, while, with a reaction time of 0.25 h, a higher degradation efficiency of BPA (99.3%) was achieved. For the same reaction conditions, the highest degradation efficiency of DBP was 78%.

The use of a continuous-flow microreactor supported by TiO₂ is a potential method for the treatment of wastewater contaminated by endocrine disruptors.



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sciforum-112464: Thermally exfoliated urea-derived g-C₃N₄/Ti₃C₂T_x MXene 2D/2D Schottky junctions as photocatalysts for the removal of pharmaceutical pollutants in aquatic matrices

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In recent decades, the most common photocatalyst used in environmental applications has been TiO₂, which exhibits a large band gap and can only be photoactivated under UV light. Therefore, the scientific interest has recently focused on the development of visible-light-activated photocatalysts such as g-C₃N₄. However, the photocatalytic performance of g-C₃N₄ is significantly hindered by the rapid recombination of photogenerated charges. An interesting approach to overcome this drawback is to fabricate Schottky junctions by combining g-C₃N₄ with materials demonstrating high metallicity.

In the present study, g-C₃N₄ was synthesized by forming a urea slurry that was dried and then calcinated at 550 °C for 4 h (CNU). The resulting CNU was ground and calcinated again at 550 °C for 2 h (3×) to achieve thermal exfoliation of its stacked 2D layers (CNUex3). In addition, a quantity of CNUex3 was then subjected to protonation using an HCl solution (pCNUex3). Ti₃C₂T_x MXene was prepared via a top-down methodology using HF to achieve wet-chemical etching of the Al layers from the Ti₃AlC₂ Max Phase. Subsequently, low amounts of Ti₃C₂T_x were coupled with either CNUex3 or pCNUex3 via a simple sonication methodology to form x%-CNMX or x%-pCNMX 2D/2D Schottky junctions (x = 1, 3 or 5), respectively. The structural, morphological and optical characteristics of all the synthesized materials were investigated using various characterization techniques (PXRD, SEM, ATR-FTIR, Raman spectroscopy, DRS, etc.). Furthermore, their photocatalytic performance was evaluated through laboratory-scale experiments using the antihypertensive drug Valsartan as a model pollutant, since it is commonly detected in various aquatic matrices. The results revealed that the combination of either CNUex3 or pCNUex3 with low amounts of Ti₃C₂T_x improves their photocatalytic performance due to the successful suppression of exciton recombination as a result of the formation of a Schottky barrier at the interface of the two materials.



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Session D. Electrocatalysis

sciforum-112680: *Juniperus brevifolia* as a potential biomass source for the construction of efficient oxygen (electro)catalysts

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The global economy's sharp growth, extreme fossil fuel consumption and the continuous increase in the population have been forcing the development of more sustainable catalytic processes as well as renewable energy technologies to overcome environmental degradation and the current energy crisis. Unfortunately, renewable energy sources are often unreliable and intermittent, limiting their large-scale applications. Among the most viable electrochemical energy storage and conversion systems are fuel cells, metal-air batteries, and supercapacitors. The oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) are crucial in electrochemical devices like metal-air batteries and reversible fuel cells [1]. However, these reactions have high activation barriers, limiting the effectiveness of energy conversion devices that use these processes. In addition, both ORR and OER require expensive and scarce precious metal electrocatalysts, making them difficult to use on a large scale. This has stimulated the quest for new, non-expensive, and highly active electrocatalysts during the last few years [2,3].

Therefore, with this in mind, a series of Co/N-doped biochar catalysts were prepared by mechanochemical synthesis using the different parts of *Juniperus brevifolia* (leaves, bark and wood). Cobalt was chosen taking into consideration the biochar's potential (electro)catalytic performance as ORR and OER electrocatalysts.

Activation under chemical/physical experimental conditions resulted in surface areas of $972 > \text{BET} > 145 \text{ m}^2/\text{g}$. The successful preparation of electrocatalysts was confirmed by XPS, XRD, Raman spectroscopy and SEM/EDS. The best-performing electrocatalyst, Co/N-JBL, showed similar ORR performance to the state-of-the-art Pt/C catalyst. Regarding the OER, Co/N-JBL also showed the most promising results, with an overpotential (η_{10}) of 0.45 V vs. RHE.

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sciforum-115534: NiO/Co₃O₄ composite: A noble-metal-free bifunctional catalyst for oxygen evolution reaction and oxygen reduction reaction applications

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Oxygen evolution reaction (OER) and oxygen reduction reaction (ORR) are critical for the efficient functioning of fuel cells, electrolyzers, metal–air batteries, etc. It is well known that Pt-based catalysts are excellent for ORR but are poor for OER; similarly, Ru,Ir-based materials are excellent for OER but poor for ORR. However, these materials (Pt, Ir, Ru) are expensive and less abundant. Therefore, there is a need to develop cheaper and sustainable alternatives that are good at both ORR and OER (bifunctional) so that they can be used in regenerative fuel cells, which can operate as a fuel cell and water electrolyzer. Herein, we report a simple synthesis method for the formation of a NiO/Co₃O₄ composite, as confirmed by a multitude of characterization techniques, namely X-ray diffraction, Raman scattering, X-ray photoelectron spectroscopy (XPS), etc. The noble-metal-free composite, i.e., NiO/Co₃O₄ composite, was tested as a bifunctional catalyst for OER and ORR. The composite exhibited excellent performance in ORR and OER with very low catalyst loading. An onset potential of 0.73 V vs. RHE at 0.1 mA/cm² for ORR and an overpotential of 0.48 V vs. RHE at 10 mA/cm² for OER were obtained for the composite. The redox couples Ni²⁺/Ni³⁺ and Co²⁺/Co³⁺ and oxygen defects in the composite are attributed to the enhanced OER and ORR performances. These results are quite encouraging given that the synthesis of the composite is simple, and the precursors used for the same are environmentally benign.



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sciforum-112713: CuCo₂O₄ as Catalyst for Oxygen Evolution Reaction in Anion Exchange Membrane Water Electrolysis

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Abstract

The UK government aims to achieve net-zero greenhouse gas emissions by 2050 [1]. Water electrolyzers (WEs) represent a promising solution for generating high-purity hydrogen fuel without environmental pollution. Among WE technologies, Anion Exchange Membrane Water Electrolyzers (AEMWEs) offer a unique combination of the benefits of alkaline water electrolyzers (AWEs) and proton exchange membrane water electrolyzers (PEMWEs). However, the performance of AEMWEs heavily depends on precious metal catalysts for the oxygen evolution reaction (OER), making them cost-prohibitive. This study investigates Copper Cobalt Oxide (CCO) spinels as a low-cost, high-performance alternative to precious metal catalysts.

Methods

A hydrothermal synthesis approach, adapted from Abu Talha Aqueel Ahmed et al. [2], was used to synthesise CCO spinels. Reaction parameters, including precursor ratios, temperatures, and synthesis durations, were systematically varied to optimise catalyst composition and morphology. Synthesised materials were characterised using SEM/EDX and XRD to confirm structure and composition.

Results

Physical characterisation revealed the successful synthesis of CCO nanoparticles with distinct morphologies, including flower-like and needle-like structures. Increasing the hydrothermal synthesis temperature to 180°C enhanced purity and homogeneity. Electrochemical testing via cyclic voltammetry (CV) demonstrated that incorporating Cu into the CCO structure improved OER activity, reducing the onset potential and increasing the current density.

Conclusions

This study highlights the potential of CCO spinels as cost-effective, efficient OER catalysts for AEMWEs. The optimised hydrothermal synthesis protocol and resulting nanostructures significantly improved catalytic activity, paving the way for sustainable hydrogen production technologies.

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sciforum-112686: Development and Characterization of a Bismuth-based MOF Electrode for the Electrophoto-catalytic Degradation of Rhodamine

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Introduction:

Environmental pollution, particularly from organic contaminants, poses a growing challenge to public health and the environment. Photocatalysis and electrocatalysis are promising technologies for pollutant degradation, and their integration can enhance the efficiency of this process. Metal-organic frameworks (MOFs) are of increasing interest for such applications due to their high surface area and tunable structure, which can improve both electrocatalytic and photocatalytic performance.

Methods:

In this study, a bismuth-based MOF using a 2,6-dicarboxynaphthalene linker was synthesized on an FTO substrate modified with TiO₂. The MOF was grown through a reflux reaction in DMF at 110°C for 12 hours. The electrode was characterized using morphological and spectroscopic techniques. Its electrochemical properties were evaluated using chronoamperometry, linear sweep voltammetry, and EIS analysis. Its active surface area and electron transfer coefficient were determined to assess its performance. Its catalytic efficiency was tested in a pH 7 Na₂SO₄ solution for rhodamine degradation, both in electrocatalytic and photo-electrocatalytic modes.

Results:

SEM analysis showed a uniform MOF distribution on the FTO-TiO₂ substrate, while FT-IR spectroscopy confirmed carboxylate formation, consistent with the MOF structure. Raman analysis validated the successful formation of MOF and demonstrated its stability post-experiment. Electrochemical tests showed that the Bi-MOF-modified electrodes had a larger electroactive surface area compared to bare TiO₂/FTO electrodes. The EIS analysis provided insights into the charge resistance and electrochemical behavior of the system. The Bi-MOF system demonstrated excellent rhodamine degradation, with a photo-electrocatalytic performance surpassing electrocatalysis alone.

Conclusion:

The MOF-modified system showed enhanced photo-electrocatalytic properties compared to bare TiO₂/FTO electrodes, making it a promising candidate for environmental applications in organic pollutant degradation.



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sciforum-111310: Electrocatalytic layers for medium-temperature polymer membrane water electrolysis

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Medium-temperature (up to 200°C) polymer membrane water (steam) electrolyzers are attractive due to improved thermodynamics and kinetics, and reduced specific electric energy consumption for electrolytic gas generation. Moreover, applications of alternative polymer membranes (such as acid-doped polybenzimidazoles) less sensitive to the presence of the impurities in water (in contrast to Nafion® and its analogs) significantly simplify the water treatment system.

The aim of this study is to develop electrocatalytic layers with high and stable proton and electron conductivity and mass transfer efficiency under conditions of strong electric/thermal/chemical fields for medium-temperature polymer membrane water electrolysis. The most severe conditions are associated with anodes, in which active oxygen and oxygen radicals are generated at increased temperatures and low pH values. Both mathematical modeling and experimental techniques have been applied to create a three-dimensional stable conducting network of pores, electrolytes, and supported catalytically active nanoparticles. The results show that IrO₂ supported with Ta₂O₅ or TaC could be potentially used as catalysts for anode of medium-temperature electrolyzers with polybenzimidazole-based membranes doped with H₃PO₄. In particular, even a few % of Ta₂O₅ improves IrO₂ activity and stability towards the oxygen evolution reaction, as well as reducing noble metal loading. It was shown that the optimum catalyst structure and composition depend on the applied synthesis method (chemical or physical). Electrocatalytic layers with a component concentration gradient are recommended. Numerical calculations have shown that in the anode electrocatalytic layer, the main reaction zone is shifted towards the gas diffusion electrode. Hence, during the formation of the catalyst layer, it is recommended to increase the concentration of the catalyst across the catalyst layer thickness (from the membrane towards the gas diffusion electrode). For the cathode, the use of carbon-supported Pt nanoparticles with a reverse concentration gradient is recommended.

