Poster Presentations

Poster Sessions

Monday, 7th September 2026

16h20	Poster Session / Coffee Break
18h30	Poster Session

Tuesday, 8th September 2026

10h40	Poster Session / Coffee Break
16h00	Poster Session / Coffee Break

Wednesday, 9th September 2026

10h50	Poster Session / Coffee Break

Coupling electro- and thermo- catalytic approaches for CO_2 conversion to C_2+ compounds

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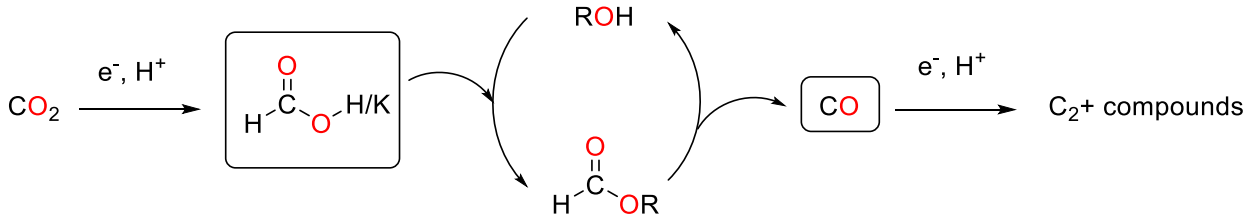
Abstract

The electrochemical reduction of CO_2 is a promising strategy for the sustainable production of value-added chemicals, although the selective formation of multi-carbon (C_2+) products remains challenging.[1,2]

Within the PowerCO_2 PEPR program, we investigate a coupled electro- and thermocatalytic strategy in which CO_2 is first electrochemically converted into a 2.4 M aqueous formate solution and subsequently upgraded to CO via methyl formate (Scheme 1). The resulting CO can then be electrochemically converted into C_2+ products.

Reactive distillation conditions were successfully transferred from a synthetic model solution to an electrochemically produced formate solution, affording 50% methyl formate yield with 62% purity. Methyl formate decarbonylation reached 70% conversion, while gas chromatography confirmed CO as the only gaseous product detected. In parallel, the CO electroreduction showed high selectivity toward C_2+ products, supporting the proposed integrated strategy.

These results demonstrate the feasibility of the individual electro- and thermocatalytic steps and provide the basis for the future integration of the complete CO_2 → formate → CO → C_2+ process.



Scheme 1. Proposed electro- and thermocatalytic strategy for CO_2 conversion to C_2+ products via methyl formate.

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Keywords

CO_2 electroreduction; CO_2 valorization; formate; thermocatalysis; CO electroreduction; C_2+ products

POWER CO_2

First principles investigation of optoelectronic properties of BiOF materials for photocatalytic CO_2 reduction

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Abstract

Bismuth oxyfluoride (BiOF) has emerged as a promising photocatalyst for CO_2 reduction, with experimental studies highlighting a strong dependence of reactivity on exposed surface facets [1,2]. Within the Plasmon sub-project of PowerCO_2, ICCF, in collaboration with IFPEN has shown that Bi/BiO_xF_y may catalyze the CO_2 photoreduction into CO in the presence of water. To rationalize these observations, a better understanding of the structural and electronic properties of BiOF surfaces under reaction conditions (T, water partial pressure) and of their interaction with CO_2 is expected.
As a preliminary benchmark, three Bi-based bulk systems (BiOF, BiF_3, and Bi) are studied using density functional theory (DFT) with two functionals: PBE-D3 and hybrid HSE06. This comparative approach enables validation of the theoretical parameters and showed that HSE06 (resp. PBE-D3) provides a reliable band gaps (resp. structure, energetics) consistent with available experimental data [3].
In the next step, surface energies and electronic properties are evaluated for three low-index BiOF facets: (001), (010) and (101) - using optimized computational parameters. Surface energies calculated through the linear-fit method [4] combined with Wulff morphology reveal the evolution of the facet proportions as a function of (T, $p(H_2O)$) conditions. The (001) and (101) facets are stabilized over a wide range of (T, $p(H_2O)$) conditions, whereas the (010) facet is stabilized at high temperature only (corresponding to specific thermal pretreatment). Moreover, the (010) and (101) facets predominantly expose hydroxyl groups, whereas the (001) facet exhibits weakly bonded molecular water.
In the presence of molecular water, the CB edge position of the (001) facet is weakly negative at the PBE level (-0.2 V vs SHE at pH=7), close to the CO_2/CO reduction potential (-0.11 V), while CO_2 molecule is weakly physisorbed. By contrast, the (010) and (101) facets exhibit more negative CB positions (below -1.1 V) and both facets chemisorb CO_2, leading to carbonate species (in the absence of OH groups) or to hydrogen carbonate (in the presence of OH). Moreover in the presence of O-vacancy, the (101) facet may thermodynamically convert CO_2 into CO.
This theoretical analysis provides a rationalization of the surface properties of BiOF materials and suggests that the (101) and (010) facets may be more efficient for CO_2 photoreduction than the basal (001) facet. To minimze the proportion of (001) facet and maximize the (101) facet, well chosen (T, $p(H_2O)$) synthesis conditions should be targeted. In perspectives, we expect to build the bridge with experiments (such as IR spectroscopy) undertaken within the Plasmon sub-project.

