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# Proceedings of the 10th International Conference on Catalysis and Chemical Engineering™ (CCE Boston-2026)

## Sustainable Catalysis Routes for Greenhouse Gas Valorization to Value-added Chemicals

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### Abstract

Methane and carbon dioxide are major greenhouse gases whose emissions have contributed significantly to global warming over the past several decades. In this presentation, I will provide an overview of my group's research on developing advanced catalyst technologies for the efficient and emission-free utilization of these gases through their conversion into value-added products. I will then present our work on integrating our developed catalysts with membrane systems to enhance reaction conversion and product selectivity in greenhouse gas valorization reactions. One of these catalyst–membrane platforms offer a carbon-free pathway for hydrogen generation and is being further developed toward industrial-scale deployment in support of Singapore's low-carbon energy initiatives. Finally, I will highlight our collaborative research with shell on electrified catalysis for methane coupling to produce light olefins under ambient conditions, enabled by low-temperature dielectric barrier discharge plasma.

## Recent Advances in Asymmetric Catalysis

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### Abstract

The ability to readily access small-molecule building blocks at will has important consequences for the discovery and development of novel medicines and materials. It is particularly beneficial when the chemical methods are convenient while at the same time economically and environmentally tenable and sustainable. A focus of our research program at ETH-Zurich is the identification, study, and development of novel reactions and methods for preparation of functionalized structures. We are especially interested in catalytic processes that are easily executed and utilize readily available starting materials. We will discuss several new reaction processes that provide ready access to a host of fundamentally versatile building blocks for synthesis. The presentation focuses on the unique reactivity of iridium- and ruthenium complexes with a novel ligand as well as recent progress with earth-abundant metal catalysts combined with photochemistry.

## Synergistic Effects of *Ex-situ* Doping and *In-situ* Ion Insertion in Electrochemical Ammonia Synthesis

**Huixin He[1*], Oguz Kucukosman[1], Zhiyuan Zhang[1], Junjie Ouyang[1], Miaofang Chi[2,3], John Mark P. Martirez[4], Aditya Dilip Lele[5] and Yiguang Ju[6]**

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## Abstract

Electrochemically controlled ion insertion and extraction in transition metal oxides (TMOs), generally described as xM+ + xe- + TMO → MxTMO (where M+ = H+ or Li+), is the fundamental mechanism behind batteries and electrochromic devices. In this presentation, using tungsten oxide ($WO_3$), a prototypical TMO with excellent ion-insertion capability, as an example, I will highlight two largely underexplored features of ion insertion that can advance electrocatalysis in the electrochemical nitrogen reduction reaction (eNRR): (1) tuning the d-band electronic structure of TM centers, and (2) generating highly active, mobile hydrogen atoms. In addition, I will also show how these features enhance eNRR while suppressing the hydrogen evolution reaction using two heteroatom-substitutionally doped $WO_3$ catalysts. The first is phosphorus-doped $WO_3$ with abundant oxygen vacancies (P-OV-$WO_3$), where doping and vacancies are uniformly distributed across the nanostructure. The second is a WOxNy/$WO_3$ catalyst, developed via non-equilibrium plasma-assisted surface nitridation, featuring a unique heterogeneous interfacial complexation structure that preserves proton intercalation behavior. The findings demonstrate that combining *ex-situ* substitutional doping with *in-situ* ion insertion provides an effective strategy for designing highly selective and active eNRR catalysts in aqueous systems.

# Efficient Precious Metal Catalysts for Solid Oxide Fuel Cell Systems

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## Abstract

With the advancing energy transition and the need for further decarbonization in the mobility and industrial sectors, technologies used here are also bound to change. Switching to carbon neutral e-fuels or even to a completely carbon-free green hydrogen economy, using hydrogen or ammonia directly poses completely new challenges to the catalytic exhaust gas aftertreatment in an internal combustion engine. Furthermore, even regardless of whether these fuels are then used in a combustion engine or for a fuel cell, additional catalytic requirements arise from the fuel management. In the present article, we focus on the development of catalytic solutions in various fields such as hydrogen economy, catalytic combustion and emission management, catalysts for balance of plant components in a solid oxide fuel cell (SOFC) system etc. We are pleased to present examples of corresponding application developments for our catalysts. The focus of the present work targets the performance of rhodium-based catalysts, with different preparative routes, for pre-reformer applications under different gas compositions and at different space velocities. The operation is near isothermal, but at higher temperatures, the endothermic heat load of the methane conversion lowers the outlet temperature. We show that rhodium catalysts can be specifically tailored to maintain a high conversion of higher hydrocarbons while allowing either for a higher or lower conversion of methane, tailored to the needs of the SOFC or downstream application.

# The Gold Standard of Excellence in Reporting Experimental Results of Permeability in Closed Conduits

**Hubert M. Quinn***

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## Abstract

A new model of fluid dynamics has emerged in the published literature. This new model goes by the nomenclature of the Quinn fluid flow model and establishes a novel methodology of defining from first principles the underlying physics of fluid flow in closed conduits. This technique gives rise to a new "gold standard" for reporting the results of empirical studies in both packed and empty conduits. The use of supported catalysts on particles of various sizes and shapes is an application at the very core of this technology. Accordingly, this new gold standard is of great importance to practitioners in this field of study. In this presentation we will describe this novel technology by focusing on the fundamentals of this physics driven model.

## Electrochemical Sensors for Monitoring Nitrogen Compounds in Water: Advances and Applications

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### Abstract

Monitoring nitrogen compounds (N-compounds) in both drinking and agricultural water is essential for safeguarding environmental and human health. The most monitored compounds include nitrate, nitrite, and ammonium, primarily from fertilizers, animal waste, sewage, and industrial activities. In drinking water, high levels of nitrate pose significant health risks, such as methemoglobinemia ("blue baby syndrome") in infants and potential associations with certain cancers. In agricultural water, excess nitrogen can disturb soil nutrient balances, damage crops, and lead to runoff that pollutes waterways, promoting eutrophication and harmful algal blooms. Portable test kits and sensors are increasingly used for rapid, on-site analysis, especially in agriculture, where real-time data supports timely decision-making. This presentation focuses on electrochemical sensors for N-compounds detection. We developed a nitrite sensor based on a manganese and copper oxide electrodeposited on a carbon electrode, showing a sensitivity of 10.69 μA/μM, a detection limit of 0.071 μM (the World Health Organization (WHO) limit for drinking water is 65.2 μM), and a linear range of 2 - 60 μM. A nitrate sensor using copper micro-flower structures on screen-printed carbon electrodes demonstrated a sensitivity of 44.71 μA/mM and a detection limit of 0.87 μM (WHO limit is 0.8 mM). Ammonium detection was achieved with gold nanoparticles on a polyaniline/carbon electrode, reaching a detection limit of 0.03 μM. All three sensors showed good reproducibility and repeatability. Data on their full characterization, performance, and real sample analysis, including interferents, will also be presented.