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sciforum-112695: Gold Nanoparticle-Modified Nickel–Iron Coatings for Efficient Sodium Borohydride Electrooxidation

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Sodium borohydride is regarded as a potential alternative fuel for direct liquid fuel cells due to its high energy density and ease of handling. However, the efficient electrooxidation of sodium borohydride (BOR) requires the development of advanced electrocatalysts with high activity, low cost, and long-term stability. Transition metal-based catalysts, particularly nickel–iron alloys, have shown considerable promise due to their affordability and favourable catalytic properties. This study explores the synergistic effects of gold and nickel–iron components in achieving high current densities and low overpotentials, which makes these materials promising for applications in direct borohydride fuel cells (DBFCs) and energy storage systems. Herein, we investigate the fabrication, characterization, and electrocatalytic properties of nickel–iron (Ni–Fe) coatings decorated with gold nanoparticles (AuNPs) for BOR. The objective of incorporating AuNPs onto Ni–Fe coatings is to enhance their catalytic activity and stability. Ni–Fe coatings were prepared using two techniques: electroless metal plating and galvanic displacement.

It was determined that AuNPs of a few nanometers in size were deposited on the NiFe coatings through the immersion of a NiFe/Cu electrode in a gold-containing solution for various periods. The BOR was evaluated in 0.05 M and 1 M NaOH solution using cyclic voltammetry and chronoamperometry. The fabricated NiFe catalysts with different AuNP loadings demonstrated significantly higher electrocatalytic activity towards the BOR as compared to bare Au or NiFe/Ti. This indicates the potential of AuNP-decorated NiFe coatings as a promising material for BOR in DBFC applications.

Acknowledgement

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sciforum-112447: Intermetallic compounds from the non-noble metals as the catalysts in the electrochemical reactions of ammonia synthesis

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Introduction.

Intermetallic compounds (IMCs), which have a homogeneous structure of active centers with controlled electronic structures and an atomic ensemble size, can be used to create catalysts with unsurpassed practical characteristics, including for demanding and stable electrochemical reactions such as nitrogen reduction (NRR), nitrate reduction (NO₃RR), and nitrite reduction (NO₂RR), which can serve as a replacement for the industrial Haber–Bosch process. An urgent task is to develop efficient electrocatalysts using cheap base metals, with partial or complete replacement of noble metals. For this purpose, the use of IMCs based on cobalt, iron, and silicon as well as some rare earth elements is proposed.

Methods.

IMCs were synthesized using a facility for electric arc melting in a rarefied argon atmosphere. In this work, the following physicochemical methods for the characterization of the IMC samples were used: UV-vis spectroscopy, optical microscopy, SEM, EDX, XPS, and XRD. For electrochemical characterization, impedance spectroscopy and the method for determining the capacitance of the electrical double layer were employed. Linear voltammetry and chronoamperometry were used to determine the optimum conditions for the reactions and ammonia synthesis.

Results and Discussion.

The results show the advantages of using electrocatalysts in the form of IMCs, which demonstrate increased values of Faraday efficiency and ammonia yield rates. Schemes of the mechanism of the studied reactions for IMCs and exhaustive clarifications of the actions of electrocatalysts are proposed. The chosen strategy, as well as methods, make it possible to confidently predict the advantages in the NO₃RR reaction.

Acknowledgment.

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sciforum-115715: NiFe-LDH and Manganese-Based Catalysts for Advanced Metal–Air Battery Applications

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Metal–air batteries offer high energy density but suffer from sluggish oxygen electrochemistry. This work focuses on developing efficient bifunctional catalysts, combining NiFe-LDH with manganese-based materials, to address this challenge and enable the practical application of these promising energy-storage devices.

Manganese-based catalysts were synthesized via a sol–gel autocombustion method. NiFe-LDH materials were prepared through a hydrothermal method. The synthesized materials were subsequently compounded with pristine and nitrogen-doped carbon nanofibers to create composite electrodes. This combination aimed to improve the overall electrochemical performance of the materials. Electrochemical measurements were conducted in a conventional three-electrode cell configuration. An alkaline electrolyte was used, with a Hg/HgO electrode serving as the reference electrode and a graphite rod as the counter electrode. The electrocatalytic activity of the materials towards the ORR and OER was assessed through a series of electrochemical techniques, including cyclic voltammetry, linear sweep voltammetry, and electrochemical impedance spectroscopy.

Electrochemical evaluation using CV and LSV in a three-electrode cell revealed promising electrocatalytic activity of the synthesized NiFe-LDH and manganese-based materials towards both OER and ORR. The materials exhibited significant current densities and favorable onset potentials, consistent with their structural and compositional characteristics. These findings demonstrate their potential for high-performance metal–air battery applications.

This study demonstrates the feasibility of NiFe-LDH and manganese-based spinels as bifunctional electrocatalysts for metal–air batteries. A comprehensive characterization confirmed their desired properties, and an electrochemical evaluation revealed promising activity for both ORR and OER. While promising, further research is crucial to optimize their performance, including long-term stability studies and the exploration of strategies such as doping and support engineering. These findings contribute significantly to the advancement of sustainable energy technologies.



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sciforum-115752: Optimized magnetron-sputtered CuFeO₂ thin films for PEC water splitting application

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CuFeO₂ (CFO) has been recently identified as a promising photocathode material for photoelectrochemical (PEC) water splitting. However, this p-type semiconductor suffers from poor photo-induced electron-hole separation and charge collection. In this study, CFO thin films were successfully sputtered via a magnetron sputtering technique, and their PEC experiments were carried out under front-side chopped illumination in 1M NaOH electrolyte against a Ag/AgCl reference electrode. In argon, the thin films produced low photocurrent, while in oxygen, it enhanced the photocurrent and rose to 0.55 mAcm⁻² at 0.4 V vs. RHE (V_{RHE}). The synthesis parameters dictated the water splitting efficiency; when the power of the Fe target increased from 160 W to 200 W, the photo-current density enhanced and reached the highest value of 0.55 at 0.4 V vs. RHE (V_{RHE}) due to its lower charge transfer resistance according to EIS data. Similarly, the Cu power was optimized in which the highest J-V was produced with a power of 40 W rather than 60 and 80 W. The other constituent of CFO that affects the PEC activity is oxygen; an oxygen flow rate of 2 sccm (with O₂:Ar = 1:9) was optimal; increasing this further reduced the J-V. AFM spectroscopy revealed that the roughness of the thin films increased as a function of Fe and Cu sputtering power, whereas SEM-EDAX inferred a homogeneous distribution of the elemental constituents.



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sciforum-114515: PEM fuel cell conditioning for subzero storage and cold start using electrocatalytic heating

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In a number of proton-exchange membrane (PEM) fuel cell applications, the storage and subsequent start-up under subzero temperatures is required. If water (the product of an electrochemical reaction) is frozen in the bipolar plate channels, gas diffusion electrodes, and membrane-electrode assemblies in a switched-off fuel cell at subzero temperatures, their destruction may occur as a result of an increase in the volume occupied by water when it is converted to ice by, ca., 9%. The original methods of PEM fuel cell conditioning before storage and subsequent start-up at subzero temperatures are suggested in this communication. In particular, the electrocatalytic self-heating of PEM fuel cells in the maximum power mode is proposed to increase its temperature up to 100-130 °C, which makes it possible to transfer water from a liquid to a gaseous phase, and effectively remove it by purging the internal cavities of the fuel cell with reagent gases (hydrogen, oxygen, or air). Corresponding strategies developed by the author and the engineering solutions realized in the experimental set-up are reported and discussed. It is shown that the suggested approaches for PEM fuel cell conditioning before it is shut down allows one to work out the issues of the storage, transportation, and cold start of PEM fuel cells at deeply negative temperatures. This work was supported by the Ministry of Science and Higher Education of RF under the project FSWF-2023-0014.



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sciforum-112707: Polyoxometalate-Decorated MWCNTs as High-Performance Electrocatalysts for Oxygen Reactions

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The ongoing and significant growth in global energy demand makes it crucial to develop new, cost-effective, high-quality materials on a large scale to serve as effective electrocatalysts (ECs) in clean energy storage and conversion devices. Among these, fuel cells (FCs) and water splitting devices have emerged as promising candidates. However, their application has been constrained by the reliance on noble metal-based electrocatalysts. In oxygen reactions, specifically O₂ reduction (ORR) and evolution (OER), conventional electrocatalysts are based on noble metals and their oxides, including Pt, Pd, RuO₂, and IrO₂. However, in addition to being scarce and expensive, these materials have poor stability under operating conditions. For this reason, the practical application of these technologies requires the development of efficient electrocatalysis for these processes, which has prompted a recent search for new, cost-effective, and highly active electrocatalysts. Polyoxometalates (POMs) have been proposed as a potential alternative to traditional electrocatalysts, offering a cost-effective solution with high efficiency.

This work involves the preparation of two hybrids based on Dawson Sandwich-type polyoxometalates and multi-walled carbon nanotubes doped with melamine (CoNi₃@MWCNT_N8 and NiCo₃@MWCNT_N8). The two electrocatalysts exhibited excellent electrocatalytic performance in OER in an alkaline medium (0.1 M KOH), with maximum current densities of 86.70 and 68.32 mA cm⁻² and overpotential values of 0.45 and 0.49 V vs. RHE. Furthermore, the two electrocatalysts showed favorable performance in ORR in the same electrolyte, with diffusion limiting current densities of -2.98 and -2.33 mA cm⁻² and potential onset values of 0.82 and 0.78 V vs. RHE.



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sciforum-112398: Sodium Borohydride-Induced Surface Modification of Manganese Oxides for Optimized ORR Active Electrocatalysts

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Abstract

Introduction:

Manganese oxide octahedral molecular sieves (OMSs) are promising catalysts for oxygen reduction reactions (ORRs) due to their cost-effectiveness and durability. However, their practical application is hindered by inherent limitations, including low electrical conductivity and insufficient intrinsic catalytic activity.

Method:

To address these challenges, we employed a novel surface reduction etching treatment using sodium borohydride (NaBH_4) to optimize the oxygen vacancy content of OMS materials. This method involves immersing OMS samples in varying concentrations of NaBH_4 solution followed by vacuum annealing, leading to the controlled introduction of oxygen vacancies.