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Keywords

Density Functional Theory; BiOF surfaces; Wulff morphology; hydroxyls; CO_2 adsorption.

Up-converting photonic structures for CO2 reduction

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Abstract

Recently, the CO_2 reduction reaction via photocatalysis has gained attention, with the perspective of utilizing CO_2 molecules to produce low-carbon footprint fuels such as solar fuels, by solar excitation [1]. However, it is necessary to use UV light, which is strongly filtered by the atmosphere. The up-conversion phenomenon, which consists in the absorption of low-energy photons followed by the emission of higher-energy photons, allows for UV emission following multi-wavelength absorption steps in the visible and near infra-red (NIR), using a co-doped system consisting of Yb^{3+} and Tm^{3+} rare-earth ions [2], as showed in figure 1. As a matter of fact, the efficiency is relatively low, and limited mostly by the low absorption cross-section of the rare-earth ions [3]. As a result, photonic approaches such as coupling with a photonic crystal have been studied to enable the control, and strengthening of the targeted energy transitions with overlapping guided mode resonances [4,5]. The work of our project is related to the fabrication of the up-converting Y_2O_3 host-matrix co-doped with Yb^{3+}/Tm^{3+}, and the different ways of coupling it with a photonic crystal that has been designed to support the targeted transitions. The up-converting material has been deposited using spin-coating and integrated into all of the photonic structures showed in figure 2, selected by earlier simulation work. The research is currently ongoing regarding the coupling and characterization of the up-conversion phenomenon. The perspectives are to extend the work on the design of the structures, allowing for efficient up-conversion and CO_2 reduction reaction yields.

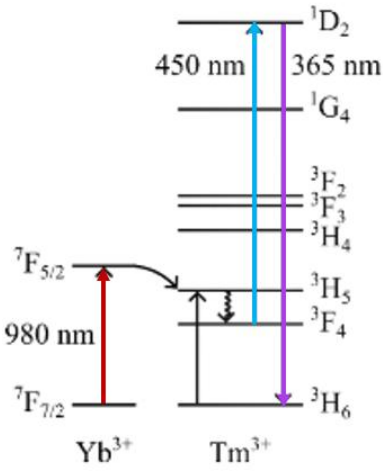

Figure 1: Multi-wavelength up-conversion mechanism of the co-doped Yb^{3+}/Tm^{3+} system [5]

