Science 4 Technology – Poster Exhibition 2024

Department General, Analytical and Physical Chemistry

Chair of Physical Chemistry

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Poster Exhibition 2024

Science 4 Technology @MUL

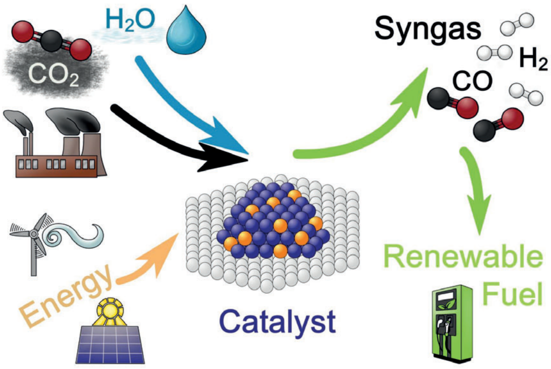
Transforming CO_2 and H_2 into renewable Chemicals and Fuels

Research Group of Christoph Rameshan

T. Berger, T. Cotter, H. Drexler, L. Lindenthal, J. Michalke, J. Rollenitz, R. Rameshan, T. Ruh, F. Schrenk

Chair of Physical Chemistry, Montanuniversität Leoben

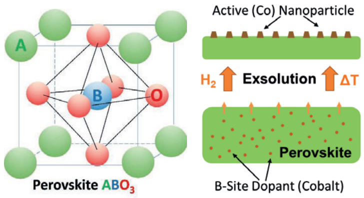
Development of New Catalytic Systems

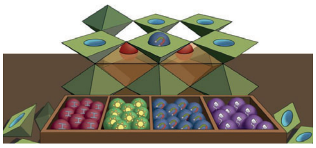


We develop and test new catalytic materials based on **complex oxides**. They facilitate a **rational design approach**, which cuts down development time and increases efficiency.

In recent studies, we have shown the applicability of these catalyst not only for **CO_2 utilisation** but also to reactions useful for **H_2 storage** and **CH_4 conversion**.

In the end, our novel materials could help mitigate climate change by **transforming greenhouse gases** and creating a **carbon neutral circular economy.**



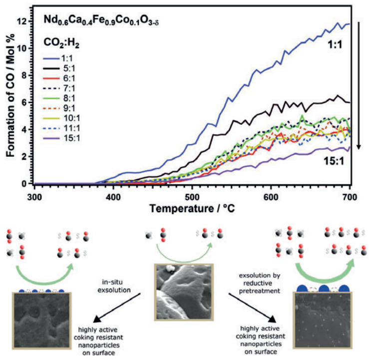


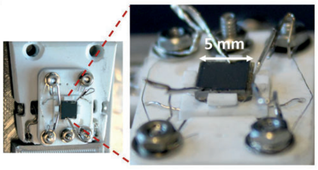
Material Characterisation: In-situ Studies and Theory Predictions

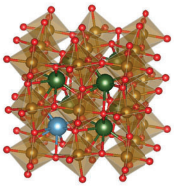
For a rational catalyst design, it is crucial to obtain insights into how desired reactions work on a molecular level. To achieve this, we utilise a multitude of **high-end, state-of-the-art in-situ/operando methods,** both in our laboratories and at **international research facilities.**

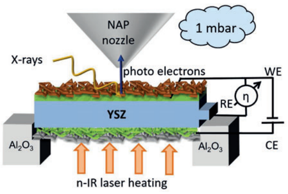
Combined with predictions via theoretical models, a direct correlation of catalyst structure and its reactivity is possible.

In the past years, we expanded our research focus to electro-catalytic processes, particularly focused on CO_2 reduction and green H_2 generation.