Results:

The NaBH_4 treatment significantly increased the number of oxygen vacancies on the OMS surface. These vacancies act as crucial active sites, facilitating the adsorption and dissociation of oxygen molecules, thereby improving ORR activity. Furthermore, the treatment was found to regulate the $\text{Mn}^{3+}/\text{Mn}^{4+}$ ratio on the nanorod surface, further promoting catalytic efficiency. Notably, the OMS material treated with 6mmol/L NaBH_4 exhibited a remarkable half-wave potential of 0.74 V in an alkaline medium of 0.1M KOH electrolyte, which is comparable to the state-of-the-art platinum catalyst (0.837 V).

Conclusions:

The optimized OMS materials exhibited significantly improved ORR performance compared to pristine OMS. This enhancement is attributed to the increased availability of active sites and the improved interaction between oxygen molecules and the OMS surface. The NaBH_4 surface etching treatment provides a simple and scalable approach to unlock the full potential of OMS materials for ORR catalysis, paving the way for advancements in energy storage and conversion technologies.



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sciforum-114990: Theoretical insights into how to inhibit an undesirable reaction while catalyzing a desirable reaction: hydrogen peroxide production during the hydrogen oxidation reaction in a proton-exchange membrane fuel cell

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In practical catalysis, it is often required to focus not only on catalyzing a desirable reaction but also inhibiting an undesirable reaction. Such is the case of the hydrogen anode in the proton-exchange membrane fuel cell (PEMFC), which is an attractive power source for long-distance trucks, where it has a weight advantage in comparison with battery power. The desirable reaction is the hydrogen oxidation reaction (HOR), but an undesirable reaction can also occur simultaneously, namely the production of hydrogen peroxide at the hydrogen anode from oxygen gas diffusing from the oxygen cathode. This hydrogen peroxide can attack the membrane, either directly or after it decomposes, to produce hydroxyl radicals in a Fenton reaction. This attack can severely limit the membrane's lifespan, thus increasing the operational cost. We recently found that a platinum alloy with cobalt was effective in inhibiting peroxide production, because the coverage of adsorbed hydrogen on the catalyst was smaller than that on pure platinum. In order to make further progress, it is necessary to carefully examine all of the possible reaction pathways involving various types of adsorbed hydrogen with O₂, including bridging and on-top hydrogen on (111) facets, bridging hydrogen on (100) facets, and on-top hydrogen at (110) steps (V configuration) and (110) edges. Based on our recent density functional theory (DFT) calculations, the V configuration is particularly important, especially since it is also involved in the HOR itself, so we must be careful to preserve the high activity of this reaction while inhibiting peroxide production. We predict that pure Rh and Ir as well as PtRh and PtIr alloy catalysts will all be effective, since they adsorb less H overall at given potentials, require more negative potentials to adsorb H, and also adsorb O₂ in a bridging configuration, making it unable to produce H₂O₂.



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Session E. Biocatalysis

sciforum-112101: Comparing the secretome response of *Aspergillus* and *Fusarium* species on chemically treated plastics

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Nowadays, plastic pollution represents one of the most pressing environmental challenges, with millions of tons of synthetic polymers accumulating worldwide in landfills as well as in water bodies. Polyethylene terephthalate (PET), widely used in packaging and textiles, is resistant to natural degradation, while polylactic acid (PLA), although considered biodegradable, requires specific industrial conditions. Biological approaches, particularly those utilizing fungal strains, offer a sustainable alternative for addressing plastic waste. In this study, thirteen fungal strains were screened for their ability to grow on solid media containing chemically treated PET or PLA as the sole carbon source. The two most promising strains, *Fusarium oxysporum* BPOP18 and *Aspergillus parasiticus* MM36, demonstrated significant growth and polymer clearance halos on both PET and PLA solid media. However, enzymatic assays in liquid cultures revealed notable protease and esterase activity only in the presence of PLA, while in the presence of PET, the fungi showed no detectable enzymatic activity. To further investigate the enzymatic mechanisms underlying PLA degradation, proteomic analysis was conducted on the secretome of both fungi from PLA cultures. This revealed the presence of key proteins potentially involved in PLA breakdown, providing insights into enzymatic pathways and supporting the development of fungal-based biotechnological solutions for plastic waste management.



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sciforum-114745: Screening biocatalysts for the selective enzymatic separation of polyester blends

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Packaging materials account for 40% of Europe's annual 50 million tons of plastic demand, and are primarily used in food applications. Their short lifespan and increasing use contribute significantly to environmental pollution. Mechanical recycling addresses only a small portion of food packaging waste due to the complexity of mixed-polymer packaging. These unsorted blends exhibit poor mechanical, thermal, and optical properties, rendering conventional recycling methods inefficient. Although incineration provides energy recovery, it contradicts circular economy principles, while chemical recycling lacks economic feasibility and fails in specificity for plastic mixtures containing polymers of the same type, such as polyesters. Enzymatic recycling offers a promising, sustainable alternative. This selective depolymerization method can address challenges associated with complex packaging waste streams by enabling the targeted breakdown of polymers like PLA and PET.

Herein, 17 serine hydrolase enzymes (esterases and proteases), both in-house and commercial, were investigated for their specificity in polyester degradation. In-house enzymes were heterologously expressed in *Escherichia coli* or *Pichia pastoris* and their degradation potential was tested through reactions with semi-crystalline PET and two PLA grades: semi-crystalline PLLA and amorphous PDLLA. The degradation yield was evaluated by measuring the variation in molecular weight, through Gel Permeation Chromatography (GPC) for PLA and the concentration of hydrolysis products, and through High Performance Liquid Chromatography (HPLC) for PET.

The results show that most esterases cannot distinguish between PET and PLA, while proteases are specific to PLA. LCC^{ICCG} was the most efficient PETase (15 $\mu\text{g}_{\text{prod}}/\text{mg}_{\text{PET}}$) that could not degrade PLA, while Protease K and Savinase effectively degraded both amorphous ($M_{w,\text{reduction}} = 16.5\%$) and semi-crystalline ($M_{w,\text{reduction}} = 28.2\%$) PLA, respectively, but not PET.

Consequently, the treatment of packaging waste streams with the aforementioned PETase and PLAases could lead to the selective degradation of these polymers, purifying the mixture and facilitating further recycling, providing a sustainable pathway for advancing plastic waste management.



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sciforum-111261: A novel xyloglucanase from the white rot fungus *Abortiporus biennis* and its potential role as an accessory biocatalyst in the enzymatic degradation of xyloglucan-containing substrates

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Lignocellulosic biomass is a composite material consisting of cellulose, hemicellulose, and lignin. Xyloglucan is a complex, highly substituted plant biomass hemicellulose that covers cellulose fibrils. Xyloglucanases, the enzymes responsible for its degradation, can be utilized for the design of efficient bioprocesses by incorporating them in enzyme cocktails that target cellulose-containing substrates. In order to shed light on the enzymatic degradation of xyloglucan, a novel xyloglucanase was studied from the basidiomycete *Abortiporus biennis*. Initially, a bioinformatic analysis of the xyloglucanase was carried out based on its amino acid sequence, followed by the heterologous production of *AbxKega* with the methylotrophic yeast *P. pastoris* acting as the host. Afterwards, the enzyme was purified to determine its biochemical and catalytic properties. Finally, its activity was investigated in 2 lignocellulose substrates (apple pulp, corn bran) to determine the synergism of *AbxKega* with a commercial cellulase preparation. From the results of these experiments, *AbxKega* was found to be a monomeric glycoprotein with a β -jelly roll structure with relatively strict substrate specificity, since it is only active in xyloglucan and β -glucan in an endo-dissociative way. The main hydrolysis products were the oligomers XXXG, XLXG/XXLG, and XLLG, and the optimum activity conditions are pH 4.5 and 55 °C. *AbxKega* was applied together with cellulases on the saccharification of corn bran and apple pulp. Overall, the importance of xyloglucanases on the saccharification of xyloglucan-containing substrates was demonstrated in this study. The results could contribute to the design of more efficient, tailor-made enzyme cocktails for the saccharification and subsequent valorization of lignocellulose.



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sciforum-108546: Electrochemical oxidation of lignin biomass to promote low-cost hydrogen

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Lignin is one of the most abundant renewable materials on Earth. Despite representing a significant carbon and energy resource with great potential as a source of aromatic compounds, lignin is often treated as waste in the context of lignocellulosic biomass biorefineries. The electrochemical oxidation of biomass waste (e.g., lignin) from biorefineries and pulping mills represents a potentially renewable development for hydrogen production with the co-generation of valuable marketable chemicals. By using a low-voltage anodic oxidation process, this method might significantly lower the cost of producing hydrogen and industrial, value-added compounds. Biomass compounds such as lignin have primarily been studied electrochemically on costly metal electrodes up to this point. Therefore, non-precious metal-based electrocatalysts, such as Iron (Fe), Nickel (Ni), Copper (Cu), Manganese (Mn), etc., were synthesized with a simple innovative method, thoroughly characterized, and tested for the electro-oxidation of Phenol, 4-phenoxy phenol, and lignin. The surface area available for electrochemical reactions is increased by nanoparticle electrocatalysts, which may result in better mass transport of reactants and products across the electrocatalyst layer. Non-precious metal electrocatalysts also enable special alloying and the synergistic interaction of several metals. Our research explores the utilization of non-precious metal nanoparticle electrocatalysts for the electrochemical lignin oxidation approach to promote hydrogen production.



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sciforum-112666: Enzymatic oxidation of lignocellulosic biomass-derived furans using novel redox biocatalysts

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Lignocellulosic biomass, a readily available and abundant organic material, is an ideal source of high-value compounds that can replace petroleum-based products. Among these, 5-hydroxymethylfurfural (HMF), obtained by the catalytic dehydration of biomass sugars ^[1], is a significant intermediate that can be converted into valuable compounds, including 2,5-furandicarboxylic acid (FDCA), a promising precursor for biopolymers ^[2]. Biocatalysis offers an environmentally friendly and efficient alternative to traditional chemical methods ^[3-5]. This study explores the biotransformation of HMF towards its oxidized derivatives using novel fungal enzymes from the Auxiliary Activity family AA5 of the CAZy database. Using the targeted exploration of fungal genomes, two promising enzymes, a glyoxal oxidase (*GGlyOx*) and a galactose oxidase (*FoGalOx*), were identified and expressed heterologously in *Pichia pastoris*. The recombinant proteins were purified and tested for their ability to oxidize model furans (HMF and its derivative compounds). Our results reveal that both enzymes facilitate the production of oxidized monomers, with *GGlyOx* showing efficiency in the biotransformation of HMF to 5-hydroxy-2-furancarboxylic acid (HMFA) and furan-2,5-dicarbaldehyde (DFF) to 5-formylfurancarboxylic acid (FFCA), while *FoGalOx* was more efficient in oxidizing HMF to DFF and HMFA to FFCA. The enzymes were also tested for their ability to transform HMF obtained from real biomass hydrolysates from OxiOrganosolv pretreated wheat straw pulps ^[6] via enzymatic saccharification and isomerization, followed by catalytic dehydration in mild conditions. Various acidic catalysts, including homogeneous (heteropolyacids, organic acids) and heterogeneous (zeolites, supported heteropolyacids) systems, were evaluated for their efficiency in dehydrating sugars to furans. The results highlight that the type and ratio of Brønsted to Lewis acidity play a key role in determining the reaction pathways for sugar conversion, significantly influencing the product distribution. This work demonstrates the potential of enzymatic biotransformation as a sustainable route for converting lignocellulosic biomass into valuable chemicals for green polymer production and other industrial applications.