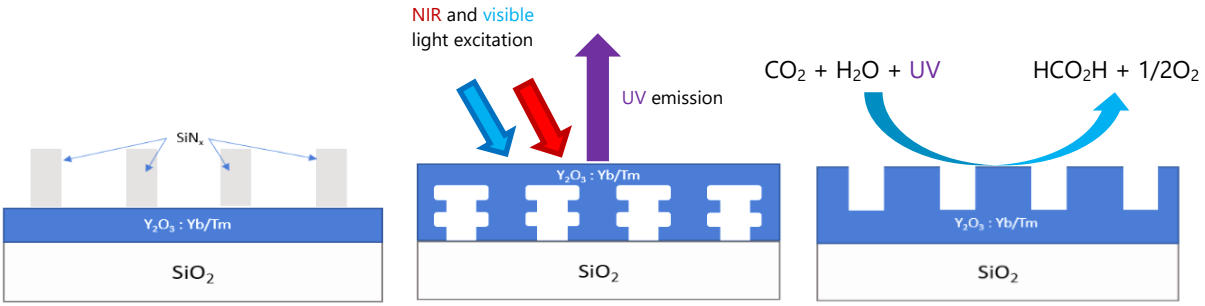

Figure 2: Different studied photonic crystal designs for the coupling with the up-converting material

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Keywords

CO_2-to-fuels; Photocatalysis; Photonic Crystals; Up-conversion; CO2 reduction; Solar fuels

Thiazolylidene-catalyzed formose reaction in aqueous conditions

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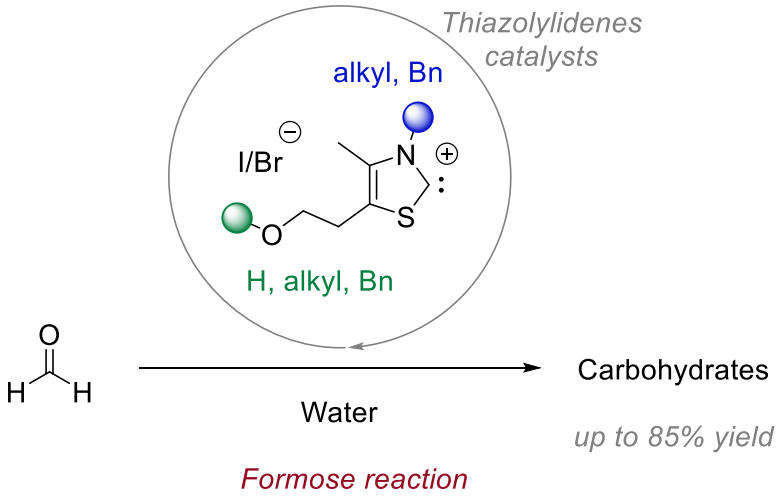
Abstract

The formose reaction (FR) converts formaldehyde into carbohydrates. With the accessibility of formaldehyde from CO_2 or CO,[1] the FR offers a promising route to transform renewable C_1 feedstocks into sugars.[2] N-Heterocyclic carbenes catalyze this reaction through the umpolung activation of formaldehyde in organic solvent but very rarely in aqueous conditions. For instance, thiazolylidenes exhibit high activity in organic solvents toward the FR, but are generally unstable in aqueous media. As a consequence, thiazolylidenes have never been shown to catalyze efficently the FR in water. Inspired by thiamine, the cofactor of formolase enzymes, in which the reactive thiazolium unit is protected by the enzyme environment, we investigated the introduction of long alkyl and aryl substituents to protect these carbenes from hydrolysis. The resulting compounds efficiently catalyzed the FR in water. The best catalyst afforded up to 85% total yield in carbohydrates.



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Keywords

Formose reaction ; C_1-to-carbohydrates ; Organocatalysis

Co-feeding CO_2 in the Isosynthesis Reaction: Competition of CO, CO_2 and H_2O Adsorption

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Abstract

The isosynthesis reaction converts syngas (CO/H_2) into C_{1-4} hydrocarbons, with high selectivity into isobutene, a useful chemical building block. This reaction is typically carried out over single metal oxide catalysts, such as ZrO_2. Metal oxides contain the acid sites that activate CO and base sites that promote the isomerization of intermediates to branched hydrocarbons. However, water is formed during the reaction and reacts with CO to produce CO_2 via the water gas shift reaction.