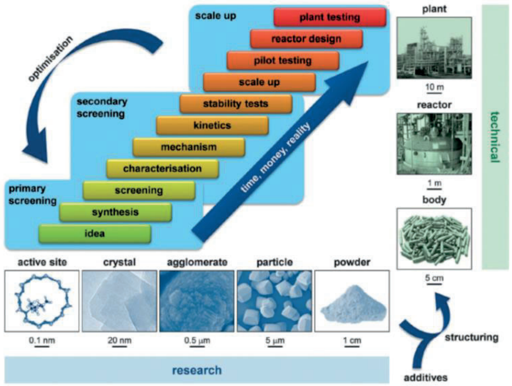


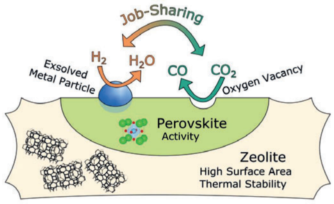


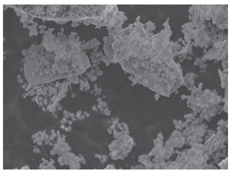




Transfer Developed Catalysts into Industrial Applications

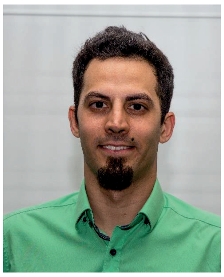






To successfully achieve global impact, the catalysts we developed need to be **implemented into existing industrial processes**. Therefore, the catalytic systems need to be optimised to guarantee **long-term stability** and **low cost** for industrial application.

We are currently researching ways to **combine our catalytic highly active materials with backbone materials already used in large- scale processes**.



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CO_2 Utilization with Citizen Scientists:

A Sparkling Science 2.0 Project

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Motivation

Closing the carbon cycle is a possible way to mitigate climate change and as such one step to **reduce the amount of CO_2 released** into the atmosphere by re-using CO_2 already in the atmosphere (in principle, a net reduction can be achieved by using CO_2 form direct air capture).

CO_2 in flue gas (1) is **captured** (2) and **converted** (3) into fuels (e.g. for aviation, 4) or feedstocks for chemical industry. Produced fuels can be stored or used (5); CO_2 set free here is then re-cycled and converted again. Operating conversion sustainably, renewable energy (6) has to be used both directly during the conversion and indirectly during the production of green H_2 (7).

The Project

In our Sparkling Science project "CO_2 Umwandlung" (CO_2 Conversion), we work on two different aspects of this step:

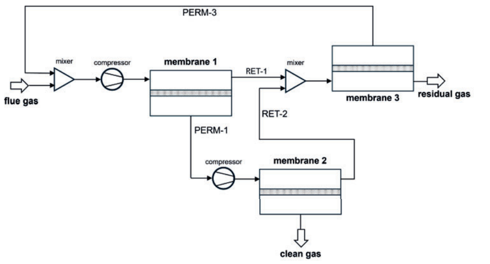
1. **Capture**:
   Together with industrial partners, we are working on approaches to **capture CO_2** from exhaust gases for further use.
2. **Conversion**:
   The captured CO_2 is converted into higher-value products (such as methanol, syngas, or e-fuels) through chemical reactions and used or stored in this form. Since CO_2 is a **very stable molecule**, **catalysts** are needed, which we aim to understand.

Carbon Capture

CO_2 must be captured from exhaust gases before its utilization in conversion reactions. This presents a **challenge** for two reasons:

1. **Flue gas parameters are process-dependent:**
   Both the composition (CO_2, residual O_2, impurities…) and temperature and pressure vary over wide ranges.
2. **Established processes require large-scale facilities:**
   This increases the costs of retrofitting CO_2 capture.

A promising **alternative** (especially regarding the retrofitting of existing processes) is **membrane technology**. In the project, we are working with **process simulations** to develop potential scenarios based on membrane modules for industrial partners.



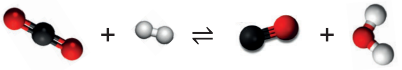
Simulated cascade consisting of 3 membrane modules:
Even for low CO_2 concentrations (<5 %), separation rates of up to 85% can be achieved. However, additional compression stages are necessary, which increase the energy costs. The residual gas has CO_2 concentrations below 1 %, while the concentration in the "concentrate" is increased by a factor of 5–6 compared to the exhaust gas.

Carbon Utilization

CO_2 can serve as a **starting material** for **base chemicals**: For example, **synthesis gas** (a mixture of CO and H_2) or **methanol** can be produced. Subsequently, **renewable fuels (e-fuels)** can be produced.