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sciforum-112693: Exploiting basidiomycetes and their enzymatic systems for the degradation of synthetic polymers

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The increasing environmental burden of synthetic polymer waste has intensified the need for sustainable solutions to plastic pollution ^[1]. Microbial enzymes, particularly those from fungal strains, are emerging as promising biotechnological tools for waste circularity ^[2]. White-rot fungi, known for producing ligninolytic enzymes (oxidases and hydrolases), can degrade complex polymers (lignin, cutin, waxes, plastics) by disrupting their chemical structure ^[3,4]. This study investigates a strain of the order Agaricales (Basidiomycota), previously isolated from a Greek habitat and identified through ITS rRNA gene sequencing, that has shown great potential for plant-litter degradation but remains largely unexplored in terms of the depolymerization of xenobiotic polymers (plastics). The strain was tested for its ability to grow on polyester- or polyether-polyurethane (Impranil® DLN-SD, Impranil® DL 2077) as the sole carbon source, demonstrating efficient substrate degradation and high biomass yield. To explore the underlying biodegradation mechanism, a spectrophotometric assessment of extracellular enzymatic activities (hydrolases and oxidative enzymes) on Impranil® DLN-SD culture supernatants was performed; the results indicated high oxidative enzyme activity. Substrate modifications were detected through attenuated total reflectance–Fourier-transform infrared spectroscopy (ATR-FTIR), while gas chromatography–mass spectrometry (GC-MS) analysis was performed to identify the biodegradation products. Proteomic analysis of culture supernatants was conducted to identify and quantify enzymes involved in polymer degradation. This study highlights the potential of this strain as an effective biocatalyst for polymer degradation, providing a sustainable approach to plastic waste management and byproduct valorization.



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sciforum-112407: Oxidation of Malachite Green by Illite Impregnated with Iron/Indium

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The contamination of aquatic systems by synthetic dyes, such as malachite green, poses significant environmental and health risks due to their toxicity and persistence. In this study, we investigated the catalytic oxidation of malachite green using illite impregnated with iron (Fe) and indium (In) as a heterogeneous catalyst. The catalyst was synthesized through a wet impregnation method, ensuring the effective dispersion of metal ions on the illite clay surface. Comprehensive characterization of the material was conducted using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM-EDX) to elucidate its structural, morphological, and chemical properties.

The catalytic oxidation process was evaluated under various conditions, including varying the dye concentration, pH, and reaction temperature, to optimize the degradation efficiency. The Fe/In-illite catalyst achieved a degradation rate of over 97% for malachite green within a short reaction time under the optimal conditions. Kinetic studies revealed a pseudo-first-order reaction mechanism. The dual functionality of iron and indium provided a synergistic effect, enhancing the catalytic activity through effective electron transfer and oxidation pathways.

This work highlights the potential of Fe/In-illite as a cost-effective and environmentally friendly catalyst for the removal of toxic dyes from wastewater. Its application could contribute significantly to sustainable wastewater management and environmental remediation efforts.



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sciforum-115169: Reaction Network Analysis and Kinetic Modeling of BHET Depolymerization as (Sub-)Network of PET

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Reaction Network Analysis and Kinetic Modeling of BHET Depolymerization as (Sub-)Network of PET

Introduction

Polyethylene terephthalate (PET) is widely used in fibers, films, and containers. Due to the low cost of virgin PET and the inferior properties of recycled PET [1-3], recycling remains economically unattractive in many regions [4]. Consequently, large amounts of PET are incinerated or end up in the environment, causing significant ecological damage [5]. Enzymatic depolymerization offers a sustainable alternative with mild conditions, energy efficiency, and environmental benefits [4]. While most studies focus on total depolymerization to terephthalic acid (TPA), this work targets the selective production of intermediates such as MHET and BHET, which are increasingly in demand for PET re-synthesis [6].

Experimental and Modeling

Two enzymes identified from prior screenings [6] were tested in different reaction media to analyze their effects on kinetics, equilibria, and product distribution. Ethylene glycol and DMSO shifted the product spectrum toward MHET. Mechanistic kinetic modeling, considering substrate, enzyme, and product inhibition, was performed to describe the reaction sub-network of BHET depolymerization with high accuracy.

Results and Outlook

A simplified reaction network for enzymatic PET depolymerization was established based on HPLC analysis. Reaction kinetics for BHET depolymerization were successfully modeled, providing a foundation for process design and optimization. Future work will extend the modeling to trimers and dimers and adapt the findings to PEF systems.



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sciforum-111412: Role of biocatalysts in biofuel production from lignocellulosic material

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Woodchips serve as a renewable and important readily available by-product of the forestry and timber sectors that can be utilized as biofuels through several methods, one of which is biocatalysis. The recent developments in biocatalysis have greatly increased the efficiency of converting wood chips into usable biofuels. Biocatalytic techniques utilize enzymes, microorganisms, and biocatalysts to decompose the intricate lignocellulosic structure of wood chips into fermentable sugars, bioethanol, biobutanol, or other forms of biofuels. The woodchips are primarily composed of cellulose, hemicellulose, and lignin, which are intricate polymers that are converted into biofuels. Prior to the biocatalysis process, woodchips typically undergo a pre-treatment process to break the lignin and other structural elements, allowing the cellulose and hemicellulose to unbind for better enzymatic breakdown. Some researchers are concentrating on producing biocatalysts which are capable of degrading both cellulose and lignin at the same time, which improves the overall process. For instance, modified enzymes or fungi such as *Trichoderma reesei* or species of *Penicillium* are utilized to improve cellulose hydrolysis, while microbes that degrade lignin are being modified for effective lignin decomposition. Enzymatic reactions play a crucial role in enhancing the efficiency of this conversion, and advancements in the development of biocatalysts are further enhancing the economic and technical viability of using woodchips as a biofuel source. This study examines the significance of biocatalysis in enhancing the conversion of wood chips into biofuels, emphasizing key enzyme systems such as cellulases and lignin-degrading enzymes that aid in the breakdown of cellulose, hemicellulose, and lignin components.



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sciforum-112705: Use of DERA in Development of Novel *N*-heterocycle-based Statin Precursors

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Hypercholesterolemia is a metabolic syndrome characterized by high levels of cholesterol in the blood plasma. Individuals with this condition have a significantly increased risk of developing cardiovascular diseases. Currently, natural or synthetic statins are prescribed to reduce cholesterol levels. In the synthesis of statin precursors, aldolases are often used. These are enzymes that catalyze the reversible and stereospecific aldol addition reaction between carbonyl compounds, forming chiral β -hydroxyketones or β -hydroxyaldehydes.

Among these enzymes, 2-deoxyribose-5-phosphate aldolase (*DERA*), which is acetaldehyde-dependent, can catalyze two consecutive aldol additions with absolute stereoselectivity, producing chiral 2,4,6-trideoxyhexoses that spontaneously cyclize into 2,4,6-trideoxy-D-erythro-hexapyranoses. However, a limitation of using DERA is that it becomes inhibited at high acetaldehyde concentrations, posing a challenge for large-scale reactions.

To obtain new statin precursors, we tested the activity of a genetically modified variant of DERA from *Pectobacterium atrosepticum*, showing a high tolerance to high concentrations of acetaldehyde, on crossed aldol addition reactions between acetaldehyde and aldehyde-based scaffolds derived from nitrogen-containing heterocycles, such as benzimidazole and substituted 4-phenyl-imidazoles, synthesized in our laboratory. The obtained products were analyzed using chromatographic and spectroscopic methods.

By replacing the heteroaromatic ring of commercial statins with different scaffolds, it may be possible to develop new hypocholesterolemic drugs that are more effective and have fewer side effects.



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Session F. Biomass Catalysis

sciforum-113698: Advancements in Biomass-Derived Catalysts for Sustainable Hydrogen and Bio-Oil Production: A Novel Integration of Catalyst Engineering, Life Cycle Assessment, and AI-Driven Optimization

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Biomass serves as an essential renewable energy source for the production of clean hydrogen (H₂) and bio-oil due to the ongoing global shift toward sustainable alternatives. The thermochemical methods of pyrolysis and gasification demonstrate potential for biomass conversion into valuable fuels which align with the European Green Deal and other sustainability goals across the world. These technologies face limiting technical and economic barriers because of catalyst performance problems, which affect cost efficiency and longevity. The authors introduce a new strategy using optimized biomass-based catalytic systems supported by progressive catalyst formulation techniques with life cycle analysis and predictive AI methods. Engineered biomass-derived catalysts possess excellent catalytic characteristics alongside advanced selectivity and superior environmental capabilities compared to traditional catalysts, as revealed by the experimental findings. A day-to-day LCA assessment shows that incorporating these catalysts leads to reduced carbon emissions throughout hydrogen and bio-oil production procedures. AI-based optimization techniques help forecast catalyst performance in different operational conditions to enable engineers to design highly stable catalytic systems. Experimental tests show that biomass-derived catalysts increase industrial output alongside sustainable processing capabilities. Economic analysis benefits from these catalysts when scaled up for industrial production. This strategy stands as a core contribution to achieving a clean energy future because it helps decrease fossil fuel usage and supports worldwide carbon emission reductions.



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sciforum-113242: Effects of Precipitation Variables on Phenolic Hydroxyl Group Content of Lignin Recovered from Black Liquor

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Black liquor, a by-product of the pulp and paper industry, is the main source of industrial lignin. Its conventional use as fuel for energy recovery underutilizes its potential and contributes to greenhouse gas emissions. Lignin, an aromatic polymer, can replace fossil fuel-based products like hydrogels, biosensors, and carbon fibers. The phenolic hydroxyl group of lignin is particularly important, as it plays a key role in determining lignin's functionality for various applications, including its antioxidant, adhesive, and polymer-stabilizing properties. Accordingly, this study employed a Box–Behnken design with 29 experimental trials to assess how pH, temperature, residence time, and acid concentration influence the total phenolic content (TPC) of lignin extracted via acid precipitation. Within the examined ranges, TPC values varied from 305.72 to 521.78 mg/g GAE, with the highest TPC achieved at pH 3, 70°C, 20% w/v H₂SO₄, and 1.5 h. In contrast, the lowest TPC occurred at pH 6, 25°C, 10% w/v H₂SO₄, and 1.5 h. A regression model and response surface methodology (RSM) were employed to analyze the data, and the model's significance was confirmed by ANOVA ($p < 0.05$), despite a moderate F value (2.7257). The model showed good explanatory power ($R^2 = 0.73$, $R^2\text{-adj} = 0.43$) and an insignificant lack of fit ($p = 0.3704$), suggesting it accurately captured the effects of the independent variables on TPC. The linear terms for pH and temperature were statistically significant, indicating that reducing pH and increasing temperature strongly enhance TPC. Interaction profiles and three-dimensional response surfaces revealed that acid concentration and residence time also affected TPC, with optimal conditions identified at 20% w/v H₂SO₄ and 1.5 h. These findings demonstrate that the careful optimization of process parameters can substantially improve lignin's phenolic properties, thereby guiding more efficient, sustainable strategies for lignin valorization.