## Engineering of Photo-Fenton-like Catalysts for Removal of Organic Pollutants from Water under Sunlight

**Nataša Novak Tušar[1,2*], Andraž Šuligoj[1,3], Ksenija Maver[1,2], Nimisha Kuruvangattu Puthenveettil[1] and Albin Pintar[1]**

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### Abstract

Pollution of water bodies by organic pollutants, so-called contaminants of emerging concern (CECs), has become an important issue. Among treatment methods, advanced oxidation processes (AOPs) are notable for generating reactive oxygen species that degrade pollutants into harmless byproducts. Fenton AOP, homogeneous catalytic process, is the most industrial applicable AOP. It uses iron (Fe) salts as catalysts and hydrogen peroxide as an oxidizing agent. However, it has drawbacks like acidic pH requirements, Fe sludge production, and excess Fe ions. To address this, Fenton-like AOP reactions as heterogeneous catalytic process at neutral pH are explored. In this work we demonstrate that the designed photocatalysts enable an advanced photo-Fenton-like AOP under visible light and neutral pH, offering a sustainable CEC removal strategy using sunlight. In the catalytic removal of bisphenol A, monometallic copper (Cu) on a silica support showed better Fenton-like activity than monometallic Fe. However, in a bimetallic (Cu-Fe) functionalized silica, the Fenton-like activity is improved. The structure-activity characterization of the material showed that only a small concentration range of Fe had a beneficial and synergistic effect between the Cu and Fe cations. Moreover, in bimetallic functionalized material, a significant increase in activity is observed when visible light is introduced into the system, making it act like a photo-Fenton-like system. *In-situ* X-ray absorption spectroscopy experiments showed that light played a positive role in the structural reorganization of the closest neighbors around the Fe ions, which remained unchanged even after the repeated cycles of photocatalytic performance.

## Synergistic Photocatalytic–photothermal Mechanisms in Interfacial Solar Distillation for Volatile and Semi-volatile Organic Compounds Rejection

**Maria Vittoria Diamanti[1*], Begüm Aksu[1], MariaPia Pedeferri[1], Syed Abdul Basit Shah[2], Vanni Lughi[2], Hady Hamza[3] and Daniela Meroni[3]**

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### Abstract

In spite of their simplicity and low cost, the technology behind interfacial solar evaporators still presents critical challenges, particularly the accumulation of volatile and semi-volatile organic compounds in the collected water. In this frame, the introduction of photocatalytic functionality can enable the degradation of organic contaminants, potentially improving water quality, as well as the reduction of biofouling, thus extending the device service life. However, the underlying mechanisms are still unclear, and the lack of standardized testing conditions affects the comparability of literature studies. This study investigates the mechanisms at play in hybrid photothermal-photocatalytic evaporators. A range of target pollutants—including dyes and phenolic compounds—were selected based on their volatility, environmental relevance, and degradability. Our results show that commonly used dyes, although prevalent in literature, are completely rejected by photothermal evaporation. Phenolic compounds are more suitable targets, as they tend to accumulate in condensed water and are partially removed through photocatalysis. To disentangle photothermal and photocatalytic contributions to phenols disappearance, we compared systems with interfacial, submerged, and vapor-exposed photocatalyst configurations, tracking reaction intermediates in both liquid and vapor phases. Our findings reveal that photocatalytic oxidation produces fewer volatile intermediates, which are more effectively rejected during evaporation. Thus, photocatalysis and photothermal effects act synergistically to achieve effective purification of water (Figure 1).

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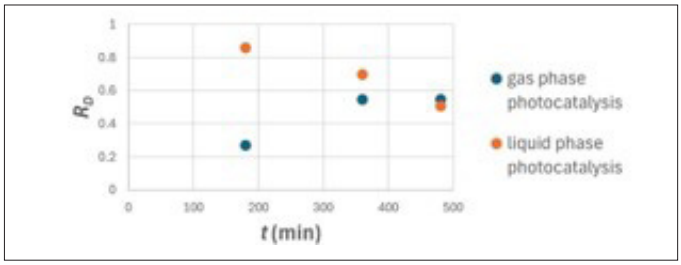


**Figure 1:** Photocatalysis phase.

## On the Stability and Photocatalytic Efficiency of Water-based Titania Sol-gels

**Begüm Aksu[1*], Daniela Meroni[2], Maria Vittoria Diamanti[1] and Mariapia Pedeferri[1]**

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### Abstract

Among many technologies that address environmental pollution, heterogeneous photocatalysis is particularly notable for its ability to transform harmful substances into benign ones. Among various photocatalysts synthesis techniques, the sol-gel method stands out for its simplicity and cost-effectiveness in producing titanium dioxide ($TiO_2$) thin films, as it operates at low temperatures, allows for large-area coverage, and relies on hydrolysis and condensation reactions of a precursor in a solvent. This study investigates the accelerated aging of water-based green sol-gels, explicitly focusing on the impact of surfactant addition on sol stability over time. In the synthesis of sol-gels, Ti (IV) isopropoxide 97% (TTIP) was used as the precursor, with deionized water (DI) as the solvent. Glacial acetic acid (AA) served as a catalyst, chelating agent, and peptizing agent,

while eco surf EH-3 (ECH3) was selected as the surfactant due to its eco-sustainable nature. The synthesis was divided into two series: surfactant-free batches (series A) and surfactant-added batches (series B). Each sol was synthesized at room temperature and then underwent varying durations of thermal aging (0 days, 1 day, and 3 days) at 50 °C in oven. In series A, the molar ratio of TTIP, DI, and AA was 1:100:5. In series B, the TTIP ratio increased to 1.2, thanks to the addition of ECH3 which allows us to stabilize a larger $TiO_2$ content. Sol natural aging was then monitored over 13 weeks through regular deposition and tested for photocatalysis. Generally higher degradation is obtained in presence of the surfactant, which likely enhances the dispersion and surface characteristics of titania, improving photocatalytic performance (Figure 1). Moreover, prolonged aging with a surfactant may create a stable, highly active structure, potentially due to enhanced crystallinity, porosity, or surface area that optimizes photocatalysis. In contrast, while with lower or no thermal aging photocatalytic films start from lower efficiency; the final reaction rate after 3 months aging almost catches up with that of B3. Therefore, thermal aging basically accelerates the sol improvement process.

**Acknowledgements:** This study was carried out within the MICS (Made in Italy —Circular and Sustainable) extended partnership and received funding from the European Union Next–Generation EU (Piano Nazionale di Ripresa e Resilienza Missione 4 Componente 2, Investimento 1.3 —D.D 1551.11-10-2022, PE00000004).