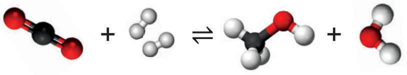
Here, two example reactions are shown:

$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$



reverse water–gas shift reaction (rWGS)

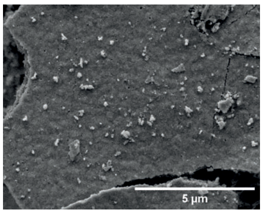
$$CO_2 + H_2 \rightleftharpoons CO + H_2O$$



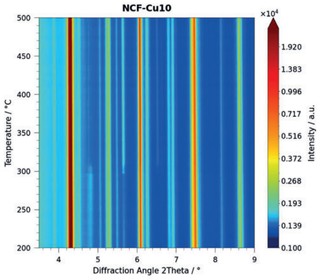
methanol synthesis

Catalyst Characterization

To understand the **relationship between the composition and the performance** of these catalysts, **thorough characterization** of the materials used is essential.
Here are examples of the methods used:



Electron microscopy image (**SEM**) of a catalyst surface with nanoparticles as active centers.



Temperature-dependent X-ray diffraction (**XRD**) reveals how the catalyst $Nd_{0.6}Ca_{0.4}Fe_{0.9}Cu_{0.1}O_{3-\delta}$ (NCF-Cu10) changes during the reaction – for example, new (active) phases may form.

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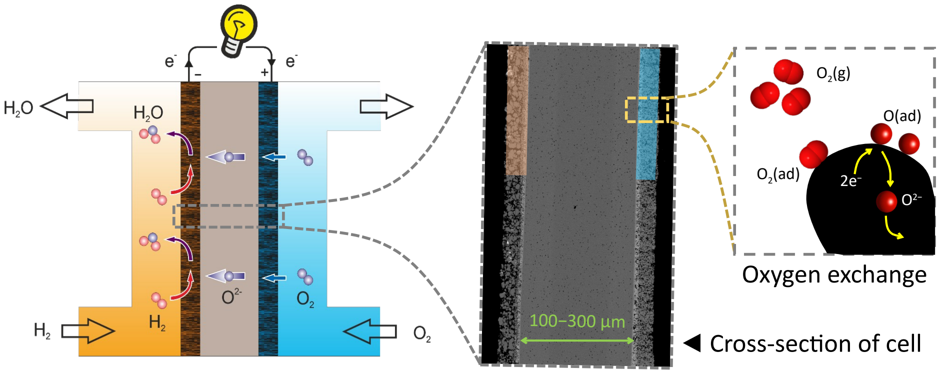
Materials for electrochemical energy conversion and storage in solid oxide cells

Research Group Bucher – Chair of Physical Chemistry

Our scientific focus is on the development of functional ceramics for highly efficient electrochemical energy conversion and storage in solid oxide fuel cells (SOFCs) and solid oxide electrolyser cells (SOECs).

Fundamental research topics

- Material synthesis and processing
- Crystals structure and microstructure
- Mass and charge transport properties
- Electrochemistry and degradation mechanisms