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sciforum-114908: Emerging Catalysts and Techniques in Microalgae-Based Biodiesel Production

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The production of biodiesel from microalgae presents a sustainable and renewable solution to the growing global energy demands, with catalysts playing a critical role in optimizing the transesterification process. This review examines the emerging catalysts and innovative techniques utilized in converting microalgal lipids into fatty acid methyl esters, emphasizing their impact on reaction efficiency, yield, and environmental sustainability. Catalysts are integral to the transesterification process, facilitating the conversion of lipids into biodiesel while reducing processing time and energy requirements. Homogeneous catalysts, such as sulfuric acid and sodium hydroxide, are widely used for their high reactivity and cost-effectiveness. Sulfuric acid demonstrates excellent performance in in situ transesterification, achieving biodiesel yields of 73% and 92% from *Nannochloropsis oculata* and *Chlorella sp.*, respectively. However, the difficulty in separating these catalysts from the reaction mixture increases operational costs and environmental concerns. Heterogeneous catalysts offer a promising alternative due to their reusability and ease of separation. Examples include NaOH/zeolite, which has achieved biodiesel yields exceeding 98%, and KF/CaO, which demonstrated a yield of 93.07% when coupled with advanced techniques like ultrasound and microwave irradiation. Metal oxides such as CuO, NiO, and MgO supported on zeolite, as well as ZnAl-layered double hydroxides (LDHs), further enhance reaction performance through their high activity and stability. Enzymatic catalysts, particularly immobilized lipases, provide a more environmentally friendly option, offering high yields (>90%) and the ability to operate under mild conditions. However, their high cost and limited reusability pose significant challenges. Meanwhile, ionic liquid catalysts, such as tetrabutylphosphonium carboxylate, streamline the process by eliminating the need for drying and lipid extraction, achieving yields as high as 98% from wet biomass.



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sciforum-112669: Exploring the Catalytic Potential of Oxide Glasses (Ceramics) in the Thermal Decomposition of Fatty Acids

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To tackle the critical issue of reducing greenhouse gas emissions, renewable fuels such as biofuels present an attractive alternative to fossil fuels due to their lower toxicity, renewability, biodegradability, and cleaner combustion [1,2]. This study focuses on developing cost-effective and innovative catalysts, specifically glasses (ceramics) derived from the $\text{Na}_2\text{O}-\text{V}_2\text{O}_5-(\text{Al}_2\text{O}_3)-\text{P}_2\text{O}_5-\text{Nb}_2\text{O}_5$ system [3], for the pyrolytic deoxygenation of long-chain fatty acids into alkanes. Stearic acid was selected as a model compound to investigate the thermal decomposition of fatty acids and assess the catalytic performance of oxide glass (ceramic) catalysts, with additional experiments conducted on oleic acid and palmitic acid to extend the study. The tested catalysts varied in V_2O_5 content, ranging up to 70 mol% V_2O_5 , with commercially available V_2O_5 used as a standard reference material. Catalytic activity was evaluated using thermogravimetric analysis/differential scanning calorimetry (TG/DSC), while coupled thermogravimetry–infrared spectroscopy (TG-IR) and simultaneous thermal analysis–quadrupole mass spectrometry (STA-QMS) provided comprehensive insights into the decomposition mechanisms. The results indicated that catalysts with a higher V_2O_5 content (≥ 55 mol%) significantly enhanced the thermal decomposition of fatty acids. This study highlights that oxide glasses (ceramics) are efficient catalysts for fatty acid decarboxylation, offering a combination of thermal and chemical stability, cost-effective and straightforward synthesis, and the flexibility to fine-tune catalyst properties through simple compositional adjustments, which is crucial for industrial applications.

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sciforum-112867: Extraction of Lignin from Sawdust (*Chlorophora excelsa*)

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Sawdust is a plentiful source of lignocellulosic biomass, offering a sustainable alternative to fossil raw materials for the production of aromatics, fuels, and chemicals. Lignin, a key component of lignocellulosic biomass, serves as a renewable feedstock that can be depolymerized into aromatics suitable for use as octane enhancers or as precursors for high-value products. Additionally, lignin's multiple hydroxyl groups enable the synthesis of diverse polymers with potential industrial applications. This study investigates the extraction of lignin from *Chlorophora excelsa* sawdust using organosolv technology. The sawdust was collected and characterized, revealing a composition of 41.15% cellulose, 28.63% hemicellulose, and 26.13% lignin. The organosolv pretreatment process was conducted at temperatures of 100°C, 120°C, 140°C, 160°C, 180°C, and 200°C for 1 hour and 30 minutes. The sawdust was mixed with an ethanol–water solution (60:40 w/w) at a solid-to-liquid ratio of 1:10 (w/w), with 20% sulfuric acid as a catalyst. The highest lignin yield of 49.81% was achieved at 160°C, while the yields at 100°C, 120°C, 140°C, 180°C, and 200°C were 14.58%, 27.29%, 28.37%, 29.57%, and 24.48%, respectively. FTIR analysis confirmed that the lignin produced at 160°C contained multiple hydroxyl functional groups. Additionally, FTIR spectroscopy indicated chemical homogeneity across the extracted lignin samples. Elemental analysis using the Walkley–Black method, flame photometry, atomic absorption spectrometry, and wet digestion revealed the carbon, sodium, sulfur, and nitrogen contents of the lignin as 60.00%, 0.02%, 0.88%, and 0.40%, respectively. The bulk density, ash content, and moisture content of the extracted lignin were determined to be 0.264 g/cm³, 0.95%, and 1.88%, respectively.



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sciforum-112711: Glucose oxidation to High-Value Products Using Heterogeneous Catalysts

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Introduction

Developing new chemical processes based on sustainable feedstocks is essential for reducing the dependence on fossil resources, lowering greenhouse gas emissions, and fostering a more sustainable chemical industry [1]. Among these chemicals, gluconic acid is one of the most important products derived from glucose, due to its biodegradability, biocompatibility, and widespread applications in the pharmaceutical, food, construction, and cleaning industries [2]. The oxidation of glucose to gluconic acid has been extensively investigated using biochemical processes, as well as homogeneous and heterogeneous catalysis. Among these methods, heterogeneous catalysis offers significant advantages in terms of recyclability and process integration [3].

In the present work, the synthesis of gluconic acid from glucose is investigated, using hydrogen peroxide as the oxidant and gold-supported catalysts. An initial catalyst screening was conducted under standard reaction conditions (80 °C, 30 min), followed by an optimization study to evaluate the influence of key reaction parameters.

Experimental

The method followed for the synthesis of all mesoporous silicas (SBA-15, MCM-41, HMS-2, HMS-3, HMS-5) was based on self-assembly processes and the sol-gel method. Au modification was achieved via a polyvinyl alcohol (PVA)-protected method with in situ parallel reduction by using NaBH₄ as a reducing agent. All synthesized catalysts were fully characterized regarding their physicochemical properties. Glucose oxidation reaction was carried out in a batch, stirred, autoclave reactor (C-276 Parr Inst., USA). The reaction products were analyzed by ion chromatography (ICS-5000, Dionex, USA). The stability of the materials after the reaction was evaluated using ICP-AES analysis of the liquid phase.

Results and Discussion

The results indicated that all synthesized catalysts exhibited excellent stability, with no detectable leaching of Au. Notably, the 1Au/TiO₂ and 1Au/SBA-15 catalysts demonstrated the most promising performance, achieving glucose conversions of 69% and 67%, respectively, along with a gluconic acid selectivity exceeding 22 %.



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sciforum-111787: Grafted polyoxometalates as recoverable catalysts for biomass valorisation

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In the permanent research on sustainable processes, chemists are now looking for clean, safe and simple processes for producing chemicals.

Following the Green Chemistry principles established 25 years ago, each step in the procedure deserves to be studied in pursuit of these greener requirements.

- The use of renewable substrates is important for facing the depletion of fossil resources. Biomass is thus an important renewable source that has to be studied. Indeed, many platform molecules can be obtained from this resource and represent a short-carbon-cycle alternative.
- Energy savings have to be pursued. Catalysis is, in this respect, an interesting aspect in terms of gains in energy consumption. These energy gains are not to be neglected.
- Safer processes have to be found. Organic solvent-free processes are interesting solvent-sober protocols since they diminish some of the hazards involved due to the handling of organic solvents.

This work will present recent results concerning the use of polyoxometalates (POMs) grafted onto a solid support and their use as catalysts to valorize biomass. These POMs contained molybdenum and vanadium metals.

Simple protocols for the synthesis of these catalytic materials and their characterisation will be presented. Improvements compared to the literature will be emphasised.

Valuable natural substrates such as terpenes will be presented, and mechanistic conclusions will be given.



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sciforum-112237: Hydrothermal carbonization as a pre-treatment to selectively remove ashes from bamboo

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Hydrothermal carbonization (HTC) is a thermochemical treatment involving the use of subcritical water, which acts not only as solvent but also exploits its acidity as a catalyst, promoting carbonization reactions in biomass. In this study, HTC is proposed as a mild pre-treatment for enhancing the combustion properties of bamboo species, focusing on reductions in fouling and particulate matter emissions through selective solubilization of the ashes. Bamboo is one of the fastest-growing plants, and it can suitably grow on poor soils, such as marginal lands, making it a promising feedstock for biorefineries, even under Mediterranean climate conditions. In this context, optimization of the HTC treatment was carried out with the aim of maximizing the ash removal and at the same time preventing the solubilization of C5 and C6 structural carbohydrates. Several HTC tests were performed using a 300 mL Parr reactor, varying the reaction temperature (160-180-200 °C) and the reaction time (1-4-8 hours), with a biomass loading of 10 wt%. The macrostructural composition of the raw bamboo and the solids recovered from the HTC tests was determined, along with the chemical composition of their ashes. Moreover, physicochemical characterization of the corresponding mother liquors was carried out to obtain useful information about their valorization. The results indicate that the mildest HTC reaction conditions (160 °C, 1 hour) could effectively solubilize certain critical inorganic elements (mainly K, Mg, and P) while preserving the macrostructural components of the pre-treated solid, thus resulting in them being more easily exploitable for energy uses. The use of carboxylate-based chelating agents to improve ash solubilization is in progress, enhancing HTC further as a mild pre-treatment for bamboo species. Remarkably, this approach could be appropriate for the development of a better-integrated biorefinery scheme, requiring the best fractionation/exploitation of each biomass component.



