Electrochemical CO_2 conversion for the synthesis of sustainable fuels and platform chemicals

Francesco Bernasconi, Alessandro Senocrate,
Peter Kraus, Nukorn Plainpan, Corsin Battaglia

francesco.bernasconi@empa.ch

Swiss Federal Laboratories for Materials Science and Technology

Technology Briefing- June 26, 2024

Empa
Materials Science and Technology

Motivation: EU/CH aim at carbon neutrality

Empa
Materials Science and Technology

More

Swiss approve net-zero climate law

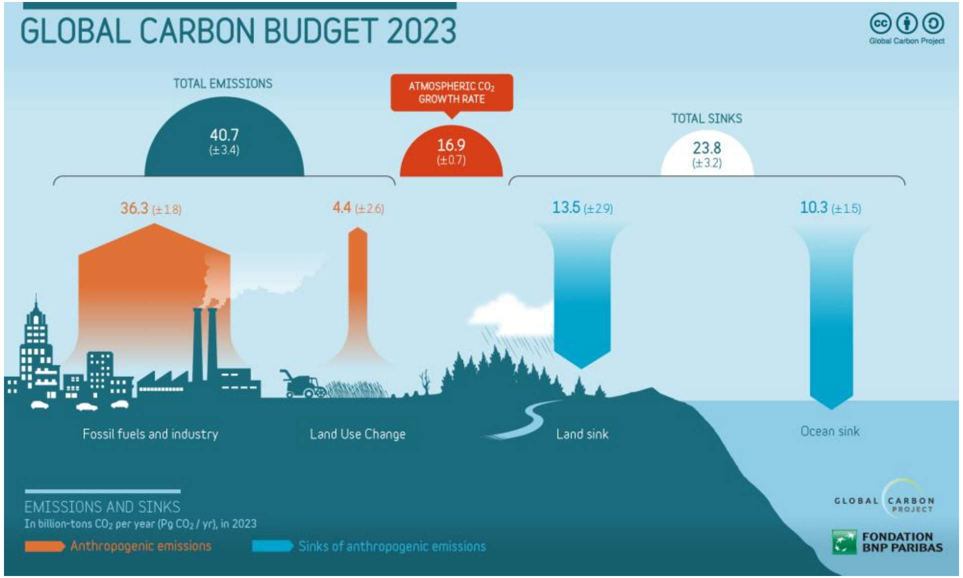
Jun 18, 2023 • Swiss voters have backed a new law to accelerate the country's shift from fossil fuels to renewable energies and reach zero emissions by 2050.

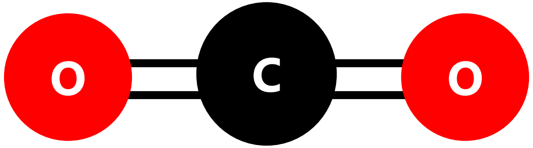
- Phase out fossil fuels
- Electrification with renewables
- Replace fossil carbon feedstock

Close the carbon loop to produce sustainable chemicals/fuels

https://www.swissinfo.ch/eng/politics/swiss-to-decide-on-net-zero-climate-law/48593158
https://www.euronews.com/2020/10/19/several-countries-threatening-eu-s-2050-carbon-neutral-goal-says-mep

CO_2 as a non-fossil carbon source





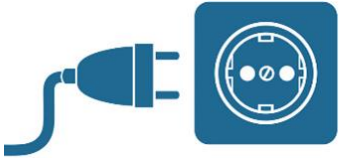
- Stable gas at RT
- Chemically (almost) inert
- Limited solubility in water

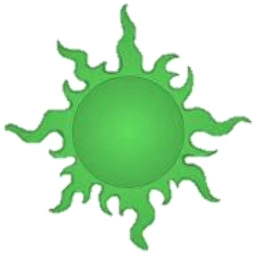
Atmospheric CO_2 as feedstock to produce goods