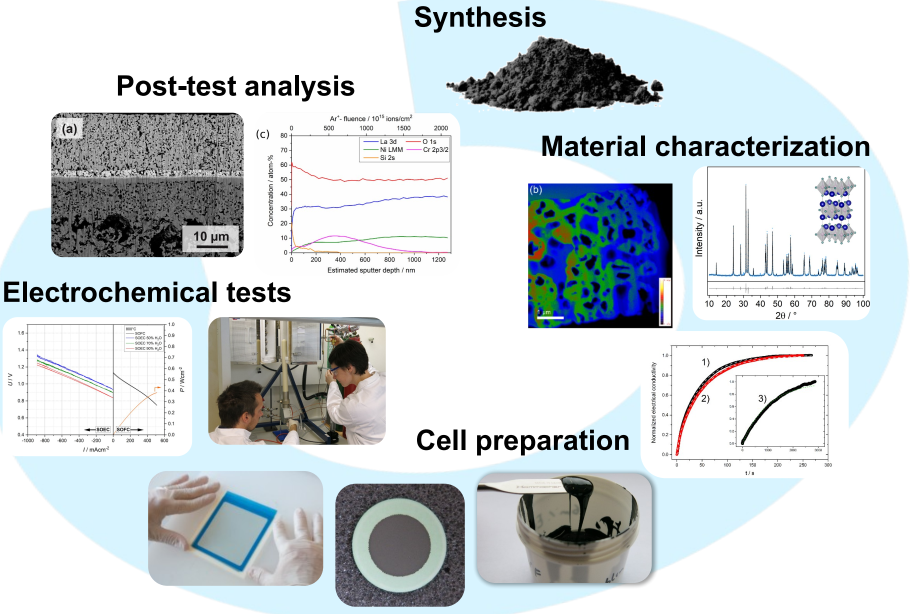


Solid oxide fuel cell (SOFC)

◀ Cross-section of cell

Oxygen exchange

Methods and expertise



Synthesis

Post-test analysis

Material characterization

Electrochemical tests

Cell preparation

Novel functional ceramics are synthesized by sol-gel processes and characterized with respect to crystal structure, phase purity, and powder morphology.

We combine ex-situ and in-situ characterization techniques to gain insights into the fundamental structure-property relationships of novel ceramics for electrochemical solid oxide cells. Promising materials are transferred to the cell level.

Performance, long-term stability, and degradation mechanisms are investigated by electrochemical characterization and post-test analyses.

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Research group Bucher

https://physchem.unileoben.ac.at/forschung/research-group-bucher

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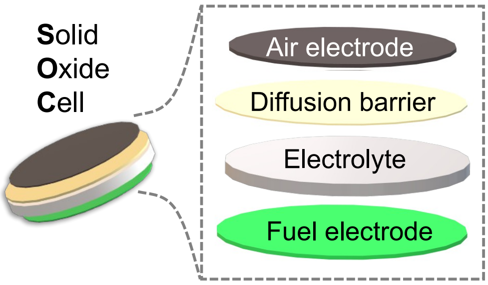
Advanced fabrication and characterisation of electrochemical solid oxide cells

Research Group Bucher – Chair of Physical Chemistry

Our scientific focus is on the development of the next generation of solid oxide fuel and electrolyser cells with excellent performance, increased lifetime, and reduced demand of critical materials.

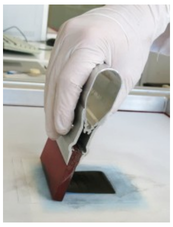
Cell fabrication

- Ceramic layers fabricated by screen printing, tape casting and sintering
- Porous air and fuel electrodes deposited on dense electrolyte and diffusion barrier

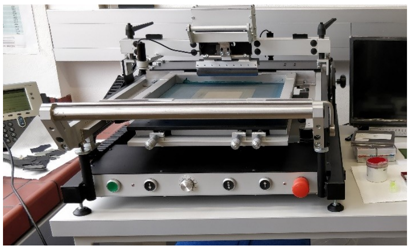


Paste made from oxide powder and ink vehicle

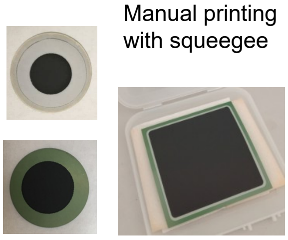
Adjustment of screen and mask on half-cell



Manual printing with squeegee



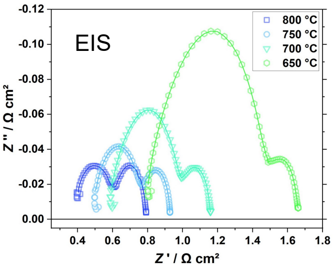
Semi-automatic screen printing system

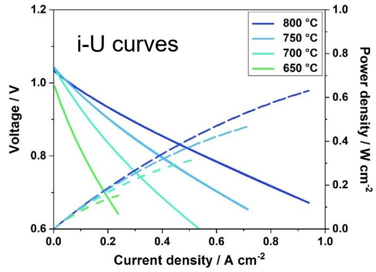


Button cells (∅ 2 cm) and square cell (10×10 cm²)