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sciforum-112734: Production of xylo-oligosaccharides from banana peel and corn husk by xylanase treatment

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Agricultural byproducts such as banana peel and corn husk are cost-effective and abundant sources of lignocellulosic biomass, offering significant potential for producing value-added biological and biochemical products. Chemical composition analysis shows that banana peels contain 13–15% hemicellulose, while corn husks contain 40–50%, making them valuable sources of xylans, particularly for Xylo-oligosaccharide production. This study explored the enzymatic hydrolysis of xylans from banana peels and corn husks using xylanase concentrations ranging from 2 to 10 mg/mL at 55 °C for 30 minutes. Samples were prepared as untreated samples or autoclaved (121 °C, 15 min). Reducing sugar concentrations were positively correlated with xylanase concentration, with the highest levels observed at 10 mg/mL. For banana peels, the maximum reducing sugar concentrations were 3.47 mg/mL for untreated samples and 3.93 mg/mL for autoclaved samples, while corn husks yielded 3.35 mg/mL and 2.88 mg/mL, respectively. Notably, banana peels exhibited higher reducing sugar values compared to corn husks, and autoclaved samples consistently outperformed untreated ones within each biomass type. Thin-layer chromatography (TLC) confirmed that the hydrolysis products of both untreated and autoclaved samples from banana peels and corn husks consisted of Xylo-oligosaccharides, including xylobiose through xylohexaose. The presence of these oligosaccharides highlights the efficiency of enzymatic hydrolysis in breaking down xylans into functional biomolecules. These findings emphasize the potential of banana peels and corn husks as sustainable and economical raw materials for Xylo-oligosaccharide production, contributing to the valorization of agricultural waste. This approach aligns with the principles of green biotechnology, supporting the development of renewable resources and advancing waste-to-value strategies for biotechnological applications.



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sciforum-106893: Sorted single-walled carbon nanotubes for catalysis

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Metallic and semiconducting fractions of single-walled carbon nanotubes (SWCNTs) attract attention from researchers because they have unique catalytic properties. The catalytic properties of sorted fractions are very important. They are needed to control the properties of metallic and semiconducting SWCNTs. For these reasons, it is important to develop and investigate the sorting process of SWCNTs. The sorting process of SWCNTs leads to metallic and semiconducting SWCNTs, as well as single-chirality samples. They possess new unique physical features, as revealed with a microscopic and spectroscopic techniques. Filled SWCNTs are important materials. Methods of obtaining sorted and filled SWCNTs are currently being developed. They allow for obtaining high-quality samples that are clean from impurities with controlled properties. In this work, the metallic fractions of nickelocene-filled SWCNTs were obtained, and the sorting process was investigated with optical absorption spectroscopy (OAS). It was demonstrated that the sorting process of 1.4 nm diameter mixed-metallicity SWCNTs leads to obtaining pure metallic SWCNTs. The OAS spectrum of the nickelocene-filled SWCNTs shows the characteristic peaks of the metallic SWCNTs. These peaks correspond to electronic transitions between the first van Hove singularities of metallic SWCNTs. This confirms the purity of the samples and their applicability for catalysis.



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sciforum-112520: Strategic Design of Copper Nanoparticles on Modified Clay as Catalyst for Efficient Domino Synthesis of γ -Valerolactone from Furfural via Transfer Hydrogenation

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Gamma Valerolactone (GVL) is an important chemical derived from the hemicellulose in biomass whose applications span across the solvent, biofuel and polymer industries. A domino reaction selectively producing GVL from furfural makes it a highly desirable transformation. In this regard, finely dispersed copper nanoparticles immobilized on zirconia-modified montmorillonite K10 clay were synthesized and examined to achieve high selectivity for GVL. The catalysts were well characterized by employing various techniques, such as PXRD, TEM, FESEM, N₂ sorption, NH₃-TPD, TGA, ICP-OES, FTIR, pyridine IR and XPS. A detailed investigation of the co-operative effect of the active sites responsible for achieving the maximum selectivity towards GVL was carried out. An intrinsic interplay between the lower particle size of copper (metal centers), the Lewis acidity (zirconia sites) and the Brönsted acidic (MMT) sites was found. Further active site masking and reaction intermediates were tested to identify and prove the synergistic effect of the active sites in the reaction pathway. To achieve the highest yield, a response surface methodology using a Central Composite Design model was formulated. Under the optimized reaction conditions, the catalyst demonstrated 99.9% furfural conversion and a high GVL selectivity of 98%, the highest obtained so far in the literature. The catalyst remained highly stable over four reaction cycles with a marginal decrease in its activity and was regenerated via an autogenous solvothermal treatment in between each cycle. Spent catalyst characterizations revealed that its structural integrity and physicochemical properties were retained.



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sciforum-115702: Thermal decomposition of 4-methoxy cinnamic acid over nanoceria

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The development of effective technologies for processing lignin has become a main area of interest in recent decades. An effective method that can be used for the conversion of lignocellulosic raw materials is pyrolysis. To establish the mechanisms of lignin decomposition under catalytic pyrolysis conditions, it is important to study the interaction of its macromolecule with the catalyst, as well as to study the thermal transformations of the lignin model compounds, cinnamic acids. Therefore, we studied the complexes of 4-methoxy cinnamic acid (4MCA) with the surface of nanoceria and the pyrolysis mechanisms of the formed complexes. The catalyst was impregnated with an ethanol solution of 4MCA. The obtained samples were investigated using the IR–Fourier spectroscopy method. Their thermal transformations were investigated using temperature-programmed desorption mass spectrometry using a MKH-7304A monopole mass spectrometer (Sumy, Ukraine) with electron impact ionization, which was adapted for thermodesorption measurements. In the 4MCA/CeO₂ samples, absorptions were detected at about 1398, 1495, and 1537 cm⁻¹, which corresponded to the vibrations of the COO⁻ group. The FTIR data indicate that 4MCA forms carboxylate complexes with bidentate bridge and chelate structures. In addition, the spectra revealed signs of interaction of the methoxyl group with nanoceria. Thermal decomposition of carboxylate complexes takes place in the temperature range of 100oC–400°C, which was confirmed based on the TPD peaks for the molecular and fragment ions of the pyrolysis products with *m/z* 107, 135, 150, and 160. The processes of decarbonylation, decarboxylation, and dehydration accompanied it. Decomposition products that may correspond to the destruction of complexes formed with the participation of methoxyl groups (*m/z* 31, 148, 164) when recorded above 250°C. The obtained results may be useful for understanding the mechanisms of pyrolysis of lignin using nanoceria.

Acknowledgments

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Session G. Industrial Catalysis

sciforum-112013: Biomass-derived mesoporous silica for sustainable flavoring production using alternative technologies

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Addressing the long-term environmental impact of chemical production has become a global challenge, emphasizing the need for sustainable and greener alternatives. In this study, a mesostructured silica was synthesized using a biomass-derived molding agent. The synthesized material was characterized by means of N₂ adsorption and desorption isotherms, Transmission Electron Microscopy (TEM) and Infrared Spectroscopy (FT-IR). A heterogeneous biocatalyst was developed by immobilizing the lipase from *Pseudomonas fluorescens* onto the material, aiming to produce isoamyl acetate—a banana-flavored compound that is widely used in the flavoring industry—as a more sustainable alternative. The catalytic activity of the heterogeneous biocatalyst was evaluated in the transesterification of vinyl acetate with isoamyl alcohol at 40 °C in three systems: a thermostated orbital stirrer, a microwave reactor and ultrasound. The best performance was achieved with a material that was prepared with 96h of immobilization between the enzyme and support at 400 mg_{enzyme}/g_{support}, achieving conversion rates of 28 %, 28.5 % and 32.5 % at 2h of reaction in the three systems, respectively. Thus, compared to traditional mechanical agitation and microwave methods, ultrasound technology improves the process productivity significantly, being a powerful tool for improving a biocatalyst's performance in this type of reaction. This research highlights the robustness of lipases in esterification reactions, showcasing their ability to adapt to different reaction systems and laying the groundwork for future studies aimed at the more sustainable production of high-value-added products in fine chemistry.



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sciforum-112138: Conversion of Carbon dioxide to hydrocarbons over hybrid catalysts containing methanol synthesis catalyst and zeolite

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The hydrogenation of carbon dioxide to C₂, C₃, and C₄ paraffins was examined by using hybrid catalysts containing a Cu-Zn catalyst with Zr-modified H-ZSM-5 zeolite, or Pd-modified β zeolite with H-ZSM-5, or Pt/SiO₂ with H-ZSM-5, or Pd/SiO₂ with H-ZSM-5 β zeolite. Various factors which affect catalyst activities were examined such as reaction temperature, pressure, and the influence of the SiO₂/Al₂O₃ ratio. The tests were conducted at 260–300°C, 2–3 MPa, a W/F of 10 g.h/mol, and with a H₂/CO₂ mole ratio of 3. The influence of the SiO₂/Al₂O₃ ratio on H-ZSM-5 zeolite played an important role in hydrocarbon distribution. When H-ZSM-5 was used on the zeolite with low alumina content (SiO₂/Al₂O₃=100), the product contained olefins and dimethyl ether with a large amount of C₅ and C₆, whereas that for the zeolite with high alumina content (SiO₂/Al₂O₃=40) showed an excellent conversion of carbon dioxide to hydrocarbon. Under mild temperature at 280°C, CO₂ conversion reached 23% with a hydrocarbon selectivity as high as 80%, while keeping the dry gas (CH₄) selectivity below 1% by using the hybrid catalysts. When Pd/SiO₂ with β zeolite was used for the hybrid catalysts, butane was produced with a high selectivity over 50% at 280°C and 3 MPa with a small amount of coke deposition.