In this study, the effect of CO_2 co-feeding on product selectivity and water formation over ZrO_2 was investigated by progressively add 9.4% and 20% CO_2 molar fractions to CO and H_2 feeds at 450°C at 30 bars. Increasing the CO_2 molar fraction promoted methanation and the formation of saturated hydrocarbon, while decreasing isobutene formation. Additionally, a significant amount of water was collected, strongly suggesting a shift in equilibrium towards the reverse water gas shift reaction (rWGS). The ZrO_2 surface is sensitive to water, as water can readily hydroxylate the surface, altering the active acid and base sites. To elucidate how the surface was influenced by CO_2 co-feeding and the concurrent increase of water vapor, CO_2-TPD analysis was conducted under dry and humid conditions.

The base sites were probed by CO2-TPD and the fresh catalysts exhibited a base site concentration of 230 µmol g^{-1}. The presence of 50% relative humidity in the feed significantly decreased CO_2 adsorption to 70 µmol g^{-1}, indicating competition for surface basic sites between CO_2 and H_2O. These results suggest that the higher CO_2 molar fraction promote rWGS reaction to produce water, which may hydroxylate basic sites, hence, the isomerization step to isobutene is partly inhibited. Overall these findings highlight the important role of CO_2/H_2O interactions and surface sites competition in controlling the product distribution ZrO_2 catalyzed Co hydrogenation.

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Keywords: CO_2-to-hydrocabon; Isosynthesis; CO_2 hydrogenation; isobutene.

Catalytic electroreduction of CO_2 by tandem catalyst to C2+ and the effect of the architecture

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Abstract

Electrochemical CO_2 reduction (CO_2RR) offers a promising route for converting CO_2 into value-added chemicals. C_2^+ products such as ethylene and ethanol are particularly attractive, but their formation remains challenging because C–C coupling generally requires high overpotentials. Cu-based catalysts can reach C_2^+ Faradaic efficiencies of about 55–60% at −0.7 V vs. RHE [1]. Here, we investigate tandem catalysts combining Cu nanocubes (CuNCs) and cobalt phthalocyanine (CoPc) and evaluate how catalyst architecture influences C_2^+ selectivity and operating potential.