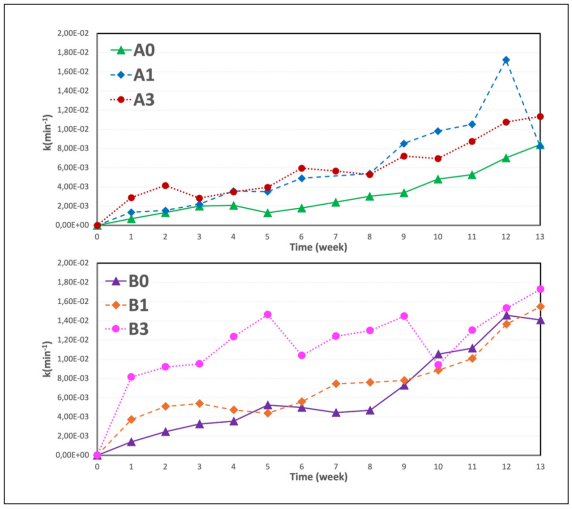


**Figure 1:** Degradation of rhodamine B on coated samples for series A, base (up) and series B, with surfactant (down).

## Multi-technique *In Situ* Assessment of Local and Long-range Stability of Metal-organic Frameworks in Alkaline Environments

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### Abstract

Approximately 90% of global hydrogen production in 2025 remains "grey", deriving from fossil fuels via steam reforming and coal gasification processes, and thus contributing substantially to $CO_2$ emissions. Electrochemical water oxidation offers a promising sustainable alternative; however, challenges related to cost, durability, and long-term stability, particularly of catalysts, still require significant optimization. Metal–organic frameworks (MOFs) have recently gained attention for water-splitting applications, especially as oxygen evolution reaction (OER) catalysts, where they can exhibit performance comparable to conventional materials. Nevertheless, OER typically occurs under highly alkaline conditions in which many MOFs rapidly degrade, resulting in reduced activity and limited operational lifetimes. In this study, monometallic and bimetallic Ce(IV)-doped MOF-808 materials were synthesized through a green, water-based method under mild conditions and characterized using a range of laboratory techniques. These analyses provided insights into their crystallinity, microporosity, crystal morphology, and

cerium incorporation. *In situ* X-ray absorption spectroscopy at the European synchrotron radiation facility further elucidated the coordination environment of the metal nodes and assessed MOF stability in alkaline solutions, simulating OER operating conditions. Complementary inelastic and deep inelastic neutron scattering experiments at the ISIS neutron and muon source (United Kingdom) strengthened these findings, offering valuable information for designing durable catalysts for sustainable hydrogen production. Overall, this study highlights the critical role of metal composition in determining MOF stability and self-reconstruction pathways under OER conditions.

## Stable Dry Reforming of Methane Enabled by High-entropy Oxides via Synergistic Redox Exsolution and Strong Metal-support Interaction

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### Abstract

Dry reforming of methane (DRM) offers a sustainable pathway to valorize greenhouse gases (Carbon dioxide ($CO_2$) and $CH_4$) by converting them into syngas (CO and $H_2$) for down-stream alkane and methanol/higher alcohols production, and the grand challenge lies in developing coking- and sintering-resistant catalysts from facile synthesis approaches. Alternative stable DRM catalyst design practical in large-scale synthesis, having no requirement on pretreatment control, and capable of surviving temperature fluctuations is highly desired and has not yet achieved. Herein, highly active and stable DRM under dynamic conditions was achieved using barium-doped rock salt structured high entropy oxide (HEO) catalyst (Ba-NiMgCuZnCoOx, denoted as BaO-HEO) facilely synthesized from metal oxide precursors. Without any pretreatment, the active NiCuCo alloy nanoparticles were generated via redox exclusion from the BaO-HEO solid solution precursor during the DRM procedure. Sintering-resistance of the active alloys was ensured by the *in situ* created strong alloy-HEO interface and BaOx overlayer encapsulation via strong metal-support interaction construction induced by $CO_2$ flow. Accelerated coking removal was achieved by enriching $CO_2$ concentration around the active sites benefiting from the strong $CO_2$ chemisorption on the as-induced BaOx overlayer during DRM. Structure evolution and intermediates formation on the surface was elucidated via combined neutron-, x-ray, microscopy, and spectroscopy-based techniques. Temperature oscillation within 25 - 800 °C was deployed and robustness of the HEO catalyst was witnessed over 150 h. This study shows the potential of easily synthesized HEO catalysts in enabling valorization of $CO_2$ and $CH_4$.

## Santa Barbara Amorphous-15 Synthesis: On the Thermal Behavior During Calcination and Pyrolysis, and Recyclability of the Pluronic 123 Template. Application for Tobacco Smoke Toxicants Reduction

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### Abstract

Santa Barbara amorphous-15 (SBA-15) has increasingly important applications in catalysis due to their high surface area, tunable pore size, and excellent thermal and mechanical stability. The synthesis of SBA-15 has been widely studied and normally uses the triblock copolymer pluronic 123 (P123) as the template. We have studied its application as a catalyst for tobacco smoke toxicant reduction where it has proved excellent results. Mixing 4% w/w of SBA-15 with tobacco leads to typically 60% toxicants reductions. This type of application would require huge amounts of the catalysts. Thus, the recovery for reused P123 in the SBA-15 production would be of great interest in reducing costs, contributing to its commercial success. In the present contribution we present the results of a deep study of the effect of the amount of sample and the atmosphere in the thermal decomposition behavior of P123 both being alone and being within the uncalcined SBA-15, clarifying certain controversy existing in the literature regarding the thermogravimetric analysis (TGA) thermal behavior of P123 in pyrolysis and combustion processes. We also present results regarding the recyclability of P123 for SBA-15 synthesis, studying different extraction procedures and the modification suffered by the copolymer during the SBA synthesis and extraction processes, using the analytical pyrolysis evolved gas analysis technique, hydrogen nuclear magnetic resonance, as well as testing the SBA-15 synthetized with the "recovered P123" in the smoking process. We concluded that only the P123 remaining in the mother liquor after the thermal treatment is susceptible to being reused for obtaining an SBA-15 yielding acceptable results in the smoking application. The extraction of the P123 after the hydrothermal treatment yields a modified copolymer leading to a material similar to SBA-15 but leading to

poor results when used for tobacco toxicity reduction.

## Advancements in X-ray Photoelectron Spectroscopy Depth Profiling using Femtosecond Laser Ablation (fs-LA) for Surfaces Relevant for Catalysis

**James Lallo[1*], Tim Nunney[2], Robin Simpson[2], Paul Mack[2], Mark Baker[3] and Charlie Chandler[3]**

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### Abstract

X-ray photoelectron spectroscopy (XPS) depth profiling is a widely employed analytical technique to determine the chemical composition of thin films, coatings and multi-layered structures, due to its ease of quantification, good sensitivity and chemical state information. Since the introduction of XPS as a surface analytical technique more than 50 years ago, depth profiles have been performed using ion beam sputtering. However, many organic and inorganic materials suffer from ion beam damage, resulting in incorrect chemical compositions to be recorded during the depth profile. This problem has been resolved for most polymers by using argon gas cluster ion beams (GCIBs), but the use of GCIBs does not solve the issue for inorganics. We have introduced a novel XPS system, hypulse, that employs a femtosecond laser ablation (fs-LA) rather than an ion beam for XPS depth profiling purposes. This novel technique has shown the capability of eradicating chemical damage during XPS depth profiling for all initial inorganic, compound semiconductor and organic materials examined. The technique is also capable of profiling to much greater depths (several 10s microns) and is much faster than traditional ion beam sputter depth profiling. fs-LA XPS depth profile results will be shown for selected thin films, coatings, multilayers and oxidized surfaces related to catalysis materials and the outlook for this new technique discussed.