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sciforum-112662: Organocatalysis originating from 1,1-Diaminoazines

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Guanabenz, a marketed antihypertensive drug, is primarily sold in its monoprotonated form, while its free base form has received little attention. Interestingly, under physiological conditions of temperature and pH, approximately 16% of guanabenz exists in its free base form. Our group recently discovered that the free base form of guanabenz is a tautomeric form of guanylhyazones, known as azines.¹ Notably, guanabenz prominently adopts the azine tautomeric state, as confirmed through both experimental and theoretical studies. This discovery has sparked a new research direction in our lab, focusing on this previously overlooked class of molecules: 1,1-diaminoazines. The unique characteristics of 1,1-diaminoazines directed us to employ them in different research areas of chemistry. 1,1-Diaminoazines are known to have applications in medicinal chemistry, material chemistry, catalysis, organic synthesis, etc.² The presence of electrophilic and nucleophilic sites in the same molecule makes 1,1-diaminoazines a unique substrate (I) for cycloaddition reactions synthesising dihydropyrazoles and different types of substituted triazoles.³ The presence of a) the conjugated double bonds, (b) the many active hydrogen atoms, (c) the N2 centre in 1,1-diaminoazines acting as a proton acceptor, and (d) the iminic C4 acting as a hydrogen bond donor makes this molecule a potential bifunctional organocatalyst.⁴ To prove the same, this molecule has been used to catalyse various types of Michael addition reactions.^{5,6} Successfully, it has been utilised in C-P and C-C bond formation. Furthermore, it has facilitated the aldol/cyclisation cascade reactions, efficiently generating small heterocycles.⁷ Additionally, it has been proven efficient in carrying out different multi-component reactions (MCRs) to generate bioactive scaffolds such as pyranopyrazoles. Quantum chemical studies have been carried out to prove the mechanistic insights and to further enhance its utility, and efforts are currently underway to develop an asymmetric version of this catalyst. This modification aims to unlock its potential for enantioselective transformations, paving the way for the synthesis of complex molecules and expanding its applicability in medicinal chemistry. Other than this, 4-pyridyl-4 methyl-1,1-diaminoazine was employed to generate the pincer complex with Pd(OAc)₂. The application of the complex in catalysing the medicinally important scaffold (e.g., benzimidazoles, quinolines, quinoxalines) synthesis using the ADC mechanism has been reported.⁸

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sciforum-115359: Structural Insights and Bioactive Potential of Coconut Shell Lignin from acid-assisted Organosolv process

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The valorization of underutilized organic waste into high-value polymeric materials is a growing topic in Thailand's industrial polymer production sector, addressing critical ecological challenges. Lignin, an abundant aromatic biopolymer found in agricultural wastes like coconut shells, has significant potential for producing high-value chemicals and contributing to a circular economy. However, its complex structure, characterized by sensitive C-O bonds, necessitates selective extraction to develop useful aromatic molecules for biotechnological applications. This study investigated the catalytic performance of hydrochloric acid in the organosolv treatment of coconut shells. Lignin was hydrolyzed in a 70% ethanol solution with 2.2% (w/v HCl) at 190 °C for 90 min, yielding up to 96% lignin. The chemical structure of lignin was characterized and discussed. Fourier-transform infrared (FT-IR) spectroscopy revealed a high intensity of hydroxyl groups, indicating the breakdown of lignin-carbohydrate linkages and interlinkages. The lignin consists of syringyl (S), guaiacyl (G), and p-hydroxyphenyl (H) units, classifying it as a grass-type (HGS). Methoxyl groups were also identified in the coconut shell monomeric units, suggesting minimal modification of the native lignin structure. Additionally, the resulting β -O-4 linkage-rich lignin fractions exhibited enhanced biological reactivity compared to commercially available lignin, demonstrating UV absorption capacity and antibacterial properties. This work proposes a sustainable biorefinery approach to transform agro-wastes into valuable resources through lignin extraction, facilitating the creation of bioactive compounds for innovative applications in cosmetics and health products.



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sciforum-114906: The Role of Industrial Catalysts in Accelerating the Renewable Energy Transition

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Industrial catalysts are accelerating the global transition toward renewable energy, serving as enablers for innovative technologies that enhance efficiency, lower costs, and improve environmental sustainability. This review explores the pivotal roles of industrial catalysts in hydrogen production, biofuel generation, and biomass conversion, highlighting their transformative impact on renewable energy systems. Precious-metal-based electrocatalysts such as ruthenium (Ru), iridium (Ir), and platinum (Pt) demonstrate high efficiency but face challenges due to their cost and stability. Alternatives like nickel-cobalt oxide (NiCo₂O₄) and Ti₃C₂ MXene materials show promise in addressing these limitations, enabling cost-effective and scalable hydrogen production. Additionally, nickel-based catalysts supported on alumina optimize SMR, reducing coke formation and improving efficiency. In biofuel production, heterogeneous catalysts play a crucial role in converting biomass into valuable fuels. Co-based bimetallic catalysts enhance hydrodeoxygenation (HDO) processes, improving the yield of biofuels like dimethylfuran (DMF) and γ -valerolactone (GVL). Innovative materials such as biochar, red mud, and metal-organic frameworks (MOFs) facilitate sustainable waste-to-fuel conversion and biodiesel production, offering environmental and economic benefits. Power-to-X technologies, which convert renewable electricity into chemical energy carriers like hydrogen and synthetic fuels, rely on advanced catalysts to improve reaction rates, selectivity, and energy efficiency. Innovations in non-precious metal catalysts, nanostructured materials, and defect-engineered catalysts provide solutions for sustainable energy systems. These advancements promise to enhance efficiency, reduce environmental footprints, and ensure the viability of renewable energy technologies.



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sciforum-112506: Transforming CO₂ Valorization: Tri-Reforming for Methanol Synthesis and Sustainable Emission Reduction in Power Plants Flue gas

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The CO₂ consumption of flue gas for methanol production is investigated as an alternative for conventional, energy-intensive CO₂ capture methods in this study. Aspen HYSYS v12.1 was used to model the tri-reforming process, which aims to lower the carbon impact of traditional methods by converting CO₂ into methanol. With a stoichiometric number (Sn) of 2.216, the ideal H₂:CO ratio was determined to be 2.293. To obtain high CO₂ conversion rates at high temperatures, guarantee the required ratios, and reduce carbon formation on the catalyst, a nickel-based catalyst was employed in the tri-reforming process. With a methanol purity of 99.1%, methanol synthesis used a Cu/ZnO/Al₂O₃ commercial catalyst for CO hydrogenation, which significantly reduced carbon emissions to 0.032 kg CO₂ per kg of methanol.

This study discovered that Ni-based catalysts could accomplish 80–95% CH₄ conversion and good syngas selectivity at temperatures between 800 and 900°C and atmospheric conditions to moderate pressures while maintaining an ideal H₂/CO ratio of about 2.0–2.5. But because carbon deposition happened at rates of about 2–10 mgC/g-cat/h, more steam was needed for steam reforming in order to increase CO₂ conversion and decrease coke development. The highest H₂/CO ratio and the highest CH₄ and CO₂ conversion rates were obtained when operating at 850°C and 1 atm. Under conditions similar to those of natural gas-based power plants, simulation results demonstrated effective CO₂-to-methanol conversion with flue gas flow rates of 1000 kmol/h and 10 mol% CO₂. In order to optimize the reforming reactions and perhaps reduce reactor volume and mitigate high operating pressures, further reactor parameter optimization is advised, including introducing O₂ and H₂O. This study underlines the need for more research into process economics and scalability for large-scale implementation, while also highlighting the potential of tri-reforming for sustainable methanol synthesis from power plant emissions.



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Session H. Computational Catalysis

sciforum-107927: A Novel Approach for First-principles Calculations of Charged Adsorbates in Periodic Metallic Systems

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Charged species are often found in various chemical processes such as catalysis, electrochemistry and acid-base reactions. DFT studies are always used to gain an in-depth understanding of these reactions. However, in periodic metallic systems, the presence of charge in supercells faces serious convergence problems, and a new method is needed to calculate charged slabs to study the reactions involving charged species.

To study the heterogeneous catalysis reactions, a simple method is proposed for the calculations of charged adsorbents. The DFT calculations are performed using the VASP package. The VASPsol solvation model and Grimme dispersion corrections are considered in all calculations. The transition state for each reaction is located using the climb-NEB method. The zero point vibrations (ZPE) are obtained using the harmonic oscillator approximation to confirm the ground state and transition state geometries.

In the proposed new approach, a counter ion is placed at a non-interactive distance in the supercell, in an aqueous medium, to maintain the neutral behaviour of the systems while the adsorbents are charged. The charged species are confirmed using the Bader charged analysis. The method is used to study the adsorption of monovalent anions such as halides, hydroxides and H^- and bivalent anions such as Se^{2-} and SO_4^{2-} . The method is later used to study the detailed mechanism of BH_4^- hydrolysis on Ag^0 and Au^0 surfaces, and the obtained conclusions are validated with experiments. This approach offers a valuable method for studying the charged species in the catalytic process.



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sciforum-108867: Dinitrogen Activation by Transition Metal Catalysts: Paving the Way for Future Energy and Sustainability

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Introduction:

The activation of dinitrogen is essential for sustainable ammonia synthesis, a critical process for agricultural and energy applications. Transition metal catalysts, including iron, ruthenium, and cobalt, along with bi-, tri-, and multimetallic alloys, are pivotal in enhancing this activation within the Haber--Bosch process.

Methods:

This study summarizes theoretical modeling techniques within the density functional theory utilizing functionals such as PBE and RPBE, as well as database investigations, to demonstrate the performance of various transition metal catalysts in activating dinitrogen. Key physical property changes, such as bond length elongation, vibrational red-shifts, and charge transfer dynamics, will be presented.

Results:

Our findings reveal that specific transition metal catalysts that contain iron/cobalt/ruthenium can enhance nitrogen activation upon adsorption, leading to measurable alterations in the nitrogen molecule's physical properties, as discussed in some recent studies. Notably, we delineate a marked decrease in activation energy for the dissociative adsorption of nitrogen, indicating improved reaction kinetics. Furthermore, detailed analysis of the hydrogenation reaction mechanism provides insights into the underlying processes that govern surface reactivity.

Conclusions:

Advancements in transition metal catalysis for dinitrogen activation not only enhance ammonia synthesis efficiency, but have also contributed to the development of more sustainable chemical processes in recent years. These insights pave the way for innovative approaches in catalysis, with the potential to significantly impact future energy solutions and agricultural practices. Continued research in this area is essential for realizing the full potential of sustainable ammonia production.



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sciforum-104448: Exploring the Catalytic Potential of Noble and Non-Noble Metals for Carbon Monoxide Oxidation: A Computational Study

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The oxidation of carbon monoxide (CO) to carbon dioxide (CO₂) is critical due to the harmful effects of CO emissions on human health and the environment. As a colorless and odorless gas, CO poses serious health risks, including headaches, fatigue, dizziness, and, in severe cases, death, primarily due to its interference with oxygen delivery to the brain. CO emissions from sources such as automobiles, power generators, and industrial processes continue to significantly contribute to air pollution, especially in developing nations. This study employs a computational approach to compare the catalytic effectiveness of noble and non-noble metals in the oxidation of CO to CO₂. The investigation explores various adsorption modes of surface oxygen, CO, and CO₂ across selected metal surfaces. The results highlight the comparative catalytic potential of noble versus non-noble metals in facilitating CO oxidation. Insights from this study could play a critical role in optimizing CO oxidation strategies to reduce harmful emissions, thereby contributing to improved air quality and environmental sustainability, particularly in communities most affected by CO pollution. The findings have important implications for the development of more efficient and sustainable catalytic converters and exhaust treatment systems. By enhancing the understanding of CO oxidation on different metal surfaces, this research can inform the design of better emission control technologies, promoting both environmental sustainability and improved air quality. Ultimately, this study emphasizes the need to continue refining catalytic processes to tackle the global challenge of air pollution and its associated health risks.