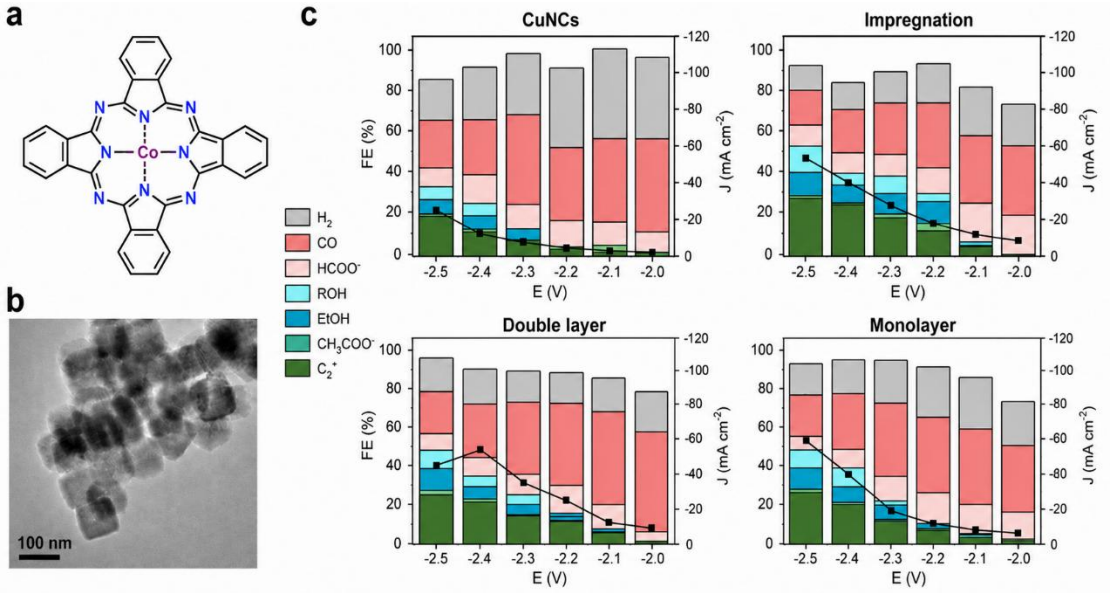

Figure 1. a) CoPc. b) CuNCs. c) CO2RR performances of the different catalysts

CuNCs (Fig. 1b) were synthesized by citrate-assisted reduction, while CoPc (Fig. 1a) was commercially available. Three tandem architectures were investigated: impregnation of CuNCs with CoPc, a mixed monolayer of CuNCs and CoPc, and a bilayer obtained by sequential deposition of CuNCs and CoPc. Catalyst inks were deposited on porous carbon gas-diffusion electrodes. CO_2RR was performed in a zero-gap membrane-electrode assembly using 1 M KOH, a Sustainion membrane, and a continuous CO_2 flow of 100 mL min^{-1}. Gaseous and liquid products were quantified by online gas chromatography and 1H NMR, respectively

Compared with CuNCs, tandem promote C_2^+ formation at lower overpotentials. The impregnation is showing the best overall performance and propanol formation at less negative potentials. This suggests that the close proximity between CoPc and CuNCs facilitates CO transfer and subsequent C–C coupling. The bilayer also improved C_2^+ formation, while the monolayer was less effective.

The Powerco2 SPLEEN project funding is greatly acknowledged.

References

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Keywords

CO_2-to-C_2+ ; Electrocatalysis ; CO_2 electrolyzers ; Tandem catalysis ; Copper catalysts

Integrating Molecular Cobalt Catalysts with Photoactive Architectures for Light-Driven CO_2 Reduction

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Abstract

Molecular catalysts offer well-defined and tunable active sites for CO_2 reduction, yet their integration into robust architectures suitable to build photoelectrochemical devices remains a key challenge.[1] This poster will first highlight our team's recent progress on the development of several functionalization strategies for the heterogenization of the molecular cobalt catalyst **CoN_4H** onto various electrode materials.[2,3,4,5] The design and photoelectrochemical characterization of a dye-sensitized NiO photocathode based on a covalent **Ru-CoN_4H** assembly for CO-rich (CO/H_2 ratio > 80:20) solar syngas production will then be more specifically described. After integration with a $BiVO_4$/CoPi photoanode in a Z-scheme tandem photoelectrochemical cell, syngas could be produced from CO_2 and water with Faradaic efficiencies of 62% and 14% for CO and H_2, respectively, under visible light and in the absence of any applied bias.[5] Building on this concept, two complementary strategies will be presented to replace the Ru photosensitizer with noble-metal-free photoactive porous organic polymers (POPs).[6] The first relies on a supramolecular approach, using pyrene-functionalized **CoN_4H** derivatives to promote π-π interactions with pyrene and perylene based POPs.[7,8] The second involves covalent coupling of the molecular catalyst directly to the POP framework through amide-bond formation. These approaches are designed to combine the well-defined catalytic properties of **CoN_4H** with the extended and panchromatic light absorption of POPs, while promoting efficient interactions between the photoactive scaffold and the catalytic center. Ultimately, this work aims at developing robust, noble-metal-free molecular photocathodes for light-driven CO_2 reduction by integrating molecular catalysis and porous photoactive materials within a single architecture.

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Keywords

CO_2 reduction; solar fuels; molecular catalyst; photocathode; porous organic polymers.

Molecular catalyst integration to electrolyser devices for selective production of CO and tandem generation of high value products

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Abstract

The increase in atmospheric CO_2 levels, largely due to anthropogenic activities, has driven global efforts to develop technologies for its capture and conversion.
Electrochemical CO_2 reduction reaction (eCO_2rr) represents a possible approach to close the carbon cycle while producing valuable chemicals and fuels, known as e-fuels. However, the efficiency and selectivity of eCO_2rr are highly dependent on the nature of the electrocatalyst.[1]

