



CORDIS Results Pack on **frontier chemistry**

A thematic collection of innovative EU-funded research results

June 2021



Helping to achieve a truly green and circular economy for Europe

*Research and
Innovation*

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Editorial

Helping to achieve a truly green and circular economy for Europe

The EU must use every tool in its arsenal to achieve its wide-reaching and ambitious climate goals, particularly the goal to be fully carbon-neutral by 2050. One of those tools is innovative chemistry research with a focus on catalysis – the process of increasing the rate of a chemical reaction by adding a substance known as a ‘catalyst’. In this CORDIS Results Pack, we highlight the efforts of 14 projects funded by the European Research Council (ERC) that work within this field and make substantial contributions to the development of greener and more sustainable industrial processes.

Catalysts are absolutely essential to many of the processes that help to sustain life on Earth. These include truly natural processes, such as Nature’s ability to turn sunlight into energy, and industrial processes developed by humans, such as the commercial production of fertilisers for agriculture. Catalysed reactions form the basis of many industrial chemical processes and catalyst manufacturing is a rapidly expanding industrial trend. Both are now widely exploited to efficiently provide solar fuels, improve fuel cells and create valuable industrial precursors from abundant feedstocks.

As a result, it’s no surprise that the continued development of catalysts is key to future human progress, particularly with regards to fighting climate change, humanity’s greatest challenge in the 21st century.

Research & Development: A crucial ingredient in greening Europe

The European Green Deal is the European Commission’s dedicated and highly ambitious plan to make the EU’s economy and societies truly sustainable whilst ensuring Europe’s global competitiveness.

No policy instrument is being left unused or untouched for achieving these goals, but at the same time, a corresponding effort to boost and promote research and technological development is also required. The ERC, founded in 2007 as an important component of the EU’s dedicated programmes for research and innovation, makes a vital contribution by providing grants to Europe’s most talented researchers, who work to advance the frontiers of human understanding and knowledge.

Taking Nature as inspiration

Whilst the ERC does not provide funding based on predefined themes, many ERC grantees have taken Nature as a direct inspiration to advance and reimagine the traditional vectors and applications of catalysis, leading to exciting contributions in line with the goals of the European Green Deal. The projects featured in this Pack show how long-established industrial processes can be converted to operate in a more environmentally friendly and sustainable way. They focus primarily on electrochemistry, photochemistry and synthesis but also touch upon the industrial domain. Many of the results presented here are highly relevant to the automotive, aviation, biorefinery and fine chemical/pharmaceutical industries.

Retracing the steps towards the origin of life

How did life emerge on planet Earth? An ERC-funded project is lending new support to the theory that self-organised chemistry could have been critical, giving rise to processes which later evolved into biological metabolism as we know it today. Reproducing these reactions in the lab could be a first step towards greener chemical processes.



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We know that metabolism is a life-sustaining process, but how did it get started – and what role did it play in the emergence of life on Earth?

The CARBONFIX (Towards a Self-Amplifying Carbon-Fixing Anabolic Cycle) project, which received funding from the ERC, has shed new light on this question by examining how simple

molecules can self-organise to trigger chemical reactions similar to those happening during biological metabolism.

The metabolism of organisms requires enzymes as catalysts, and these enzymes can only be produced in living cells. The CARBONFIX researchers identified mechanisms which are similar to those involved in metabolism, but can occur without the presence of enzymes under specific conditions. They examined

metabolic processes used by ancient life to convert CO₂ into organic compounds and recreated non-biological analogues of these CO₂-fixation pathways.

Mimicking nature

The two biological processes found in ancient life that the project attempted to replicate are most commonly known as the Wood–Ljungdahl pathway and the reverse Krebs cycle. “Both convert



Both convert CO₂, protons and electrons into a small set of molecules – which also happen to be the universal building blocks of biochemistry.

CO₂, protons and electrons into a small set of molecules made up only of carbon, hydrogen and oxygen – which also happen to be the universal building blocks of biochemistry,” says Joseph Moran, professor at the Institute of Supramolecular Science and Engineering ISIS in Strasbourg, who received an ERC grant to lead CARBONFIX. “While many

scientists think that the two pathways, possibly working together, could have played a role in the origin of life, there was little experimental evidence so far to support this idea.”

To mimic the Wood–Ljungdahl pathway, the researchers placed metallic iron, nickel or cobalt into warm carbonated water. This triggered a reaction which converted the CO₂ into formate, acetate and pyruvate – the same intermediates as in the metabolic pathway.

Work on the reverse Krebs cycle delivered similar conclusions. The researchers were able to show that metal ions and metallic iron can promote more than half the reactions that make up the cycle without the presence of enzymes. Further research is aiming to achieve the full cycle.

These results could have important implications for the origin of life, because they indicate that these biological pathways might have emerged before enzymes existed. “In this model, a complex, self-organised chemistry occurs non-enzymatically and is later

refined by evolution to give rise to metabolism as we know it today,” Moran explains. “This would also provide direct insights into why metabolism functions the way that it does – because it started that way.”

Green synthesis

In addition to providing us with new clues about our past, the CARBONFIX project may have opened up new perspectives for a greener future: producing a full reverse Krebs cycle could provide an effective way of removing CO₂ from the atmosphere.

Moreover, the reactions identified could represent a first step towards developing methods to transform CO₂ into useful chemicals by identifying cheap and simple catalysts. “Acetic acid is one of the main components of vinegar, while pyruvic acid is useful for biological research,” Moran adds. He cautions, however, that further work is required to get there: “Finding a way to convert the transiently formed products into a single useful compound could eventually make this a viable solution. We are currently collaborating with specialists in heterogeneous catalysis to explore this possibility.”

PROJECT

CARBONFIX – Towards a Self-Amplifying Carbon-Fixing Anabolic Cycle

HOSTED BY

International Centre for Frontier Research in Chemistry in France

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/639170



One step closer to green hydrogen with promising new catalyst

Hydrogen fuel produced with solar power is being hailed by some as the clean energy solution of tomorrow. The discovery of a high-performance catalyst for hydrogen production could speed up this technology's path to the marketplace.

Future energy needs could be based on hydrogen as the energy carrier. Potential applications range from vehicles including cars, boats and trains to homes and industrial processes. When hydrogen is produced from renewable power sources, it is a clean fuel: its transformation in a fuel cell produces only water.

Solar energy can be stored in the form of hydrogen fuel by splitting water into hydrogen and oxygen in a process called electrolysis. The oxygen evolution reaction (OER), which forms the key reaction in this process, requires catalysts. Enabling the large-scale production of solar hydrogen will require the development of efficient and robust catalysts using inexpensive materials.



A tenfold performance increase

The FANOEC (Fundamentals and Applications of Inorganic Oxygen Evolution Catalysts) project, supported by the ERC, has opened up new prospects in this field by identifying a catalyst which ticks all

the boxes. "We discovered a bifunctional iron-nickel catalyst that outperforms the benchmark catalyst by about tenfold," explains Xile Hu, professor of Chemistry at the Swiss Federal Institute of Technology in Lausanne and FANOEC principal investigator.

The newly discovered catalyst can be easily prepared and exhibits long-term stability. Its bifunctional mechanism, which involves two cooperative active

sites, increases the catalyst's activity, thereby improving its overall performance.