Friedlingstein et al., *Earth System Science Data*, **2023**, 15, 5301

Empa
Materials Science and Technology

Strategies to convert CO_2 into products

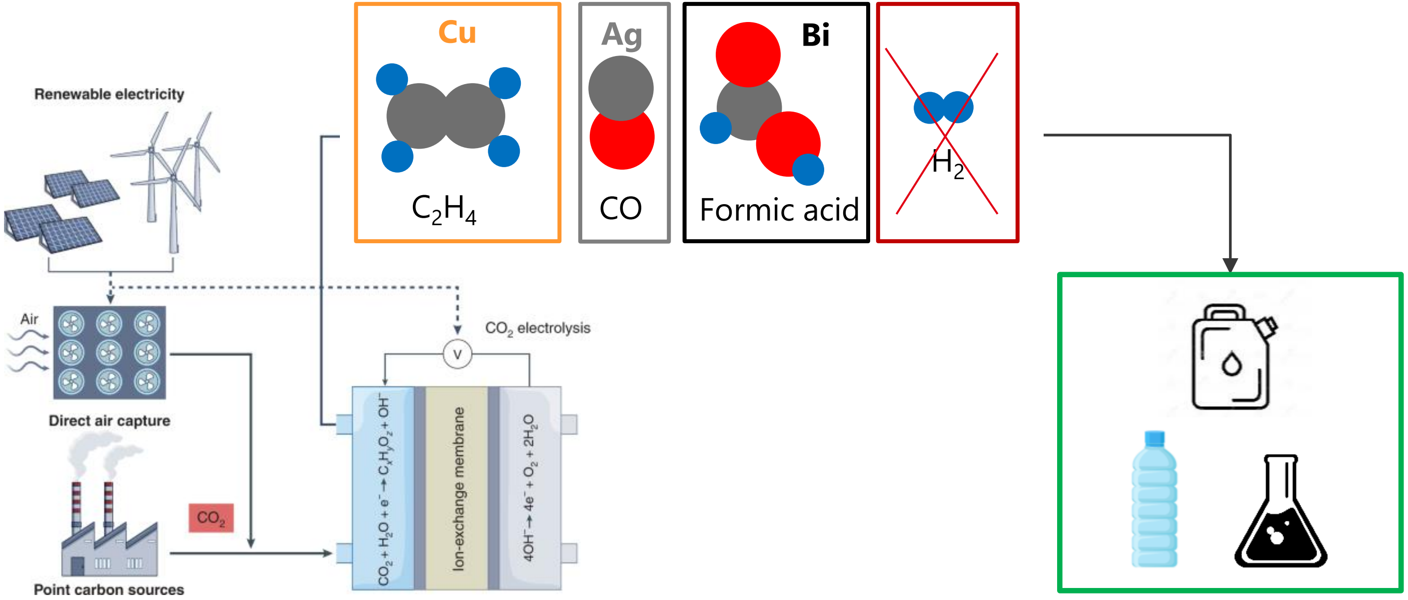




Thermochemical	Electrochemical	Photochemical
High heat and pressure	Ambient conditions	Ambient conditions
H_2 as co-reactant	H_2O as co-reactant	H_2O as co-reactant
Fossil-fuel heated	Couple with renewables	Under development
High TRL	Low/Med TRL	Low TRL