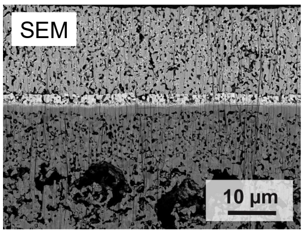
Cell characterisation

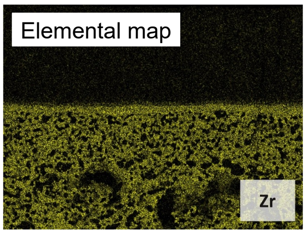
- Electrochemical impedance spectroscopy (EIS) is used to analyse processes with different characteristic frequencies
- Current density vs. voltage curves are used to study the performance and stability in fuel cell and electrolyser mode





- Scanning electron microscopy (SEM) reveals the microstructure and elemental distribution as well as mechanism of degradation
- Insights into the complex relations between electrochemistry, microstructure, and material properties are applied to improve cell design





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Research group Bucher

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FWF Österreichischer Wissenschaftsfonds

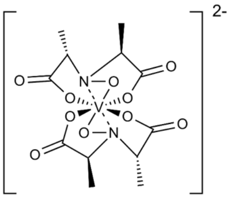
ÖAW ÖSTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN

Amanita Muscaria For Heterogeneous Redox Transformations

Amanita Muscaria (Fly Agaric Mushroom)

- **Vanadium** uptake of
  > 100 mg per kg dry mass
- Highest concentration in bulb part
  1000 mg per kg dry mass
- Not dependent on location
- < 75–96 % of the V bound in form of

Amavadin



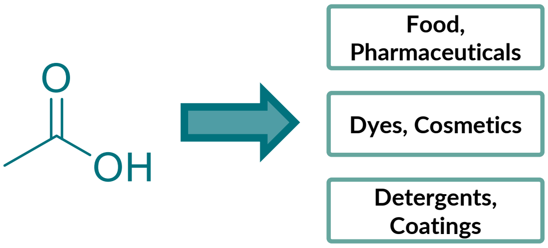
If you're looking for a Bachelor- or Masterthesis, I'd be happy to hear from you to work together on Mushroom catalysis

Use of models for oxidations

- Labor-intensive extraction steps
- Syntheses of model substrates
- Purification steps

Applications

- Acetic acid production **(> 7 Mio. t/a)**



Food, Pharmaceuticals

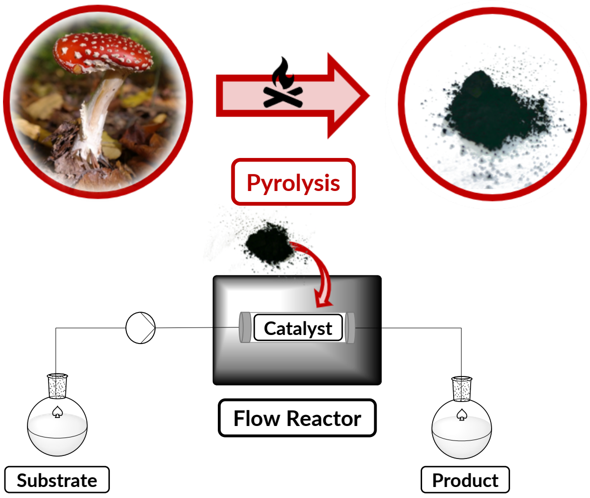
Dyes, Cosmetics

Detergents, Coatings

- *Monsanto* or *Cativa* processes rely on **Platin Group Metals** (PGMs)
  - High cost
  - Toxicity (environment & humanity)
  - Global availability

Alternative with Amanita Muscaria

- Drying & **pyrolysis** of fly agaric mushrooms
- **Direct use** of obtained material as **catalyst for oxidations**
- Use of **renewable resources** instead of exploitation
- Optimized utilization and **recycling**
- **Extended lifetime** & efficiency utilizing **flow-chemistry** with particles sealed in stainless-steel cartridge
- **Comprehensive analysis** of the material before and afterwards
- ~~**Food waste**~~ → toxic if eaten by humans



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