We discovered a bifunctional iron-nickel catalyst that outperforms the benchmark catalyst by about tenfold.

Towards next-generation devices

Their results open the way for improving electrolyzers and eventually making them fit for large-scale development. These water-splitting devices are currently still too costly and difficult to scale up, Hu points out. The project has made an important contribution to overcoming these hurdles: "It provides knowledge and even a candidate catalyst for use in next-generation electrolyzers."

Together with his colleagues, he is currently looking into new ways to integrate catalysts into electrolyzers and to develop more efficient devices.

There is, however, still lots of work to do before we could see green hydrogen fuels hit the market, Hu says: "To make large-scale carbon-neutral production of hydrogen a reality, additional system optimisation and research, as well as academic-industry collaborations are needed."

Deep understanding

While metal oxides have long been known to hold potential as OER catalysts, our knowledge of how this works exactly has so far been limited. FANOEC's team of researchers has been able to achieve a deep understanding of OER on metal oxides at the molecular level, and to develop better catalysts based on this understanding: "The project has delivered some of the best catalysts which might be used in future devices," Hu remarks.

To get there, the team developed several new tools to improve our grasp of the molecular functioning of OER catalysts. Based on these insights, they delivered new synthetic methods and described key design principles for efficient OER catalysts.

PROJECT

FANOEC – Fundamentals and Applications of Inorganic Oxygen Evolution Catalysts

HOSTED BY

Federal Institute of Technology Lausanne in Switzerland

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/681292



Clean hydrogen: deeper insights for better catalysts

To design efficient catalysts for producing solar hydrogen through photoelectrochemical water splitting, we first need a better understanding of what happens at the molecular level during the reaction. A team of EU-funded researchers has delivered just that.



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The discovery that titanium dioxide enables water to be split into hydrogen and oxygen with the help of sunlight was made almost 50 years ago. This breakthrough could turn out to be the key for unlocking 'green' hydrogen – one of the most up-and-coming energy carriers to watch.

"To generate hydrogen from water, we need only water, sunlight and a catalyst – and (by definition) the catalyst can be reused. When the hydrogen is subsequently used to produce energy, only water is released. That makes hydrogen a very clean energy

carrier,” explains Ellen Backus, professor of Physical Chemistry at the University of Vienna.

Titanium dioxide is still considered a benchmark photocatalyst and has been the focus of much research to improve the efficiency of the process. However, half a century after its discovery, we still have very limited knowledge of what happens at the molecular level during photocatalytic water splitting.

A team of researchers led by Backus has taken decisive steps towards unravelling this mystery. The FOPS-water (Fundamentals Of Photocatalytic Splitting of Water) project, supported by the European ERC, delivered new insights into the molecular mechanism behind the process.

A bottom-up approach

Crucially, the project team achieved a new understanding of how water binds to the photocatalyst, and how the acidity affects what happens at the interface between the two. The researchers analysed the orientation of the water molecules vs the photocatalyst, and how strongly they interact, both with each other and with the photocatalyst itself.

This represents significant progress towards improving our grasp of the photocatalytic water splitting mechanism, which in turn could help researchers make the photocatalyst more efficient. “Understanding the process will be an important step in designing cheaper and more efficient photocatalysts. Currently, catalyst optimisation is often achieved by trial and error. Our results could enable a more bottom-up approach,” Backus remarks.

commercially applicable devices. FOPS-water has been able to fill in this gap, Backus notes: “We made progress in understanding this process at the molecular level in environments close to real-life conditions.”

A global picture at the micro level

The team also studied what happens after putting the photocatalyst into an excited state – in other words, raising its energy level. Backus explains: “The excitation is basically mimicking the sunlight. The main result of that work is that photoexcitation changes the surface charge to which the water molecules adapt their orientation.”

In addition to these aspects, the team looked at how fast energy can be dissipated during the process, and on which timescale the reaction takes place. They also broke down the reaction into its separate steps.

Drawing on the knowledge gained from the FOPS-water project, the team is currently studying the interface between water and other photocatalysts. They aim to obtain a more global picture of how the catalysts work with a view to identifying relevant parameters for catalyst design.

These advances could help inch closer to catalysts suitable for large-scale sustainable hydrogen production as needed to support its use in applications such as passenger cars.



Understanding the [water splitting] process will be an important step in designing cheaper and more efficient photocatalysts [to produce sustainable hydrogen].

While there had been previous efforts to unravel the water splitting reaction at the photoelectrochemical electrode interface, these studies had either taken a theoretical approach or made use of extreme conditions, such as low temperatures or ultra-high vacuum (allowing the experimental ‘visualisation’ of the molecules), which do not reflect the normal working conditions for

PROJECT

FOPS-water – Fundamentals Of Photocatalytic Splitting of Water

HOSTED BY

University of Vienna in Austria

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FP7-IDEAS-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/336679



Hybrid photoelectrodes advance solar fuel generation

Solar fuel generation uses artificial photosynthesis to obtain chemicals from carbon dioxide. HybridSolarFuels developed proof of concept techniques for future renewable energy applications that could offer viable alternatives to fossil fuels.

Solar fuel generation uses artificial or natural light to convert abundant and stable molecules, such as water or carbon dioxide (CO_2), into high-energy chemicals. This photoelectrochemical process is an especially attractive sustainable energy technique, as in principle it only requires energy from light (photons), water and/or CO_2 and a catalyst.

With commercial applications still awaiting some significant technical breakthroughs, the ERC-supported project HybridSolarFuels (Efficient Photoelectrochemical Transformation of CO_2 to Useful Fuels on Nanostructured Hybrid Electrodes) is developing a high-performing approach, using hybrid photoelectrodes made of multiple components.

“The key to ensuring high solar-to-chemical conversion efficiency is to design the interfaces using nanostructured materials and sophisticated synthetic processes,” explains Csaba Janáky, principal investigator in the project from the University of Szeged in Hungary.

Another achievement is the development of scalable electrolyser flow cells. While these do not qualify as photoelectrochemical cells, as they don't directly use light, they are the first step towards achieving photoelectrochemical cells.



Inspired by nature

HybridSolarFuels initially faced two significant challenges. As CO₂ is an inert molecule, it requires a lot of energy to convert it into useful products, such as methanol. This makes the selection of the right catalyst vital. Finding suitable catalysts and integrating them into photoelectrochemical cells, is difficult.



We were among the first to use lead halide perovskite films directly as photoelectrodes.

Another challenge was that most previous research had been carried out in batch cells. It is challenging to translate these results into specific applications because industrial conversion rates can only be achieved in flow cells, where CO₂ is fed continuously.

In natural photosynthesis, each component in the system has a specific function. Inspired by this, HybridSolarFuels designed electrodes made with several components: one for light absorption, another for charge carrier transport, and one for the catalytic reaction at the surface; these are brought together at nanometre scale.

For example, various p-type semiconductors were used to absorb light in the photoelectrode assembly where the team made an unexpected discovery. “We were among the first to use lead halide perovskite films directly as photoelectrodes. This resulted in some important discoveries regarding the primary role that photo-generated holes play in the corrosion processes of these exciting materials,” says Janáky.