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sciforum-112041: First Principles Modeling of Hydrogen Oxidation Reactions on Perovskite Oxide Surfaces for Solid-Oxide Cells and Quantum Computing-Based Simulations for Molecular Vibrational Properties of CO₂ Capture Reaction with NH₃

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The simulations of electrochemical performances of perovskite materials for hydrogen oxidation reactions (HOR) in H₂ gas environments were investigated using planewave-based Density Functional Theory (DFT) modeling, and the simulation results unveiled significant findings. The impacts of the oxygen chemical potential and surface hydrogen bonding interactions, when the steam content in the H₂ gas and nonstoichiometry of the perovskite (001) slabs varied, were found to significantly alter the HOR energy landscapes. In the realm of the CO₂ capture reaction with NH₃ as a model amine solvent, the variational quantum eigensolver (VQE)-based algorithms have shown remarkable predictive quality, enhancing calculations of vibrational ground-state energies, addressing molecular anharmonicity [2], and providing results for the reacting and producing molecules in the CO₂ capture reaction with accuracy that rivals the direct diagonalization method for CO₂ and NH₃. The performances and computing cost of the VQE algorithms implemented on current quantum simulators and hardware will be further discussed.

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sciforum-109903: First-principles calculations of structural and electronic properties of FeSb_2O_6

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The aim of this work is a comprehensive study of the structural and electronic properties of the trirutile compound FeSb_2O_6 . The quantum DFT approximation used for this research was applied to iron antimonate oxide, which has a well-defined trirutile structure with the space group $P4_2/mnm$ (136). It crystallizes in a tetragonal lattice, featuring unit-cell parameters of $a = 0.466$ nm and $c = 0.924$ nm. The structural characteristics of a material can be thoroughly investigated without the need for physical measurements by employing optimized first-principles computational methods. In this case, the CASTEP code, integrated within the Material Studio software suite, was utilized based on a pseudo-potential plane-wave approach. In this study, the geometrical optimization of FeSb_2O_6 was conducted using a semi-local generalized gradient approximation (GGA), specifically employing the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional. Additional functionals used include the PBE for solids (PBESOL), Perdew–Wang91 (PW91), the revised PBE (RPBE), and the local density approximation (LDA–CAPZ). After optimization, both the band gap values and the density of states (DOS) of FeSb_2O_6 were calculated to gain deeper insight into its electronic properties. The electronic properties of FeSb_2O_6 were determined by examining its electronic band structure and DOS, establishing it as a narrow-gap semiconductor with a direct band gap, making it promising for potential electronic applications.



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sciforum-112475: From Predictive Chemistry to Machine Learning in Applied Chemistry

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Amidst the widespread enthusiasm for machine learning, one often-overlooked domain is predictive catalysis. In the realm of computational chemistry for sustainability, this research group advocates for the maximum utilization of predictive catalysis, employing machine learning principles. Their endeavors extend beyond identifying reaction mechanisms; once the rate-determining state (rds) is established, the focus shifts to exploring alternative catalysts, aiming for more benign reaction conditions. The computational research spans various domains, encompassing processes such as olefin metathesis using Ru-based catalysts, gold chemistry for organometallic reactions, and green chemistry strategies for CO₂ avoidance or reduction, including water oxidation catalysis and alcohol transformation to aldehydes with H₂ generation as an energy source ^[1].

DFT calculations have unveiled the mechanisms underlying the formation of N-substituted hydrazones through the coupling of alcohols and hydrazine, achieved via sequential processes of acceptorless dehydrogenation and borrowing hydrogen ^[2,3]. This process, facilitated by a Mn-PNN pincer-based catalyst, aligns with green chemistry principles, releasing water and H₂ as environmentally friendly byproducts ^[3].

This research also delves into the reductive amination of aliphatic carbonyl compounds catalyzed by a Knölker-type iron catalyst. Utilizing DFT calculations and a detailed chemical structure analysis, the team investigates the reaction mechanism ^[4]. Armed with insights into the mechanism, various catalyst modifications are explored with the goal of steering catalytic reactions towards milder conditions.



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sciforum-115373: Structural Modification of Graphitic Carbon Nitride to Enhance Photocatalytic Efficiency: DFT-based Physicochemical and Spectral Study

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Semiconductor-based photocatalysis presents a promising solution to the global energy crisis and environmental pollution challenges. Since the groundbreaking discovery of graphitic carbon nitride (g-C₃N₄) in 2009 for visible light-driven photocatalytic water splitting, g-C₃N₄-based photocatalysis has emerged as a highly active area of research. Herein, the structural modification of pristine g-C₃N₄ is explored to enhance its photocatalytic efficiency, employing density functional theory (DFT) with the widely adopted B3LYP/6-31g(d) theory. Furthermore, the band structure for the periodic system was determined using GGA-PBE functionals. This study investigated the effects of functionalizing g-C₃N₄ with different grafting agents, including benzofuran (BF), benzoxazole (BFz), indole (ID), and benzimidazole (IDz). Thermodynamic analyses revealed notable changes in free energy, indicating the improved binding possibility of the modified materials. Frontier molecular orbital analyses showed reduced HOMO-LUMO gaps, correlated with enhanced reactivity and improved charge transfer properties. Dipole moment analyses confirmed increased polarity, promoting higher photocatalytic activity. Band structure and density of states (DOS) analyses demonstrated shifts in energy levels conducive to visible light absorption. Theoretical FT-IR and Raman spectra confirmed successful functionalization by identifying characteristic bonds and vibrational modes. In contrast, UV-vis absorption spectra revealed a redshift absorption of modified g-C₃N₄, indicating improved light absorption. These findings highlight the potential of grafted g-C₃N₄ materials for efficient photocatalytic applications, offering a promising approach to address energy and environmental challenges.



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sciforum-115737: Structural modification of porphyrin to accelerate its electron donor nature: a physicochemical and spectral study

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The π -conjugated structures of organic photovoltaic cells offer a viable answer to meet the growing need for renewable energy sources. This research investigates how the addition of benzocyclic groups such as benzofuran (BF), benzoxazole (BFz), indole (ID), benzimidazole (IDz), benzothiophene (BT), and benzothiazole (BTz) to porphyrin systems increases their electron donation potential for use in photovoltaic devices. The electronic, optical, and thermodynamic properties of seven molecular configurations (P, PID, PIDz, PBF, PBFz, PBT, and PBTz) were assessed through density functional theory (DFT) using the B3LYP/6-31G+(d,p) basis set. A steady reduction in the free energy points to greater stability, alongside changes in the dipole moment, demonstrates substantial charge polarization effects. An analysis of the HOMO-LUMO gaps demonstrates the enhanced electronic stability in PIDz, PBFz, PBT, and PBTz, which is vital for charge transfer optimization and reactivity improvements. PBFz and PBTz demonstrate promising DOS profiles that maximize the donor-acceptor overlap and electronic transitions, leading to a superior solar material performance. The N-H, C-H, and C=C vibrational modes play a key role in the charge delocalization and light absorption, which are essential to the photovoltaic performance. The optical measurements reveal a red shift, with λ_{max} from P at 359.6 nm toward PID at 405.0 nm, while PBTz shows the maximum absorption levels, which demonstrates improved $\pi \rightarrow \pi^*$ transitions, leading to enhanced light-harvesting capabilities. The transition density matrix, alongside exciton binding energy studies, reveals PBFz and PBTz as the top choices for solar cell technologies because of their superior charge separation abilities and excitonic features. The NBO analysis confirms PBFz and PBTz as the top materials for organic photovoltaics and nonlinear optics while providing a basis for ongoing optimization and device exploration.



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sciforum-115289: The Role of Electronic and Geometric Factors in Rhodium-Catalyzed Selective Hydrogenation of Enones

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The selective hydrogenation of α,β -unsaturated carbonyl compounds (enones) versus isolated double bonds is a reaction of considerable interest in organic synthesis, particularly in the pharmaceutical and fine chemical industries. Previous studies have elucidated the mechanism of this reaction, which is catalyzed by the $\text{Cp}^*\text{Rh}(2\text{-(2-pyridyl)phenyl})\text{H}$ complex^{1,2}. However, computational research has primarily focused on substrates containing a single reactive group, neglecting systems with both enone and olefin functionalities². Moreover, the origins of the preference for enone hydrogenation remain insufficiently explored.

In this study, DFT calculations were employed to investigate the key electronic and geometric features enabling the selective hydrogenation of a dual-functionality substrate, catalyzed by the $\text{Cp}^*\text{Rh}(2\text{-(2-pyridyl)phenyl})\text{H}$ complex. The analysis integrated two complementary approaches: (1) an electron density-focused framework, including charge transfer and QTAIM/ELF analyses at critical points along the reaction force profile, and (2) quantum mechanical methods such as NBO analysis of donor-acceptor interactions and interference energy evaluations of the complex-substrate system. Additionally, coordination and deformation energies of the catalyst-substrate complex were compared for dual substrates and for substrates containing only one functionality.

The results reveal that the selective hydrogenation of enones over olefins is governed by distinct substrate-catalyst interactions, influenced by both steric and electronic factors. The interplay between electrostatic and quantum phenomena elucidates the preference for enone hydrogenation and provides insights into the coupling between electron and proton transfers along the reaction pathway. These findings suggest modifications to the ligand structure to further enhance the selective hydrogenation of enones, expanding the versatility of Rh-catalyzed transformations in synthetic chemistry.

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sciforum-109406: Theoretical study of CO₂ capture mechanisms of SrO and Sr(OH)₂×nH₂O (n=0,1,8)

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Strontium oxide (SrO) is a promising material for CO₂ capture through a reversible cycle of carbonation and calcination, where SrO reacts with CO₂ to form strontium carbonate (SrCO₃) and can be regenerated by calcination. In the presence of moisture, SrO forms strontium hydroxide and its hydrates (Sr(OH)₂×nH₂O). This study employs density functional theory (DFT) to investigate the underlying mechanism of these processes on various crystal surfaces of SrO, Sr(OH)₂, Sr(OH)₂·H₂O, and Sr(OH)₂·8H₂O. The interaction of CO₂ with these surfaces leads to carbonate formation via electron transfer, with notable differences in CO₂ orientation and bond characteristics between SrO and the hydroxylated surfaces. The hydration of SrO increases the CO₂ surface adsorption energy with the exception of the monohydrate. CO₂ adsorption reaction on the Sr(OH)₂·H₂O surface is more thermodynamically favorable than on the anhydrate and octahydrate surfaces. Reaction pathway analysis reveals that bicarbonate formation is preferred on the anhydrate and octahydrate surfaces, while carbonate formation is favored on the SrO and monohydrate surfaces. The CO₂ removal reaction from the SrCO₃ surface is also investigated. This study provides valuable insights into the fundamental mechanism for CO₂ capture using SrO and its hydrated forms.



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