## Evolution from the Titration Curve Equation through the Invention of the Diode Based on a Frozen Electrolyte Solution to the Formulation of a New Law of Electrolytic Ionization

**Stanislav V. Yefimov[*]**

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### Abstract

In this work, we combined the results of our research and data from other authors to unify and popularize a new approach to describing the behavior of aqueous electrolyte solutions. As part of this task, we briefly describe the derivation of a general equation of state for aqueous solutions of acids and bases and their mixtures, as well as the derivation of a general equation of state for semiconductors doped with p-type and n-type impurities. The identity of the mathematical models for electrolyte solutions and doped semiconductors indicates the direction for searching for semiconductor properties in electrolyte solutions. Such a property was discovered and claimed to be an invention under the name: "Diode Made of Ice". It is shown that acid is an n-type semiconductor impurity, and a base is a p-type impurity. The result of this stage of the work was the formulation of the Law of Electrolytic Ionization. The law states that water and ice are semiconductors, which is confirmed by the calculation of the band gap of water.

## Automated Software for Homogeneous Catalyst Design

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### Abstract

Identifying molecular catalysts that simultaneously achieve high selectivity, fast turnover, and robust stability remains a central challenge in homogeneous catalysis. Traditional discovery pipelines rely heavily on labor-intensive experimental screening, while existing automated computational workflows typically focus on a single performance descriptor such as enantioselectivity or rate-determining step. Here we present a next-generation, fully automated physics–artificial intelligence framework for rapid, mechanism-guided optimization of catalytic performance at scale. By substantially expanding the accessible design space, the framework accelerates the discovery of high-performing molecular catalysts. It is accessible through both graphical and command-line interfaces and requires minimal user input or prior expertise.

# Catalytic Methane Splitting Technology: A Decarbonization Pathway

**Prem Kumar Seelam* and Samuli Räsänen**

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## Abstract

Methane splitting technology is one of the key decarbonization strategies for the fossil-driven industries. At industrial scale, hydrogen is traditionally produced by methane steam reforming and coal gasification. However, both technologies are highly carbon dioxide emitting and energy intensive processes. The thermocatalytic methane decomposition (TCD) has been a well-known process for decades and it is a potential methane splitting technology for $H_2$ and valuable solid carbon production. Moreover, TCD offers many benefits in terms of cost, energy consumption, and scalability compared to other technologies i.e., thermal, plasma, and molten catalyst. Successful commercialization of TCD is still a big challenge in terms of catalyst and reactor technology upscale. Separation of carbon from metal particles, catalyst stability, and efficient reactor design are some of the key issues that must be addressed in TCD scale-up. The nickel, copper, cobalt, and iron-based catalysts are found to be the most active and selective transition metal catalysts in TCD. The type of carbon structure or allotrope is formed solely depending on the metal type and the catalyst composition. A case study of hycamite TCD process is successfully demonstrated at pilot scale with low-cost and zero carbon $H_2$-production. The most common reactor technologies operated in TCD are fluidized and fixed bed reactors. Thus, TCD is a promising cost and environmentally efficient technology in $H_2$ production. Innovation in sustainable catalysts and novel reactor design are key in successful implementation at commercial scale. Overview on current status of TCD technology in comparison with hycamite process

# Photocatalytic α-ketoaziridine Intermolecular Ring Expansion to Synthetize Dihydrofuran Derivatives

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## Abstract

Visible-light photo redox catalysis has become a powerful tool for generating radical species under mild conditions, offering a milder alternative to traditional radical-based methods. This approach has significantly impacted various reaction classes, including cross-couplings, cycloadditions, and more recently, radical/polar crossover processes - emerging as promising strategies for synthesizing cyclic structures. In this study, we report a photocatalytic intermolecular aziridine ring expansion, using α-ketoaziridines and olefins in the presence of an iridium-based photocatalyst and an organic base under visible light irradiation. This reaction proved high levels of chemoselectivity, providing the desired amino-substituted dihydrofuran products 3 in good yields. Reaction optimization, substrate scope, and mechanistic insights will be discussed in detail in this communication (Figure 1).

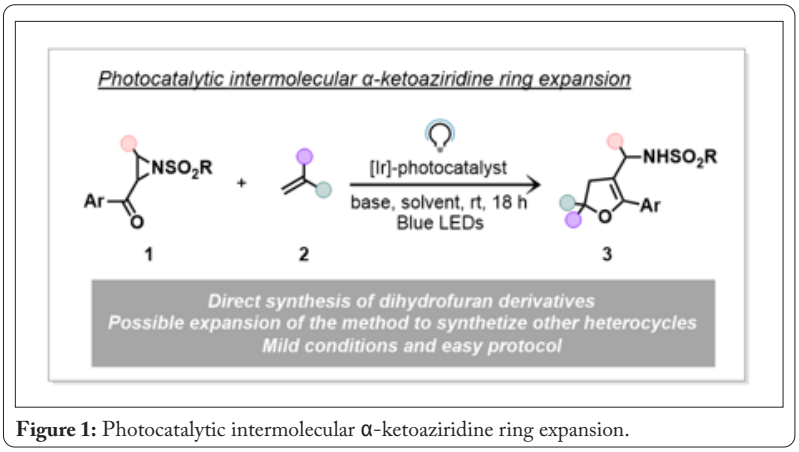


**Figure 1:** Photocatalytic intermolecular α-ketoaziridine ring expansion.

## Highly Stable Defect-free HZSM-5 Nanocrystals for Enhanced Conversion of Biomethanol to Sustainable Aviation Fuel Components

**Judith Hernandez Cabello*, Ming Zhou, Liang Yu and Jonas Hedlund**

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### Abstract

The aviation sector is responsible for 2 - 3% of global human-induced carbon dioxide emissions, and this value is rising. Therefore, one of the efforts to decrease carbon footprint is sustainable aviation fuels. Zeolites, and specifically Zeolite Socony mobil-5 (ZSM-5), have been continuously reported as good candidates for methanol to hydrocarbon processes. This work is focused on the synthesis and evaluation of defect-free hydrogen-form ZSM-5 (HZSM-5) nanocrystals with a size of about 10 nm for conversion of biomethanol to heavy hydrocarbons (C8+), considered jet fuel components. This novel one-step process was evaluated at different experimental conditions in a fixed-bed reactor, showing best performance at 340 °C and 2 bar. The nanocrystals show a clearly better performance than the commercial HZSM-5 catalyst used for comparison. Pure ethylene was also used as feedstock. The condensed C8+ fractions for both feeds and catalysts were aromatic-rich, proving the high potential of these nanocrystals, since aromatics are an essential fraction of jet fuels, and a highly demanded blending component for other new alternative jet fuels. The long stability test with a running time of up to 1000 h shows that the defect-free HZSM-5 catalyst maintains excellent performance with a high and stable C8+ yield of 35% and methanol conversion of about 90%. This enhanced activity is attributed to the lack of defects within the catalyst structure, reducing the likelihood of coke formation within the silanol groups.