Copper is a particularly interesting candidate due to its unique ability to reduce CO_2 to hydrocarbons and alcohols, but it generally lacks of selectivity toward a specific product. [2] In order to overcome this limitation, copper complexes have come into play as highly adaptable platforms for CO_2 reduction and the combination of these two components has attracted significant scientific interest.[3]

However, in many cases, the molecular nature of the catalyst (or precursor) doesn't completely resolve copper selectivity issue. Hence, in order to overcome this, several approaches have been proposed such has varying the conductive supports where the complex has been immobilized [4,5]. In some particular and recent examples, direct coupling of metallic copper with other molecular catalysts in a tandem system has allowed to enhance the selectivity toward CH_4 or C_2^+ products.[6,7]

In this work, a combination of two molecular catalyst, Co(II)Phthalocyanine (CoPc) and Cu(II)Phthalocyanine (CuPc) , is studied in order to tune the selectivity of the copper based catalyst by exploiting the capability of the CoPc to generate CO locally. Additionally, in order to better appreciate the performances of the tandem system in application relevant conditions, a zero gap electrolyzer configuration had been chosen.

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Keywords

CO_2-to-fuels ; Electrocatalysis ; CO_2 electrolyzers ; Tandem Systems ; Copper

Development of Operando IR Methodologies for CO_2 Photoreduction Investigations

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Abstract

Understanding the dynamic behavior of photocatalysts under reaction conditions is crucial to unravelling the mechanism underlying CO_2 photoreduction. Operando spectroscopy, particularly when combined with the Modulation Excitation (ME) approach and chemometric analysis, enables the detection of transient surface species often hidden within complex spectral responses. In this context, we investigated the photocatalytic conversion of CO_2 and H_2O to short hydrocarbons on Pt/ and PtCu/TiO_2 using operando ME-IR spectroscopy coupled with Mass Spectrometry (MS) detection.

Thanks to the PEPR-SPLEEN funding program, we developed a dedicated operando experimental unit, including an in-house developed transmission IR cell for photocatalytic experiments, enabling the acquisition of operando IR-MS data while actuating sharp ME perturbations. Phase-resolved spectra obtained from operando ME-IR under light/dark cycling (Figure 1) shows that Cu incorporation (i) enhances CO_2 adsorption as carbonate species, (ii) reduces the surface population of Pt^0-CO and (iii) increases the amount of acetate[1] and methoxyl species responding to the modulation. As surface Pt^0-CO formation has been shown to drive H_2 and CO production,[1] Cu incorporation suppresses this route, thereby favoring CO_2 conversion to CH_4 through acetate intermediates. These observations highlight a cooperative interplay between Pt and Cu, with Cu modifying surface reactivity and facilitating the hydrogenation of C-species. A methodological study is ongoing to assess advantages and pitfalls of transmission IR and DRIFTS for operando IR studies of CO_2 photoreduction with particular interest in disentangling the competing effects of photoexcitation and heating under irradiation in relation to the employed photoreactor. These results underscore the potential of operando ME-IR spectroscopy as a relevant approach for investigating complex photocatalytic mechanisms. The unveiled synergistic role of Cu in PtCu/TiO_2 enhances our understanding of CO_2 photoconversion and provides a rational basis for designing more efficient bimetallic photocatalysts for solar fuel production.