After performing characterisation studies to determine the optimum crystallinity, morphology and chemical composition of the new photoelectrodes, they were incorporated into continuous-flow electrolyser cells, which underwent various photoelectrochemical studies, namely to assess the solar-to-chemical conversion efficiency – the number of photons in the sunlight which are actually converted to chemical energy. “The hybrid photoelectrodes were shown to outperform single component electrodes,” adds Janáky.

A green disruptor

The success of the European Green Deal, with its target of carbon neutrality by 2050, will depend on new disruptive technologies. The conversion of solar energy to high-value chemicals and fuels could be such a technology. The photoelectrochemical conversion of CO₂ could generate chemicals such as formic acid, carbon monoxide, methanol and ethanol, reducing the demand for fossil fuel feedstocks and so CO₂ emissions from the chemical industry.

The team are currently exploring the substitution of water oxidation in the electrochemical CO₂ reduction process with something of higher economic value. “As a by-product of biodiesel production, we now have a surplus of glycerol which could be transformed into high-value chemicals such as formic acid, which is used for livestock feed preservation amongst other uses,” says Janáky.

As for applications, the team continue to develop their continuous-flow photoelectrochemical cells.

PROJECT

HybridSolarFuels – Efficient Photoelectrochemical Transformation of CO₂ to Useful Fuels on Nanostructured Hybrid Electrodes

HOSTED BY

University of Szeged in Hungary

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/716539



Hybrid photocatalysts transform CO₂ into environmentally friendly solar fuels

Using artificial photosynthesis, HyMAP has achieved a breakthrough in solar fuels and chemicals production. Hybrid materials, designed for water splitting and CO₂ conversion, were demonstrated from laboratory scale through to a solar reactor prototype.



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Mimicking nature, artificial photosynthesis uses sunlight to convert CO₂ and water into energy-giving and -releasing compounds. But instead of producing sugars, as with green plants, artificial photosynthesis can produce carbon monoxide (CO), methane (CH₄), methanol (CH₃OH) and hydrogen (H₂) – of interest as green fuels.

The HyMAP (Hybrid Materials for Artificial Photosynthesis) project, funded by the ERC was set up to develop a new generation of hybrid organic-inorganic materials and devices to perform the chemical transformations necessary for artificial photosynthesis. This would open the door for the development of green alternatives to electrochemical storage electrodes for batteries.



Our results, especially those increasing yield, are at the forefront of knowledge in the field of CO₂ conversion, marking a milestone for this research area.

The team investigated photo(electro)catalysis, at different scales, from nanoscaled catalysts to pilot-plant reactors, creating novel photoactive hybrid materials.

“Our results, especially those increasing yield, are at the forefront of knowledge in the field of CO₂ conversion, marking a milestone for this research area,” says principal researcher Víctor A de la Peña O’Shea from the IMDEA Energy Institute. Accordingly, scientific findings are being widely disseminated in high-profile journals.

The project’s new family of organic semiconductors, made from conjugated porous polymers, have already been patented for solar fuel production.

Hybrid materials

HyMAP’s main objective was to develop multifunctional systems with improved capabilities to harvest light from the whole solar spectrum. To achieve this, the team explored hybrid photocatalysts, investigating several materials and approaches.

The different strategies adopted were (i) band gap engineering of inorganic and (ii) organic semiconductors; (iii) as well as their related heterojunctions; (iv) metal-organic frameworks (MOFs) and (v) up-conversion (UC).

The first four options can harvest ultraviolet along with the visible regions of the light spectrum, while UCs improve the harvesting of infrared wavelengths. Crucially, inorganic and organic semiconductors enhance charge generation and transfer, increasing the photocatalytic yield.

“Combining different materials, with each specialising in the separate functions of photocatalytic reactions – principally of light absorption, charge separation and catalysis – improved overall efficiency,” explains de la Peña O’Shea.

The reaction mechanisms of these materials were characterised in the laboratory using a variety of advanced *in situ* techniques, including near-ambient pressure X-ray photoelectron spectroscopy, X-ray diffraction and synchrotron radiation.

Solar reactor

As the team’s studies revealed the hybrid organic/inorganic semiconductor heterojunctions made from a conjugated porous

polymer to be particularly highly performing, they designed a gas phase solar reactor.

It comprised a solar reflector – a compound parabolic collector – that redirects all solar radiation received towards the reactor, and a tubular annular reactor made out of borosilicate glass, which is more resistant to high temperatures.

This prototype reactor was demonstrated to successfully produce solar hydrogen from both water and biomass, as well as from other fuels or chemicals, such as CO, CH₄ and CH₃OH, using CO₂ as a reagent.

“These excellent results for solar fuel production have already led to a pilot plant, increasing our knowledge and allowing us to fine-tune processes before considering market opportunities,” says de la Peña O’Shea. “We need to broaden the use of these hybrid materials for other reactions, beyond photo- to include photo(electro)catalysis, for more sophisticated fuels and chemicals, such as ammonia, ethylene and dimethyl ether.”

Scaling up to meet new challenges

The HyMAP team has already started an associated ERC-funded proof of concept project NanoCPPs, to develop a proof of concept which scales up their nanostructured conjugated porous polymers. “This polymer’s nanostructure offers enhanced properties, opening the door to better performance,” he adds.

A remaining challenge is to truly maximise the electronic properties of these systems so that the proposed environmentally friendly alternatives to current electrochemical storage electrodes for batteries can really be brought forward and made a reality.

PROJECT

HyMAP – Hybrid Materials for Artificial Photosynthesis

HOSTED BY

IMDEA Energy Institute in Spain

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/648319

PROJECT WEBSITE

hymap.eu

Advancing knowledge of sustainable biorefining

Lignocellulosic waste biomass is one of the world's most abundant raw materials, yet it is underutilised. LIGNINFIRST has advanced the knowledge necessary to biorefine lignocellulose, opening up new avenues for a sustainable bioeconomy.

Lignin is a natural polymer present in plant tissues and one of the main components of lignocellulose or biomass. Annually, the pulp and paper industry releases about 130 million tonnes of lignins. Yet, despite accounting for 30 % of plant biomass and 40 % of its energy content, lignin is underutilised, serving mainly only as a source of low-energy solid fuel.

'Lignin-first' biorefining is a technique that uses chemical catalysis and considers lignin valorisation in the design phase of biomass deconstruction. The ERC-supported project LIGNINFIRST (The Lignin-First Approach for the Full Valorisation of Lignocellulosic

Biomass), hosted by Imperial College, London, was set up to investigate the complex processes of biomass deconstruction and develop new strategies to improve the individual yield of valuable compounds released during lignin-first biorefining.

"Our research group has pioneered the lignin-first biorefining approach using organic molecules as a hydrogen source to control the reactivity of lignin fragments," explains the principal investigator, Roberto Rinaldi. "Further understanding the complex chemistry involved will improve our patented process."



Stabilising lignin products

Lignin has a complex chemical structure, with no two molecules alike. In the early days of lignin biorefining, researchers discovered that no matter how good the catalysts were, conventional approaches consistently resulted in very complex mixtures of compounds, making their use difficult.