## Expanding Sulfur Ylide Chemistry for the Synthesis of Cyclic Compounds

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### Abstract

Strained and medium-sized ring systems hold immense value in drug discovery and material science, due to their unique conformational and biological properties. In this work, we present new uses of sulfur ylides as versatile platform for the construction of cyclic compounds such as cyclopropanes and benzazepines - valuable motifs in pharmaceuticals and natural products. Sulfur ylides are zwitterionic compounds defined by a carbanion and a neighboring positively charged sulfur atom, which allows a rich reactivity to produce simple, effective transformations, including insertion and formation of (hetero) cyclic systems. Our research explores the development of different protocols utilizing sulfur ylides to access both strained and medium-sized ring frameworks under mild, metal-free conditions. By activating sulfur ylides through photo redox catalysis, a new visible-light-mediated approach to cyclopropanation of alkenes using sulfoxonium ylides under mild conditions, without external oxidants or metal carbenes is presented. Moreover, we have also proven that sulfur ylides can be used as safe, easier to handle alternative reagents to diazomethane derivatives for the insertion-ring expansion of N-heterocycles such as quinolines to build added-value 7-membered benzazepines. This work demonstrates how S-ylide-based both radical and polar approaches can provide innovative access to complex molecules with medicinal potential, while aligning with sustainable and scalable synthetic practices.

## Embedded Correlated Wavefunction Theory for Accurate Predictions of Adsorption Energies on Transition Metal Surfaces

**Connor Fawcett* and Qing Zhao**

*Northeastern University, United States*

### Abstract

Density functional theory (DFT) is the most widely used method in simulating heterogeneous catalysis, due to its balance between computational efficiency and accuracy. Still, it suffers from electron self-interaction and energetic delocalization errors arising from the approximate exchange-correlation functional, and most importantly, a single-reference description of the electronic structure. These issues can lead to quantitative and even qualitative errors in the description of transition metal chemistry and charge transfer processes which are crucial in heterogeneous catalysis. Instead, embedded correlated wavefunction theory (ECW) is a more suitable approach to describe electronic structure and to predict reaction barriers in complex catalytic systems. Within ECW, the periodic system is partitioned into two subsystems – a cluster containing the important catalytic

center and its surrounding environment. We then generate an embedding potential to recover the interaction, i.e., electron density, between the cluster and its environment using density functional embedding theory (DFET). This allows for a drastic reduction of computational cost in CW calculations on the cluster in presence of the embedding potential compared with that on the periodic system directly, extending the applications of CW from small and medium-sized molecules to heterogeneous catalysis. Here, we couple DFET with multireference wavefunction methods, including complete active space second-order perturbation theory using reference wavefunctions generated from complete active space self-consistent field theory to examine its accuracy in predicting experimentally measurable adsorption energies on metallic surfaces. Our work explores new computational framework that goes beyond standard DFT to enable qualitatively and quantitatively reliable modelling of heterogeneous catalysis.

## Efficient Visible-light Photocatalysis of Textile Dyes via Multi-block Doped Anatase Nanocrystals

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### Abstract

Industrial dye pollution poses a major environmental threat, with conventional treatment methods often falling short in efficacy or sustainability. This study presents a novel photocatalyst, a four-nuclear oxide nanocrystal, synthesized via a solvothermal route and doped with elements across s-, p-, d-, and f-blocks. The photocatalyst exhibited complete degradation of a broad spectrum of textile dyes-including cationic, anionic, and azo types-under low-intensity visible light-emitting diode illumination light within 2 h. Extensive characterization revealed that nitrogen and cerium dopants tune the energy bandgap, while the transition metal introduces lattice strain, improving surface reactivity and reducing crystallite size. Statistical optimization over 81 reaction conditions and mechanistic studies, including cyclic voltammetry and electron paramagnetic resonance, confirmed superoxide radicals as the key active species. The catalyst also demonstrated high stability over multiple cycles and outperformed traditional titanium dioxide-based systems in both efficiency and environmental relevance. This work highlights a scalable approach for designing advanced photocatalysts tailored for low-energy, high-efficiency water purification systems.

## Designing High Entropy Janus Particles for Economical Catalytic Conversion of Polyolefins to Benzene, Toluene, and Xylenes

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### Abstract

Catalyzed conversion of polyolefin waste to value-added products such as benzene, toluene, and xylenes is one of the most economically productive methods of recycling plastics. However, polyolefin recycling methods such as hydrogenolysis are significantly limited by the cost effectiveness of catalysts due to its short lifespan caused by cumulative coke formation. By designing the high entropy Janus particle (HEJP), which requires a spherical metal cluster consisting of an equimolar combination zirconium, hafnium (Hf), palladium (Pd), ruthenium (Ru), and titanium and 4,4'-azobenzene dicarboxylic acid (AZ-BDC) as linkers, reaction kinetics can be significantly improved. Thus, AZ-BDC linkers were added asymmetrically to simulate the photoactive properties of azobenzene, which is an enantiomer oscillating between cis and trans conformations subsequent to optical excitation. Grand canonical Monte Carlo simulations were utilized to replicate the high entropy conditions of the Janus particles and to identify the optimized active sites for which ligand adsorption was maximized, which showed a ratio of 4 Hf:2 Pd:1 Ru. By utilizing the coherent potential approximation–Korringa–Kohn–Rostoker method, the local density of states of the particle was identified, revealing that plasmonic activity was recorded at 0.52 rydberg (Ry), 0.59 Ry, 0.67 Ry, 0.73 Ry, 0.81 Ry, 0.88 Ry, 0.94 Ry, and 0.96 Ry, confirming electron transfer through AZ-BDC. This was confirmed by the molecular dynamics simulation to monitor the adsorption of polystyrene (PS) oligomers, which showed a high degree of adsorption of PS at 11 molecules per particle. Therefore, it can be concluded that HEJPs are a highly favorable candidate to economically process polystyrene waste.