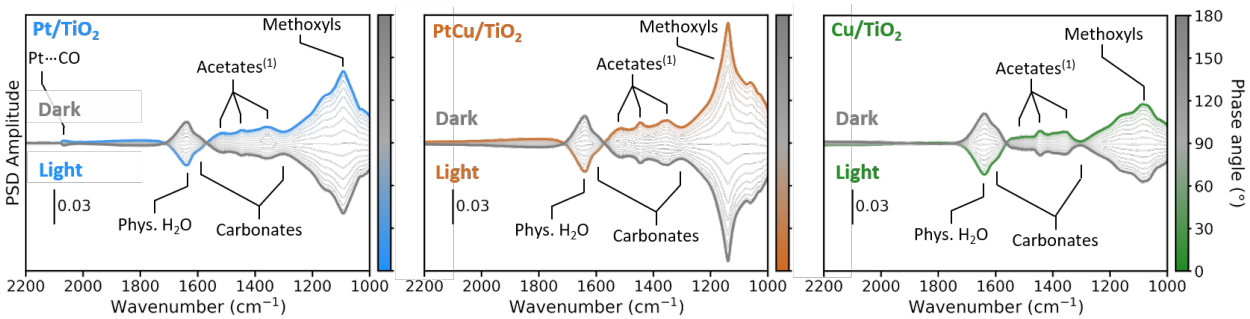

Figure 1. Phase-resolved spectra obtained from ME-IR under light/dark cycles for Pt/, PtCu/, and Cu/TiO_2.

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Keywords

CO_2 photoconversion, IR spectroscopy, operando, Modulation-Excitation, Phase-Sensitive Detection

Size-Tuning Porphyrinic Metal–Organic Frameworks for Photocatalytic CO_2 Conversion

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Abstract

Porphyrinic PCN-type MOFs offer a modular photocatalytic architecture that combines accessible porosity, visible-light-harvesting porphyrins, tunable framework functionality, and functionalizable Zr_6 nodes for photocatalytic CO_2 reduction.[1-3] Here, PCN-222 MOFs[4] with four distinct particle sizes, MOF-XL (~30 μm), MOF-L (~1.5-2 μm), MOF-M (~600 nm), and MOF-S (~70 nm), were prepared to examine how particle-size-dependent structural tuning affects their photosensitizing properties and photocatalytic performance. The framework porphyrins were first metallated with Zn(II), followed by loading of a guest Fe-porphyrin catalyst to form PCN-222(Zn)/Fe-porphyrin composites. Under green-light irradiation with 100 mM 1,3-dimethylbenzimidazoline (BIH) as the sacrificial electron donor and 50 mM water as the proton source, the assemblies exhibited a clear particle-size-dependent catalytic response. MOF-XL produced CO with a turnover number (TON) of 655 and a production rate of 7.81 mmol g^{-1} h^{-1}, whereas MOF-M reached a TON of 1570 and a CO production rate of 18.9 mmol g^{-1} h^{-1} after 64 h. Further photocatalytic investigations across the particle-size series are ongoing to establish a more comprehensive structure-activity relationship. The results nevertheless highlight particle-size control as an important parameter governing the performance of photosensitizing MOF-molecular catalyst assemblies. Selected particle sizes also showed good film-forming behavior upon spin coating, supporting their potential for the development of photoactive MOF films and future photoelectrocatalytic CO_2-reduction systems.

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Keywords

CO_2-to-fuels; Photocatalysis; Metal-organic frameworks (MOFs); Solar fuels; Carbon monoxide

The impact of substrate channel mutations on the O_2-sensitivity of CODH

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Abstract

Carbon monoxide dehydrogenases (CODHs) are able to reversibly catalyse the conversion of CO_2 into CO with very high TOF. They are, however, extremely O_2 sensitive as a result of the rapid degradation of their active site C-cluster, which lies buried in the centre of the protein matrix.[1] O_2 reaches the active site using CODH's forked substrate channel.[2] Two recent publications showed improved O_2-resistance upon mutation to a single channel-arm with little impact on substrate affinity.[3,4] Here we characterize these mutants[5] in detail using protein film electrochemistry and find no significant impact on the substrate affinity. In contrast, we show that a series of mutations to the common section of the channel can improve O_2-resistance, but at the cost of decreased substrate affinity.[2] This forms an important limitation on the use of substrate channel modification for improving the O_2-resistance of CODH.