The catalysts, which deconstruct lignocellulose, work through depolymerisation, which breaks down large molecules into fractions of cellulose, hemicelluloses and lignin. Rinaldi's pioneering work contributed to the realisation that the problem was not the catalysts themselves, but rather lignin degrading in the extraction process and how this impacts on its receptiveness to chemical processing.



By better understanding the interplay of chemical processes in lignin-first biorefining, LIGNINFIRST has contributed not only to lignin valorisation efforts but also to maximising biomass as a renewable feedstock for sustainable manufacture.

As lignin fragments are reactive, the biorefining process often causes them to recombine, forming less reactive but more complex polymer structures or 'technical' lignins. The LIGNINFIRST project enabled the team to further develop their strategy of processing lignin in its 'native' form.

"We discovered that using a catalyst at the lignin extraction stage – hence 'lignin-first' – instead of processing extracted lignin in the presence of a catalyst, controlled the recombination of lignin fragments. This produced a few high-value compounds rather than a complex mixture of many," says Rinaldi.

The team also demonstrated that the relationship between catalysis and lignin valorisation is no longer limited to downstream processing: the processing of technical lignin waste generated by the pulping and paper industry. Catalyst solutions for the

pulping process itself introduced methods for lignocellulose deconstruction, referred to as 'Catalytic Upstream Biorefining'.

Additionally, proof of concept membrane filtration to refine the lignin was also achieved. "It is crucial to develop processes for separating the compounds in the lignin-first liquor, to help with recycling liquor solvents and transform lignin products into advanced biofuels," he notes.

Benefitting the bioeconomy

The pulp and paper industry directly creates more than 180 000 jobs in Europe and 1.5 million indirectly. With a turnover of EUR 90 billion, the sector adds EUR 20 billion to the EU's GDP. LIGNINFIRST's fundamental research benefits efforts to increase the value of lignocellulose from wood and crop residues.

"We don't view a barrel of crude oil as waste because we have the technology to transform it into useful materials, unlike bags of wood chips despite their potential," says Rinaldi. "By better understanding the interplay of chemical processes in lignin-first biorefining, LIGNINFIRST has contributed not only to lignin valorisation efforts but also to maximising biomass as a renewable feedstock for sustainable manufacture."

PROJECT

LIGNINFIRST – The Lignin-First Approach for the Full Valorisation of Lignocellulosic Biomass

HOSTED BY

Imperial College of Science, Technology and Medicine in the United Kingdom

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/725762



Metal-organic structures for electrolyser improve the efficiency of their chemical reactions

Using electric currents, electrolyser 'split' water into hydrogen and oxygen and can reduce carbon dioxide, making them a key technology for the EU's Green Deal.

MOFcat developed an electrolyser based on metal-organic frameworks, improving the efficiency of the process.

Metal-organic frameworks (MOFs) are porous crystalline materials of organic molecules ('linkers'), that interconnect with metal ion clusters to form three dimensional structures. These small structures, up to around 100 micrometres, are ordered and highly modular, and form materials of vastly different properties.

They have been used to improve the efficiency of hydrogen storage in gas cylinders and are being explored for their potential

as a mechanism to load and release therapeutic drugs for medical treatments.

Recently, MOFs have been developed to act as electrocatalysts with catalytic units (an internationally recognised unit of measurement for quantifying the catalytic activity of enzymes) included in the metal nodes, in the linker molecules or even trapped in the MOF pores.





The ERC-supported MOFcat (Fundamental and Applied Science on Molecular Redox-Catalysts of Energy Relevance in Metal-Organic Frameworks) project explored MOF-based electrolyzers which oxidise water, generating the electrons and protons necessary to produce hydrogen and reduce carbon dioxide (CO₂).

In the MOFs developed, the metal nodes provide scaffolding, ensuring the MOF's structural integrity and longevity, while the linkers provide the sites for the catalysts that drive the desired chemical reactions.

"To enable the most efficient electrocatalysis, we developed new methods to analyse charge transport in these crystalline materials," says Sascha Ott, the project's leader, from Uppsala University. "We found that limitations were often not caused by the turnover frequency of the catalytic units, but by limitations to the speed of electrical charge transportation through the MOFs."

The advantages of MOFs

As MOFs are highly ordered materials, they hold a significant advantage over solution-based approaches where the catalyst isn't controllable. Precisely placing the catalyst within the MOF offers possibilities for controlled and site-specific interactions that improve its performance.

MOFcat developed a photoelectrochemistry platform which harnesses light energy to speed up chemical transformations. This new methodology can be applied to both fuel production and for organic photoredox catalysis.

To demonstrate the latter, MOFs were used to coat semiconductors which, when illuminated, provided electrical energy to carry out chemical transformations.

The team then made several MOF-based electrode materials. One, dubbed 'UU-100', was synthesised using the relatively abundant metal cobalt. UU-100 generated hydrogen for 18 hours without decreasing its catalytic activity. "Incorporating molecular cobalt catalysts into the MOF increased hydrogen turnover by a factor of over 1 000, compared to catalysts in homogenous solutions," explains Ott.

Most of the materials' characterisation was done using electrochemistry techniques, sometimes coupled to ultraviolet-visible spectroscopy. For example, a MOF was grown onto a transparent electrode where the linkers change colour when electrochemically reduced, making it possible to observe charge transport through the film over time.

To enable the most efficient electrocatalysis, we developed new methods to analyse charge transport in these crystalline materials.

'Door opening' technology

MOFcat's platform offers a technology that is both more efficient and cleaner than many alternatives. For example, in photoredox catalysis, the so-called sacrificial chemical reagents that generate the electrons and oxidising equivalents necessary for catalysis remain in the mixture as waste chemicals. This can be avoided using the MOFcat platform.

The precise molecular chemistry of MOFcat, can also fine-tune catalyst reactivity. This reduces CO₂ while giving higher yields with fewer by-products that would otherwise be difficult and expensive to remove. Another example could be the electrochemical reduction of CO₂, for carbon capture or the generation of products such as methanol or ethylene, which is currently not very selective. This is especially true when materials such as metal oxides are used as catalysts.

"Our electrochemical MOF-based electrocatalysis technology could, in principle, be placed at CO₂ emitting sources such as fossil fuel power plants or oil refineries, to reduce their CO₂ emissions," adds Ott.

The team is now seeking further support to test more MOFs in different electrolyser designs and to develop a prototype for their catalytic MOF materials.

PROJECT

MOFcat – Fundamental and Applied Science on Molecular Redox-Catalysts of Energy Relevance in Metal-Organic Frameworks

HOSTED BY

Uppsala University in Sweden

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/681895



Clean hydrogen production with bio-inspired catalysts

For hydrogen to help meet our low-carbon future energy needs, its production will have to be greener. The PRODUCE-H2 team has tweaked an existing method to convert water into hydrogen, so that they can work with bio-inspired cost-effective catalysts rather than noble metals.



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If hydrogen (H_2) is to truly offer revolutionary clean energy solutions, its production must avoid greenhouse gas emissions, such as carbon dioxide (CO_2). This is currently only possible if H_2 is produced from water using electrolysis, using renewable electricity, or by photo(electro)catalysis, using sunlight.

For the former, one clean H_2 production technique uses proton-exchange membrane electrolyzers (PEMELs) – devices that use electricity to split water molecules (H_2O) into H_2 and oxygen (O_2) in an electrochemical process.