## Synthetic Fuels and Chemicals from Plastic Waste with Scalability

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### Abstract

Plastics is a common material in our daily lives. The widespread applications of plastics in building, construction, automotive and packaging have resulted in a rapid increase in the use of plastic and the generation of plastic waste. Plastic waste cannot be broken down by microorganisms easily and must be destroyed by incineration process which emits the greenhouse gas, carbon dioxide that contributes to global warming. The issue of plastic waste should be addressed to reduce the carbon emissions resulting from incineration of plastic waste. In addition, the current market lacks scalable cost-effective low carbon fuel technologies to increase the supply of synthetic fuels for the hard to decarbonize sectors such as aviation. The transformation of plastic waste into valuable products that are required by society such as sustainable aviation fuel should be explored. The scalability of most lab based hydroconversion technologies also poses as a barrier for further translation to pilot scale demonstrations. In this work, the design of cost effective catalytic hydroconversion processes of polyolefin waste towards continuous flow production of synthetic fuels and chemicals are investigated to develop pilot scale demonstrations for environmental solutions with possible economic value.

## Elucidating the Formation Mechanism of Yellowing During the Production of Bio-based Poly(ethylene Furanoate)

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### Abstract

Under dual pressures of energy scarcity and environmental pollution, the biobased polyester poly(ethylene furanoate) (PEF) is poised to dominate the industry in the future, overtaking conventional petroleum-based polyesters. Nonetheless, PEF discoloration is a critical impediment to its commercial success. An in-depth analysis of esterification products from 2,5-furandicarboxylic acid (FDCA) and ethylene glycol was conducted. The decarboxylation byproducts which resulted in the yellowing were accurately separated and identified using ultrahigh-performance liquid chromatography/high-definition mass spectrometry techniques. In the production of PEF, two different types of decarboxylation reactions may occur for oligomers with a carboxyl terminal: (i) intramolecular decarboxylation reaction: removal of carbon dioxide ($CO_2$) to generate a furan monoacid; and (ii) intermolecular decarboxylation reaction: removal of water and $CO_2$ to produce a structure in which the two furan rings are attached to the same carbonyl group. To trace the origin of the decarboxylation reaction, a comprehensive characterization of FDCA monomers corresponding to PEF of varying color phases was performed. Gas chromatography-mass spectrometry and desorption electrospray ionization-mass spectrometry identified organic impurities such as 2-furoic acid, while inductively coupled plasma–optical emission spectroscopy revealed residual metal ions including aluminium, calcium, iron, potassium, and sodium (Na). Crucially, the integration of density functional theory calculations and thermogravimetric analysis demonstrated that residual $Na^+$ in the monomer promotes the decarboxylation process. This decarboxylation action leads to the formation of chromophoric compounds, ultimately causing polymer discoloration. This work provides a solid scientific foundation and theoretical guidance for producing high-quality and color-stable PEF.

# Visible Light-mediated Organic Photoredox-catalyzed S-difluoromethylation and S-trifluoromethylation of Aromatic and Heteroaromatic Thiols

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## Abstract

Visible light-mediated difluoro- and trifluoromethylation protocols are developed for the conversion of aromatic and heteroaromatic thiols to their respective S-difluoromethylated and S-trifluoromethylated derivatives employing difluoromethanesulfonyl chloride ($CHF_2SO_2Cl$) and trifluoromethanesulfonyl chloride ($CF_3SO_2Cl$; Ered = -0.18 V vs saturated calomel electrode (SCE)) as cost-effective sources of difluoromethyl radical ($CHF_2$·) and trifluoromethyl radical ($CF_3$·), respectively. While S-trifluoromethylation of thiols takes place in the presence of a highly reducing organophotocatalyst, 3DPA2FBN (E1/2 ($PC^{•+}/PC^*$) = –1.60 V vs SCE), the S-difluoromethylation of thiols produces best results with 3DPAFIPN (E1/2 ($PC^{•+}/PC^*$) = –1.38 V vs SCE). The developed photochemical synthetic methodologies are operationally simple, providing access to a diverse range of the corresponding products in up to quantitative yields (>99%). Plausible mechanisms for both cases have been postulated based on preliminary mechanistic studies, including irradiation on-off, ultraviolet–visible spectroscopy studies, radical trapping experiments, and triplet energy quenching studies (Figure 1).

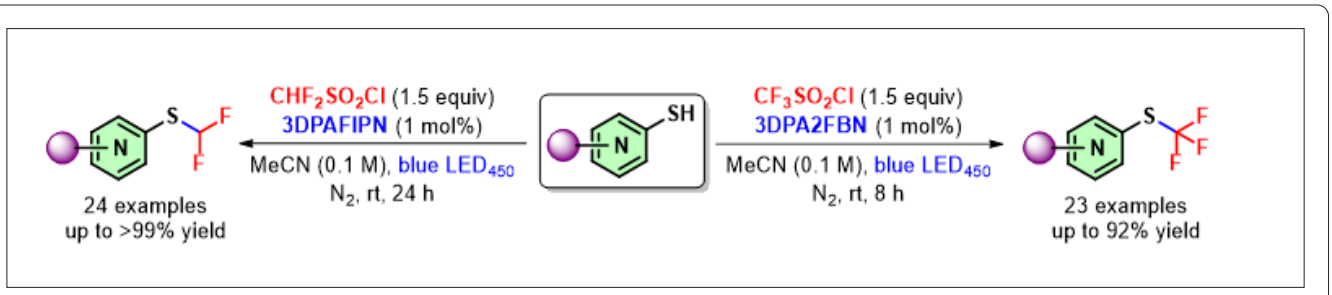


**Figure 1:** Visible light-mediated S-difluoromethylation and S-trifluoromethylation of aromatic and heteroaromatic thiols using $CHF_2SO_2Cl$ and $CF_3SO_2Cl$, respectively.

# Green Catalytic Hydrogenation-challenges and Opportunities

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## Abstract

Catalytic hydrogenation is an important industrial process for many important molecules. It is a chemical reaction where hydrogen gas is added to a molecule, specifically unsaturated compounds like alkenes or alkynes, in the presence of a catalyst. The catalyst, often a metal like platinum, palladium, or nickel, lowers the activation energy of the reaction, allowing it to proceed at milder conditions. This process converts unsaturated bonds (double or triple) into single bonds, effectively reducing the molecule. As hydrogen gas is highly inflammable, special safety measures are followed for handling the reaction. An option of producing hydrogen from water is gaining momentum and use of green hydrogen in catalytic hydrogenation is an area of current industrial interest. Producing hydrogen from wastewater generated helps in managing water treatment load along with producing necessary raw material in house i.e., hydrogen gas. Sayaji industries is an 85-year young organization and always remains at the forefront to adopt new ideas which is evident from company's initiatives on zero discharge of hazardous chemicals, carbon disclosure project, zero liquid discharge, etc. Process for a sweetener produced at the Ahmedabad plant is being greenified by the company as company believes in long term strategies even at the expense of initial high capital. Present paper discusses challenges in getting green and opportunities involved.