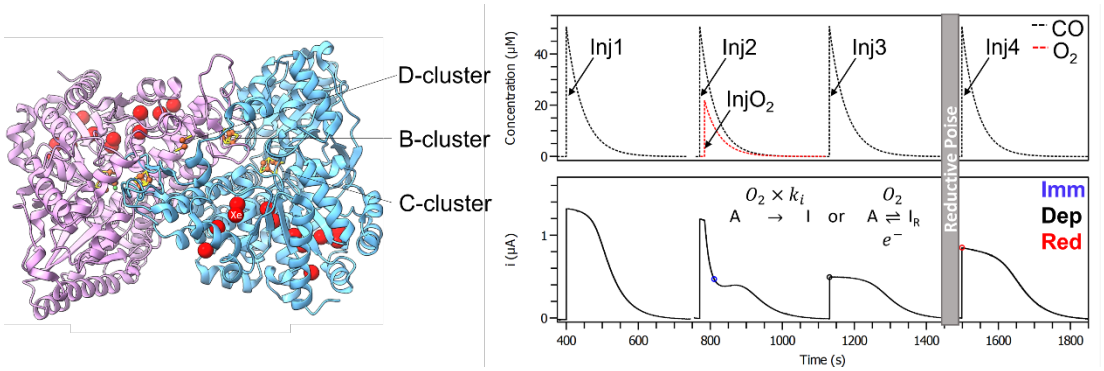

Figure 1. Left: Structure of CODH with the xenon atoms (red) in the substrate channels. Right: Protein film electrochemistry of CODH in presence of CO and O_2.

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Keywords

Protein Film Electrochemistry; CODH; Substrate channels; Oxygen resistance; Enzyme stability

Plasma-Assisted CO_2 Methanation: Experimental Evaluation of Catalysts for CO_2 Conversion to CH_4

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Abstract

Plasma-assisted single-atom catalysis is an emerging approach for CO_2 conversion that combines the high metal atom utilization and well-defined active sites of single-atom catalysts (SACs) with the unique activation capabilities of non-thermal plasma [1]. Unlike conventional thermal catalysis, where the catalyst plays a central role in activating the reactants, plasma-assisted catalysis involves the interaction of the catalyst with excited and reactive species generated in the plasma. Therefore, the development and evaluation of catalysts under plasma conditions is essential for improving CO_2 conversion and product selectivity [2]. In this work, a Ni–Y_1/CeO_2 catalyst containing atomically dispersed Y^{3+} species on Ni nanoparticles supported on CeO_2 was investigated for plasma-assisted CO_2 methanation. The catalyst was synthesized by coprecipitation followed by impregnation with NiO nanoparticles, and the single-atom dispersion of Y was confirmed using HAADF-STEM, STEM-EDS, XANES and EXAFS characterization [1].

The catalytic performance was evaluated in an atmospheric-pressure dielectric barrier discharge (DBD) tubular reactor using CO_2 and H_2 at flow rates of 40 and 160 mL min^{-1}, respectively, corresponding to an H_2/CO_2 ratio of 4:1. Prior to the reaction, the catalyst was reduced using H_2 plasma. CO_2 hydrogenation experiments were subsequently performed at different discharge voltages and frequencies, with a GHSV of 48,000 h^{-1} maintained throughout the experiments. The plasma operating conditions were varied within the available power-supply limitations, and the outlet gas composition was analyzed to determine CO_2 conversion and CH_4 selectivity. Repeated reaction cycles were performed to evaluate the stability and reproducibility of the catalytic performance [3].

Preliminary results indicate that increasing the plasma operating voltage led to a significant increase in CO_2 conversion. At 7.4 kV, the CO_2 conversion was approximately 20–25% higher than that obtained at the lower voltage of 5.4 kV. Frequency tuning between 2.5 and 10 kHz also influenced the discharge behavior; however, within the investigated operating window, changes in voltage produced a more pronounced effect on CO_2 conversion than frequency variations. A maximum preliminary CO_2 conversion of approximately 48% was obtained at 7.4 kV and 10kHz frequency. These results demonstrate the promising activity of Ni–Y_1/CeO_2 for plasma-assisted CO_2 methanation and highlight the importance of plasma operating conditions in determining catalytic performance. Further experiments at higher and more stable discharge voltages will be performed to establish the optimum plasma conditions and better understand the interaction between the catalyst and plasma-generated reactive species.

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Keywords

Plasma-assisted catalysis; Single-atom catalysts; CO_2 methanation; DBD plasma; CO_2 conversion.

BOOK OF ABSTRACTS

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