The proton-exchange membranes (PEMs) are made of the synthetic polymer Nafion. The electrodes typically contain

catalysts based on noble metals, i.e. iridium oxide to push the O₂ evolution and platinum to produce H₂.

While the technology has been around for a while, these components are prohibitively expensive and the low abundance of noble metals in the Earth's crust makes such technologies unsustainable. As an alternative, the PRODUCE-H2 (PROtotype Demonstration Using low-cost Catalysts for Electrolysis to H2) team supported by the ERC developed innovative H₂-producing catalysts based on Earth's abundant elements.

After testing various catalyst manufacturing methods, the team found that a synthesis method with cheap precursors and using a microwave oven, rapidly produced the most active and stable materials.

"This method is easily scalable and life cycle analysis, in collaboration with Toyota Motor Europe (which produces H₂-powered cars), indicated the environmental effects and cost benefit of such catalysts compared to noble-metal catalysts," says Artero.

Mimicking photosynthesis

PRODUCE-H2 built on the results of an earlier project, photocathH2ode, which had developed materials to convert sunlight directly into H₂ fuel, inspired by the way micro-algae produce H₂ for energy using sunlight.

The previous ERC project, photocathH2ode, developed photoelectrodes which combined light-harvesting materials – including organic dyes, conducting polymers and semiconductors – with H₂-producing catalysts inspired by hydrogenase enzymes.

"We integrated photocathodes into complete photoelectrochemical cells, able to use sunlight to split water and produce H₂," says principal investigator Vincent Artero from the French Alternative Energies and Atomic Energy Commission (CEA).

During photocathH2ode, the team discovered that the molecular structure of amorphous molybdenum sulfide – an electrocatalyst for H₂ production – could be readily manipulated to enhance performance and stability. Additionally, molybdenum had the advantage of being abundantly available.

Towards a hydrogen economy

The PRODUCE-H2 team are now working to finalise the development of a PEM electrolyser prototype, founded on bio-based plastics and using additive manufacturing.

To further advance the work, the team intend to combine their H₂-producing catalyst with other non-precious metal catalysts. They especially want to find a means to replace O₂-producing iridium oxide with a more sustainable catalyst – a more complex challenge.

"We also want to integrate these catalysts into our bioplastic PEMEL prototype and to couple this with a photovoltaic cell to produce H₂ from sunlight and water. This alternative method for H₂ generation could prove more competitive than photoelectrocatalysis in the short term," adds Artero.

PRODUCE-H2's results could help decarbonise the energy, transportation and industry systems contributing to the development of a hydrogen economy, affording the EU more energy independence and security by reducing reliance on imported fossil fuels.



This method is easily scalable and life cycle analysis, in collaboration with Toyota Motor Europe, indicated the environmental effects and cost benefit of such catalysts compared to noble-metal catalysts.

In PRODUCE-H2, various composite materials, derived from amorphous molybdenum sulfide catalysts, were formulated into catalytic inks using a patent-pending technique. These electrocatalysts were then tested in PEMELs.

"This was the first time that non-precious metal catalysts were tested in this way. Some of the materials displayed very good stability and reasonable activity, compared to platinum," explains Artero.

PROJECT

PRODUCE-H2 – PROtotype Demonstration Using low-cost Catalysts for Electrolysis to H2

HOSTED BY

French Alternative Energies and Atomic Energy Commission in France

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

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Using intrinsically fragile catalysts to generate and use chemical fuels

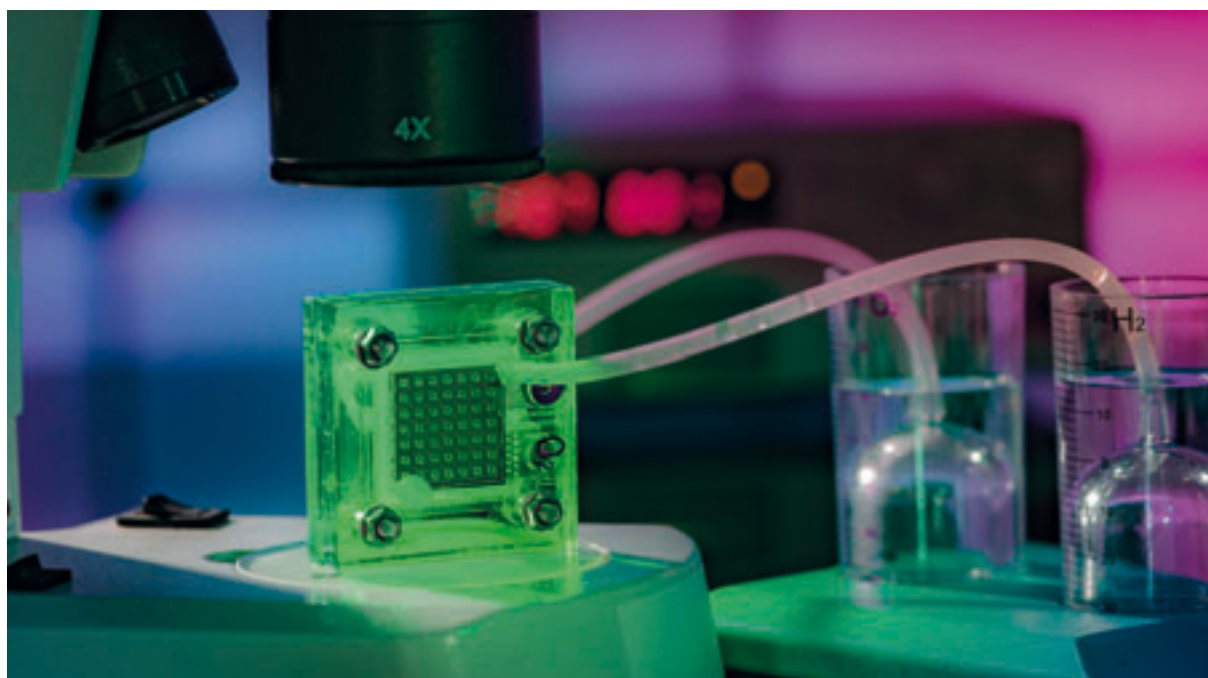
By demonstrating that fragility does not preclude catalysts' use, new EU-funded research helps position renewable energies as a competitive alternative to fossil fuel-based energy sources.

The global transition to sustainable energy requires the development of robust, highly active, and scalable catalysts. A catalyst is a substance that increases the rate of a chemical reaction without undergoing any permanent chemical change itself.

Take for example the production of hydrogen, a zero-carbon fuel that can be used for vehicles or heat production. The electrolyser that produces hydrogen from water and electricity and the fuel cells that convert hydrogen back into electricity typically use precious metals as a catalyst. However, their limited abundance and issues with sustainable sourcing have proven to be a major

roadblock to the widespread use of hydrogen. Unfortunately, alternative catalysts based on more sustainable metals fail to provide the stability these applications demand.

What is needed is a new approach to the catalyst conundrum – which is where the EU-funded REDOX SHIELDS (Protection of Redox Catalysts for Cathodic Processes in Redox Matrices) project comes in. “Popular thinking is that chemical energy conversion requires a robust catalyst,” says principal investigator Nicolas Plumeré, a professor at Technical University of Munich) “This project, which received support from the ERC, aims to demonstrate that the opposite is also true, that intrinsically



fragile catalysts can be applied to generate and use chemical fuels.”