## Simulating Electrocatalytic Thermodynamics and Kinetics Through Density Functional Theory-based Methods

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### Abstract

Electrochemistry enables the efficient interconversion of electric and chemical energy which can be harnessed in numerous electrocatalytic reactions such as hydrogen evolution and oxidation, oxygen reduction, and carbon dioxide ($CO_2$) reactions. At the heart of all electrochemical and electrocatalytic systems lies the ability to control reaction thermodynamics and kinetics at solid-liquid interfaces through the application of an external electrode potential. While experiments are readily performed under such conditions, theory and simulation of electrochemistry under conditions mimicking experiments is extremely difficult requiring the development and application of novel theoretical and modeling methods. I will present our recently developed theoretical and computational methods for simulating electro-catalytic thermodynamics and kinetics under constant potential conditions within the grand canonical ensemble approach. I will also present ways to simulate electrolyte effects on electrochemical interfaces and reactions. Illustrative applications of these methods showcase 1) the complex surface chemistry of gold electrodes as a function of potential and pH, 2) the effect cations on the $CO_2$ reduction reaction mechanism, thermodynamics, and kinetics, and 3) the effect of the electrode potential in creating localized electronic (polaron) states that activate semiconductor interfaces towards the $H_2$ evolution reaction. Overall, the presentations show how advanced theory and computational methods allow understanding of the impact of the catalyst and reaction conditions in electrocatalysis.

## Divergent Sequential Reactions of β-(2-aminophenyl)-α,β-ynones: Brønsted Acid vs Transition Metal Catalysis

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*[2]Department of Physical and Chemical Sciences, University of L'Aquila, Italy*

### Abstract

β-(2-aminophenyl)-α,β-ynones are versatile intermediates whose sequential reactions can be directed toward divergent products depending on the catalytic system employed. Their employment as building blocks allowed the development of efficient, versatile and sustainable synthetic methods for constructing complex nitrogen-containing heterocycles. The high functional group tolerance, suitable for further functionalization, expanded their utility in medicinal chemistry and drug development. Transition metals catalyzed reactions of β-(2-aminophenyl)-α,β-ynones enabled cascade or tandem transformations, including regioselective hydroamination, hydroarylation, and cross-coupling, to access a wide variety of heterocyclic scaffolds such as quinoline derivatives, indoles, diazocines, benzoxazines, and other polycyclic frameworks, with product selectivity control. Brønsted acids, on the other hand, provided simpler and more viable routes to quinolines and related products. Generally, transition metals catalysis achieved more tunable transformations, while Brønsted acids excelled in sustainability and practicality. Conversely, in some cases, transition metal- and Brønsted acid-catalysis could provide a powerful tool to direct divergent sequence reactions by distinct mechanisms and product selectivity control. Indeed, the choice of the catalyst in these later cases addressed the reaction pathway toward different outcomes. Overall, the choice of catalyst-Brønsted acid versus transition metal-enabled tunable divergent access to a wide array of heterocyclic scaffolds from the same starting ynones. Notably, synergistic combinations of transition metal catalysts with Brønsted acids can further enhance reactivity and selectivity achieving the one-pot synthesis of complex heterocycles.

## Coupled "Molecular – collective" Investigation of Electrode Processes and the Electrode-solution Layer

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### Abstract

A combined approach is proposed that consists in the coupled study of "molecular" x and "collective" X properties; the x relate to the behavior of individual specific molecules in electrochemical reactions, in particular, the product ratios when the electrolysis

conditions are changed; the X describes properties of the electrode environment as a whole. Existence of molecular effects x follows from the difference in products xdir and xhom obtained via direct electrolysis and via homogeneous electro-catalysis (HOMEC). We found these differences by studying the electrochemical reduction of the deuterated 2,4-pentadienol and its derivatives. It was explained by the hypothesis of "superviscosity" of the near-electrode layer, X-factor, which prevents equilibrium arrangement of intermediate electrolysis products. The molecular dependence x = f (L) (I) on the distance L from the electrode surface is determined using the near-electrode tomography with a gradual change in the HOMEC contribution (NELTO-method) by solving the diffusion-kinetic equations. The collective dependence, in the present case, of viscosity X = ηS = F(L) (II) was determined by our proposed, electro-chemical atomic force microscopy technique (EC-AFM). The identical character of the profiles of the (I) and (II), regression coefficients 0.99 - 1.00 confirms the hypothesis of superviscosity. Similar relations are to be expected for other properties, in particular for the dielectric constant ηS for the liquid-to-solid state transition, etc. For the first time, results are published comparing the products of HOMEC-NELTO-electrolysis and in electrochemical stopped flow EC-AFM- mode, completely free of electrode effects. The combined x, X - measurements open up new possibilities for establishing the nature of electrode phenomena.

## Synthesis of Polyesters Using Surfactant Catalysts in Microemulsions: The Role of Micelle Shape

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### Abstract

In this study, we explored traditional methods commonly found in the literature to analyze how surfactants and polymers interact during the synthesis of polyester in emulsion systems. The study justifies its focus on micellar catalysis by exploring its effectiveness and suggesting methods for enhancing the synergy among surfactants, reactants, and catalysis. We looked at factors like surface tension, critical micelle concentration, micelle shapes, aggregation numbers, and interfacial phenomena in the process of macromolecular packing in emulsion polycondensation. A surfactant-water system consisting of dodecylbenzene sulfonic acid and sodium dodecyl sulfate was employed. Polyesters were prepared from glycerol, ethylene glycol, diethylene glycol, and dicarboxylic acids in a surfactant-water system under mild conditions ranging from 70 - 150 ˚C. Fourier-transform infrared spectroscopy and proton nuclear magnetic resonance confirmed the esterification. Differential scanning calorimetry indicated no crystallinity and a glass transition temperature range of –53 to –46 ˚C, typical of soft matter. The resulting polymers had molecular weights ranging from 1180 – 6800 g/mol. We found that these polymer aggregate shapes can respond by changing their sizes, both in bulk and at the air-solution interface, when the concentration of surfactants is increased above the critical micelle concentration. The results showed narrow spherical and ellipsoidal polymer aggregates.

## Automated Reaction Discovery of Laser-driven Fragmentation Pathways in Diaminomaleonitrile

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### Abstract

Nitrogen-rich nitriles are pervasive in the interstellar medium, yet the formation and survival of larger prebiotic precursors remain mechanistically under constrained. 2,3-diaminomaleonitrile (DAMN) and hydrogen cyanide tetramer implicated in pathways toward purine chemistry-has recently been probed via laser ablation, yielding a suite of small N-bearing fragments. Here, I present a first-principles, mechanism-resolved interpretation of these laser-driven outcomes using automated reaction discovery coupled to high-level energetics. The resulting reaction network rationalizes key experimentally reported products and their accessibility: (i) formation of malononitrile via low-to-moderate barrier sequences involving C–C/C–N cleavages and hydrogen shifts; (ii) production of aminomethyl nitrile + cyanomide radical pairs, which can yield aminoacetonitrile in the presence of atomic H; and (iii) multiple routes to Z-C-cyanomethanimine, including pathways that generate two Z-isomers from a single DAMN precursor. The search also predicts additional energetically feasible products not observed in ablation measurements, highlighting how plasma-plume secondary chemistry (recombination and further fragmentation) may shape experimental product distributions beyond the unimolecular scope. Overall, this workflow links laser ablation observables to a kinetically and energetically consistent mechanistic map, offering testable targets for future laboratory and astronomical searches.