To do this, Plumeré established an innovative electron-conducting polymeric matrix to protect even the most fragile catalysts, such as the hydrogenase, nature’s catalyst for hydrogen production or oxidation. The innovative system is used for water electrolysis, the electrochemical reaction where water (H₂O) is transformed into H₂ and O₂. The challenge here is that the released O₂ can damage the hydrogenases, essentially causing them to quickly become inactive.

“Our system addresses this issues by leveraging the released H₂ and using it to protect the catalyst against the disactivating effects of O₂,” explains Plumeré. “This protection is also effective in fuel cells by using H₂ from the fuel feed.”

Several important breakthroughs

Using this novel matrix, Plumeré was able to achieve several important breakthroughs. These include, for example, the theoretical demonstration that minimal protection matrices offer quasi-infinite protection to the catalyst – even when that catalyst is the very fragile hydrogenase.

“This opens the door to the possibility of being able to protect the hydrogenase from oxygen for as long as 20000 years, according to theoretical predictions,” remarks Plumeré. “From a practical perspective, this means that degradation by oxygen can be completely prevented without having to sacrifice catalyst loading or catalytic performance.”

Next, researchers showed how hydrogenase can be operated in the presence of air, such as its use in a fuel cell for converting hydrogen into electricity. “This breakthrough showed that hydrogenases have the potential to remain active in oxygen for over a week, whereas in the past this enzyme would deactivate in just minutes,” adds Plumeré.

A competitive alternative to fossil fuels

According to Plumeré, the project’s findings are directly applicable to devices in the context of biotechnology and solar fuel generation. As a result, the project helps position the source renewable energies as a competitive alternative to fossil fuels.



I am confident that our findings will have a big impact on the way the chemical energy conversion community designs new molecular and biological catalysts for chemical fuel generation.

“The REDOX SHIELDS project successfully showcased that catalyst fragility does not preclude its use in applications,” concludes Plumeré. “As such, I am confident that our findings will have a big impact on the way the chemical energy conversion community designs new molecular and biological catalysts for chemical fuel generation.”

PROJECT

REDOX SHIELDS – Protection of Redox Catalysts for Cathodic Processes in Redox Matrices

HOSTED BY

Technical University of Munich in Germany

FUNDED UNDER

Horizon 2020-ERC

CORDIS FACTSHEET

cordis.europa.eu/project/id/715900



Using metal-organic frameworks to help build more efficient energy applications

Metal-organic frameworks have the potential to play an important role in the development of sustainable energy solutions. The challenge, however, is figuring out how to best leverage this potential. To help, researchers have developed new synthetic processes for generating sets of structurally fascinating and highly functional materials.

Metal-organic frameworks (MOFs) are porous materials defined by metal ions or inorganic clusters connected via rigid organic linkers. Thanks to their unprecedented surface areas, ability to be modified, and modular construction that allows for the replication of key features of natural enzymes, these materials

have the potential to play an important role in energy storage and conversion.

The challenge, however, is figuring out how to best exploit MOFs for use with sustainable energy applications – a challenge taken



up by the EU-funded Supramol (Towards Artificial Enzymes: Bio-inspired Oxidations in Photoactive Metal-Organic Frameworks) project. "By leveraging light-harvesting constitutional units, we aim to develop robust, porous MOFs that use light-absorption as a means of triggering the electron-transfer events needed to activate the catalytic process," says Wolfgang Schmitt, principal investigator of the project, and professor of Chemistry at Trinity College Dublin.

According to Schmitt, the ultimate goal is to provide a proof of concept for the development of photocatalytic systems capable of catalysing the highly endergonic H₂O oxidation reaction. "Doing so would be a major breakthrough and a significant step towards implementing sustainable, hydrogen-based energy concepts," he adds.

Several important outcomes achieved

Although still a work in progress, this ERC-supported project has already achieved several important outcomes. For instance, researchers were able to catalyse the oxidation of H₂O by using a bio-inspired, manganese-based species that resembles the structural features of the natural photosystem-II (PS-II). PS-II is found in the thylakoid membrane of plants, algae and cyanobacteria and is the first protein complex in the light-dependent reactions of oxygenic photosynthesis.

"This approach could open the door to a new conceptional avenue for developing effective catalysts for direct 'solar-to-fuel' energy conversion technologies," explains Schmitt.

The project also prepared highly porous MOFs in which catalytically active units are linked through light-harvesting, ruthenium-based metalloligands. "Remarkably, the system can be synthesised electrochemically from highly diluted reactant solutions and assembled directly within minutes on the surface of electrodes," Schmitt says.

Using photophysical studies, researchers confirmed that the light-harvesting attributes of the ruthenium-pyridyl metalloligands are maintained in the MOF. "This feature is key to facilitating the rapid energy and electron transfer needed to efficiently catalyse the water oxidation reaction or other energy-related transformations," adds Schmitt.

Other key outcomes include the discovery of a synthetic approach to spherical molecular cages with large cross-sectional diameters

and the discovery of materials with high affinities for CO₂ gas molecules.

Inspiring new collaborative research projects

The project has succeeded in developing synthetic processes for generating sets of structurally sound and highly functional materials. "Some of these materials are photoactive," explains Schmitt. "Others have the ability to be synthesised within minutes to form, for example, electrodes directly on the surface."

Researchers are now using these compounds to develop photoelectrocatalytic devices that can be used with a variety of photo/electrocatalytic redox transformations, including water oxidation, CO₂ reduction, and transforming organic reagents.



The materials developed during the Supramol project will inspire new collaborative research projects.

"The materials developed during the Supramol project will inspire new collaborative research projects," concludes Schmitt. "This could include not only investigations into new structure-reactivity relationships, but also bottom-up approaches to MOFs with enhanced physicochemical properties that extend beyond water oxidation catalysis."

PROJECT

**Supramol – Towards Artificial Enzymes:
Bio-inspired Oxidations in Photoactive
Metal-Organic Frameworks**

HOSTED BY

Trinity College Dublin in Ireland

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Horizon 2020-ERC

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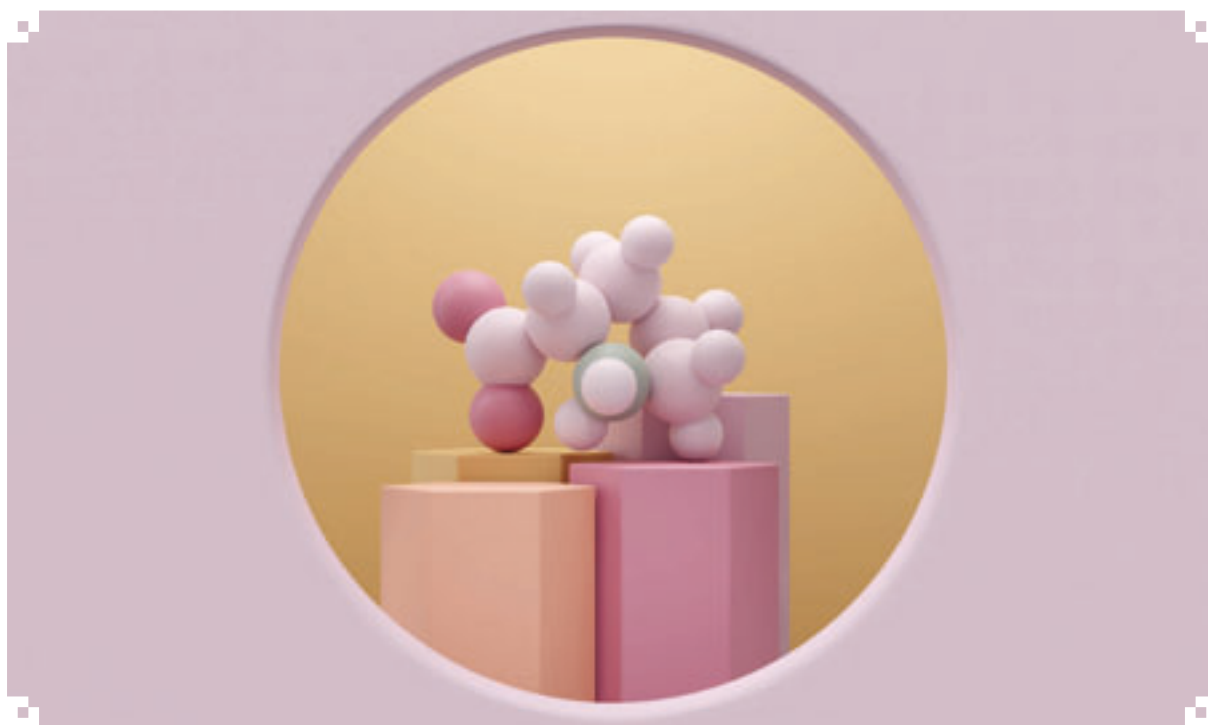
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Novel catalytic reactions to make the world a greener, cleaner place

Research into developing green catalysts will go a long way towards making many key industries more environmentally friendly. The EU-funded SUSCAT project has made impressive contributions to this research, including the development of new sustainable catalytic reactions for green chemical synthesis, and towards the development of the efficient, safe storage and use of hydrogen as a green energy carrier.

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The SUSCAT (New Directions in Sustainable Catalysis by Metal Complexes) project, funded by the ERC has its basis in several fields, including fundamental organometallic chemistry,

coordination chemistry, organic synthesis, kinetics, spectroscopy, catalysis and density-functional theory (DFT) calculations that are based on quantum mechanical computation.



"Overall, our key aims in SUSCAT were to discover and then develop novel, sustainable and environmentally benign catalytic reactions," begins David Milstein, principle investigator of the project, professor and the Israel Matz Professional Chair of Organic Chemistry at the Weizmann Institute of Science. "Such reactions are useful for 'green' organic synthesis methodology which generates no waste and uses sustainable substrates, as well as the development of liquid organic hydrogen carrier (LOHC) systems."

Whilst our LOHC system does require further development, we believe that it has the potential to be a top LOHC system, considering it's a cheap, abundant sustainable hydrogen carrier, its use of a single catalyst, its mild operational conditions and its compatibility with existing infrastructure at petrol stations.

A flurry of catalyst successes

The catalyst development method used by SUSCAT is based on a mechanistic approach, employing both experimental and computational methods. Particularly significant for its work has been the use of pincer complexes as catalysts. In a nutshell, pincer complexes are a family of compounds that have had an important impact on the recent catalytic development of organic synthetic methods thanks to being stable and capable of versatile reactivity modes. SUSCAT has used these pincer complexes to pioneer several green and sustainable catalytic reactions useful for organic synthesis that can feasibly replace currently used polluting processes.

"For example, one of our recently developed, unprecedented reactions is catalysed by a novel pincer manganese complex and leads to a family of compounds (acrylonitrile derivatives) that are valuable intermediates in the organic synthesis of a variety of products such as dyes, herbicides, fragrances, pharmaceuticals and natural products," says Milstein. "Traditional methods of generating these products create harmful waste and so our new method is truly greener and better for the environment."

Another example of SUSCAT's successes in green catalytic reactions includes a waste-free, one-step direct synthesis of amides (crucial for the pharma industry but traditional amide synthesis generates copious waste) and, as a happy consequence, the production of valuable hydrogen gas.

A third, and very environmentally significant, example of a reaction accomplished by SUSCAT is the unprecedented hydrogenative depolymerisation of widely used, robust Nylons to form amino alcohols, efficiently catalysed by a ruthenium pincer complex. "Nylons are widely used and are non-biodegradable, which has increased both land and ocean pollution, posing a severe ecosystem threat," Milstein comments. "This is why our accomplishment is so significant as the amino alcohols can be polymerised back to Nylons of similar molecular weight, thus providing a green and sustainable closed loop cycle for recycling Nylon waste."

as a green energy carrier. "Hydrogen is considered an attractive energy vector due to its high gravimetric energy capacity, and the fact that it generates only water upon combustion," explains Milstein. "However, its volumetric energy capacity is very low, requiring its storage (e.g. in cars) at very high pressure if in a gas state or as a liquid at a very low temperature (-253 °C) – both of which cost considerable energy investment and could be potentially dangerous. Using LOHC systems can avoid these problems."

The SUSCAT solution is founded on the fact that many of the project's reactions generate or consume hydrogen gas and as a natural next step, they developed a LOHC system for hydrogen storage. "The theoretical hydrogen capacity of this system is 6.5 wt%, higher than the United States Department of Energy's target for on-board hydrogen storage for light-duty vehicles, which is 5.5 wt%," Milstein continues. "Whilst our LOHC system does require further development, we believe that it has the potential to be a top LOHC system, considering it's a cheap, abundant sustainable hydrogen carrier, its use of a single catalyst, its mild operational conditions and its compatibility with existing infrastructure at petrol stations."

Looking to the future, Milstein and his team plan to continue their work on new catalytic reactions for green synthesis and hydrogen, possibly in collaboration with industrial partners. "What I'm most proud of in terms of SUSCAT is that we have hopefully made some contribution to the development of a truly greener world," Milstein concludes.

PROJECT

SUSCAT – New Directions in Sustainable Catalysis by Metal Complexes

HOSTED BY

Weizmann Institute of Science in Israel

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Horizon 2020-ERC

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cordis.europa.eu/project/id/692775

The hydrogen connection

SUSCAT has also been at the forefront of developing a new LOHC system to safely and sustainably store hydrogen that can be used

Converting greenhouse gases into valuable liquid chemicals

With the support of EU funding, researchers are designing more efficient and economical processes for converting natural gas and carbon dioxide into high-value chemicals.



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Today, most people are well aware of the fact that CO₂ causes climate change. However, many are unaware about another, even more potent form of greenhouse gas: natural gas, or CH₄.

“With natural gas production on the rise, there is an increasing need to simultaneously address both CO₂ and CH₄ emissions,” says Bert Weckhuysen, a professor at Utrecht University in the Netherlands.

The urgency of the climate crisis and the increase in natural gas production accelerate the need for an efficient way to convert methane into liquid fuels and other commodity chemicals. Working to meet this need is the ERC-funded project ZeoMemRx (Greenhouse gases to valuable liquid chemicals: High-flux zeolite membrane-based reactor for the efficient conversion of CH₄ and CO₂).