## High Surface Area Zinc Oxide

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### Abstract

Zinc oxide (ZnO) is a high-volume chemical with numerous applications including vulcanization aid in car tires, sulfur trap and guard bed to protect downstream platinum-group metal (PGM) and nickel catalysts. Low surface area ZnO is commercially produced by air oxidation of zinc metal vapors. We have investigated various routes to synthesize high surface area ZnO, including wet digestion in aqueous ammonium carbonate, soft combustion synthesis using the Pechini method and dry decomposition, 1-step spray calcination, and in particular 2-step spray drying and subsequent calcination which is directly scalable and allows high productivities at very large commercial scale. Brunauer–Emmett–Teller (BET) surface areas >70 $m^2/g$ have been achieved so far by high throughput screening. BET can likely be further enhanced by optimization.

## Onion-like Carbon as a Robust Support for Palladium and Palladium–nickel Catalysts in Low-temperature Methane Oxidation

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### Abstract

Utilization of carbon supported catalysts in the thermal oxidation of methane is precluded by the instability of carbon in the high operating temperatures. However, optimization of carbon can improve its thermal stability, resulting in robust catalysts. Hence, palladium (Pd) has been supported on onion-like carbon (OLC), which, as far as we know, has not been investigated in the oxidation of methane. The OLC was prepared from nanodiamond powder by annealing at 1300 °C, providing high thermal stability and high surface area, which led to high catalytic performance. In addition, inserting nickel (Ni) into the Pd/OLC catalyst offered higher surface area, improved the metal distribution on the support, and slightly decreased the particle sizes. The monometallic Pd/OLC showed a complete methane conversion at 450 °C, while the bimetallic Pd-Ni/OLC presented higher catalytic performance, as it achieved the full methane conversion at 400 °C only. This work paves the way for utilizing the OLC, as an excellent support in the thermal gas phase reactions, not only in the methane combustion (Figure 1).

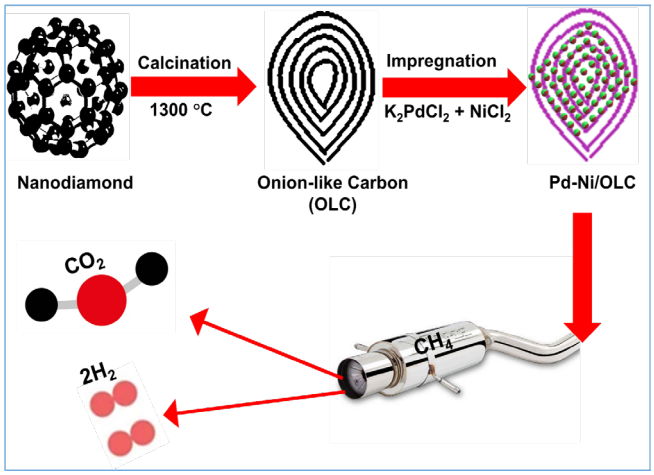


**Figure 1:** Schematic representation of OLC-supported Pd and Pd–Ni catalysts for methane ($CH_4$) oxidation to $CO_2$.

# Zeolites Effect of La-promoted Iron/Titanium Dioxide Catalyst for Production of $C_2^+$ Hydrocarbons in Carbon Dioxide Hydrogenation

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## Abstract

Considerable efforts have been made to convert one of the major greenhouse gases contributing to global warming, carbon dioxide ($CO_2$), to hydrocarbons. Additionally, the depletion and unfavorable environmental impact of fossil crudes have led to an increased focus on alternative feedstocks such as $CO_2$ for hydrocarbon chemical production. However, direct production of a reasonable quality of hydrocarbon products is still a great challenge. Products that are mostly produced from $CO_2$ hydrogenation are $C_1$ chemicals, such as methanol, methane, formic acid and carbon monoxide because of the low reactivity of $CO_2$ to produce $C_2^+$ hydrocarbon products. Currently, the use of iron (Fe) and zeolites in $CO_2$ hydrogenation reaction to directly produce gasoline-range hydrocarbons, $C_5$ - $C_{12}$, for clean and environmental-friendly fuels has gained much attention. However, in this study, we present the use of La-promoted Fe/titanium dioxide ($TiO_2$) catalysts and zeolites for the conversion of $CO_2$ containing-hydrogen to $C_2^+$ hydrocarbons via the $CO_2$ hydrogenation. The catalysts were characterized and evaluated in tubular fixed-bed reactors. The results of the effect of zeolites on the La-promoted Fe/$TiO_2$ catalysts showed an increase in the production of $C_2^+$ hydrocarbon products during the $CO_2$ hydrogenation reaction.

# Metal Oxide Nanocomposites for Dye Removal from Water

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## Abstract

Water resources are increasingly threatened by pollution resulting from untreated industrial effluents, particularly those containing synthetic dyes such as methylene blue (MB), a common pollutant used extensively in the textile industry. In recent years, nanomaterials-particularly metal oxide nanoparticles-have emerged as efficient and environmentally friendly candidates for the removal of such contaminants from water. In this study, a nanocomposite composed of magnesium oxide and zinc oxide (MgO-ZnO) was synthesized using simple and cost-effective methods. The composite was employed as an adsorbent for the removal of MB dye from aqueous solutions. To enhance its physicochemical properties, the prepared samples were subjected to thermal treatment at various temperatures. Characterization techniques including X-ray diffraction, scanning electron microscopy, Fourier transform infrared spectroscopy, and thermogravimetric analysis were used to investigate the crystal structure, surface morphology, and functional groups of the composite. The dye removal efficiency was assessed using ultraviolet-visible spectrophotometry by monitoring the absorbance of MB. Results revealed that MgO-ZnO nanocomposites calcined at optimal temperatures achieved removal efficiencies exceeding 85% within 40 min of treatment. These findings are on par with, or superior to, conventional adsorbents such as modified silica gel, treated sand, and other metal oxides like $MnO_2$ and $V_2O_5$. Adsorption kinetics followed a pseudo-second-order model, while the Freundlich isotherm provided the best fit for describing the adsorption equilibrium. Furthermore, the thermal stability of the material suggests its suitability for regeneration and multiple reuse cycles, enhancing its practical and economic appeal. Overall, the MgO-ZnO nanocomposite demonstrates considerable potential as a low-cost, high-efficiency, and sustainable alternative for the treatment of dye contaminated industrial wastewater.

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