"The conversion of CH₄ and CO₂ are interconnected goals," explains Weckhuysen, the principal investigator. "A promising strategy for accomplishing this dual conversion is to transform the two gases into easily transported liquid chemicals."

This approach is particularly attractive because such a conversion reduces the amount of emissions released into the atmosphere. Furthermore, it also produces commodity chemicals that can be used either as fuels or as precursors for many industrial processes. "Unfortunately, actually doing this transformation is easier said than done," says Weckhuysen.

Challenges to conversion

According to Weckhuysen, several major issues exist in the current approaches to CH₄ and CO₂ conversion, separation, and use. For example, converting CO₂ into more valuable chemicals requires a dependable source of hydrogen. There's also the fact that CO₂'s high thermodynamic stability makes it very difficult to transform it into other chemicals.

Then there's the matter of CH₄'s fast deactivation, not to mention that CH₄ often only exists at wells located in very remote areas. This latter problem makes current gas-to-liquid technologies, such as conversion to syngas followed by upgrading via the Fischer-Tropsch Synthesis (FTS) process, uneconomical.

These challenges require innovative approaches to designing more efficient and economical processes for converting CH₄ and CO₂ into high-value chemicals – which is exactly what the ZeoMemRx project is attempting to do. "We are proposing a high-flux zeolite membrane reactor capable of effectively converting a mixture of CH₄ and CO₂ into hydrocarbons and aromatics – including benzene, a versatile platform chemical," remarks Weckhuysen.

A key feature of the envisioned system is a highly oriented zeolite membrane with a tunable composition fabricated on a porous substrate. This will give the system the ability to shift the reaction

equilibrium and decrease the contact time, resulting in a high catalytic performance.

The right people, right skills and right goals

Although still a work in progress, researchers have succeeded in preparing the highly oriented zeolite and related catalyst materials needed to activate CO₂ and CH₄. They've also developed the first prototype membrane reactor system for initiating the reaction, which is now undergoing further assessment.

"Everything from the transfer of knowledge to the build-up of the new reactor system and the creation of new materials are the result of the teamwork and collaboration that have defined this project," concludes Weckhuysen. "You can have a great idea, but without the right people, the right skills, and the right goals, it will remain only that – an idea."

PROJECT

ZeoMemRx – Greenhouse gases to valuable liquid chemicals: High-flux zeolite membrane-based reactor for the efficient conversion of CH₄ and CO₂

HOSTED BY

Utrecht University in the Netherlands

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Horizon 2020-ERC

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A sustainable method for producing amines from agricultural and forestry waste

Amines are crucially important classes of chemicals, widely present in pharmaceuticals, agrochemicals and surfactants. However, a systemic approach to obtaining this essential class of compounds from renewable sources has not been achieved. The CatASus project set out to change this by enabling the production of amines from alcohols, in turn derived from renewable resources, specifically lignocellulose waste.



Lignocellulose – plant dry matter – is the most abundantly available raw material on Earth for the production of biofuels, mainly bioethanol. It is produced in large quantities as part of agricultural and forestry waste but is currently not fully valorised because of its challenging structure.

The ERC-supported CatASus (Cleave and couple: Fully sustainable catalytic conversion of renewable resources to amines) project, carried out at the University of Graz, Austria, aims to fully tackle this by developing a novel and efficient means to depolymerise (decompose) lignocellulose into platform chemicals and then convert them into useful compounds, primarily amines (a nitrogen-containing compound).

This would be highly beneficial as amines, ubiquitous in the chemical industry, are in high demand in medicinal polymer chemistry and as fine chemical intermediates. By utilising lignocellulose, the production of amines could become fully sustainable. CatASus aims to deliver groundbreaking approaches in catalysis that are necessary to establish an entirely new lignin valorisation platform. Its core focus is devoted to catalysts relying on cheap, Earth-abundant materials in contrast to methods that use expensive, noble metals that are becoming ever scarcer and could be fully depleted in the coming decades.

Whilst constituting a major innovation in being able to produce amines in a truly sustainable novel-to-waste value chain, the project's results would also offer important economic benefits, creating new sources of revenue for the agricultural and chemical sectors and contributing to the growth of a European bioeconomy.

CatASus began in May 2016 and is due to run until April 2022.

PROJECT

CatASus – Cleave and couple: Fully sustainable catalytic conversion of renewable resources to amines

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Introducing HY-CAT, a project devoted to finding better catalysts to spur a CO₂ circular economy

The electrochemical conversion of CO₂ can generate a variety of valuable products, such as liquid fuels used to power transportation. However, as CO₂ is a very stable molecule, efficient catalysts to break its bonds are needed. The ERC-supported HY-CAT project aims to identify and develop better catalytic systems to convert CO₂ into value-added chemicals whilst storing renewable energies.



The world's current dependence on fossil fuels requires us to capture and store the CO₂ human civilisation produces, to prevent unacceptable CO₂ levels in the Earth's atmosphere. However, there are also limits to CO₂ storage. What if excess CO₂ could be converted into useful chemicals instead, thus creating, in effect, a CO₂ circular economy?

The HY-CAT (Multifunctional Hybrid Platforms based on Colloidal Nanocrystals to Advance CO₂ Conversion Studies) research team, based at the Swiss Federal Institute of Technology, Lausanne, is working to synthesise hybrid materials comprised of atomically well-defined CO₂ sorbents, which are thin, porous layers of the so-called metal-organic frameworks (MOFs), and nanocrystalline catalysts intimately bound in a single integrated system. They will use three different classes of hybrids, each characterised by one specific absorption/preactivation mechanism, to make a detailed investigation of the effect of mechanisms on the catalyst activity. Such a methodical approach enables the team to compare structure and activity, determining the design principles upon which better catalysts can be made.

HY-CAT has already reached some notable milestones. This includes learning how to synthesise hybrid electrocatalysts, including silver nanocrystals embedded in MOFs. They found that MOFs make the nanoparticles more selective, thus making them more energetically favourable as a reaction channel, for CO₂ reduction and more stable towards aggregation during catalysis. They have also successfully developed an approach to form a copper/ceria oxide (Cu/CeO_x) system, finding that such a

combination of nanoparticles also makes copper more selective towards converting CO₂ to methane.

From a commercial standpoint, HY-CAT has also designed and built a state-of-the-art electrochemical cell that is fed by gas instead of aqueous electrolyte. This device makes it possible to test the catalysts under commercially relevant conditions, a crucial step for making real progress towards true sustainability.

HY-CAT began in January 2017 and will run until June 2022.

PROJECT

**HY-CAT – Multifunctional Hybrid Platforms
based on Colloidal Nanocrystals to Advance
CO₂ Conversion Studies**

HOSTED BY

Federal Institute of Technology Lausanne in
Switzerland

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RESEARCH*EU MAGAZINE ISSUE 94

Hydrogen's growing role in sustainable energy systems

Hydrogen is a real contender for being the world's next big solution to ensuring more sustainable energy and transport systems and in this edition of Research*eu, we meet seven EU-funded projects that are demonstrating how hydrogen's time to shine may finally have dawned.



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