Electrochemical route requires coupling CO_2 with H_2O and electrons

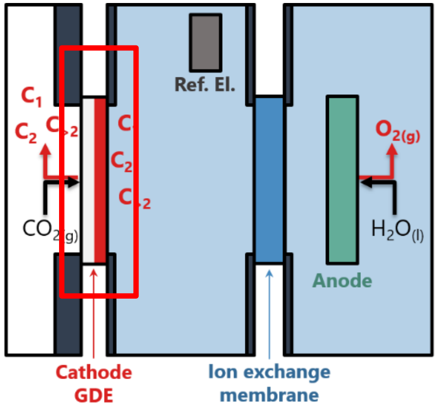
Target platform chemicals

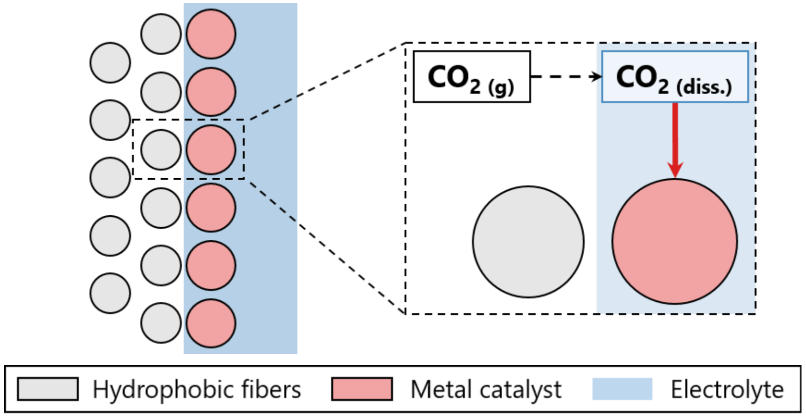


Electrochemical CO_2 conversion using renewables yields sustainable fuels/chemicals.

Jordan, and Wang, *Nat. Catal*, **2021**, 4, 915

CO_2 conversion on gas diffusion electrodes (GDEs)





CO_2R | $CO_2 + H_2O + 2e^- \rightarrow CO + 2OH^-$

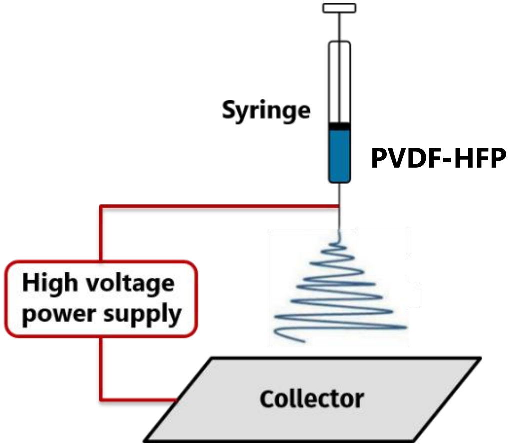
CO_2R | $2CO_2 + 8H_2O + 12e^- \rightarrow C_2H_4 + 12OH^-$

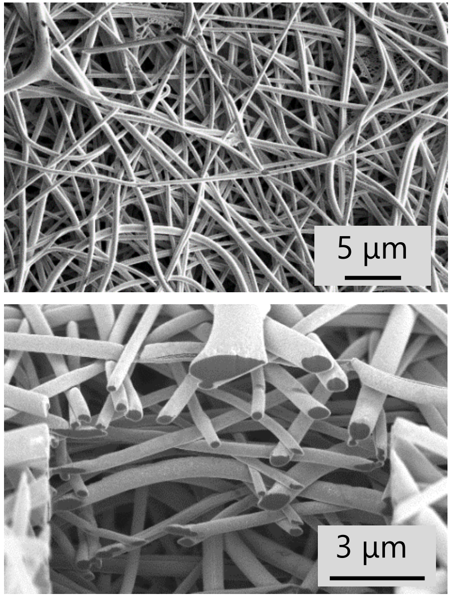
HER | $2H_2O + 2e^- \rightarrow H_2 + 2OH^-$

A key challenge is to reduce H_2O reactivity to favor CO_2 reduction

Ju, Jiang, Ma, Pan, Zhao, Pagani, Rentsch, Wang, Battaglia, *Adv. Energy Materials*, **2019**, 9, 1901514
Bernasconi, Senocrate*, Kraus, Battaglia, *EES Catalysis*, **2023**, 1, 1009.

Electrospinning: scalable substrate fabrication



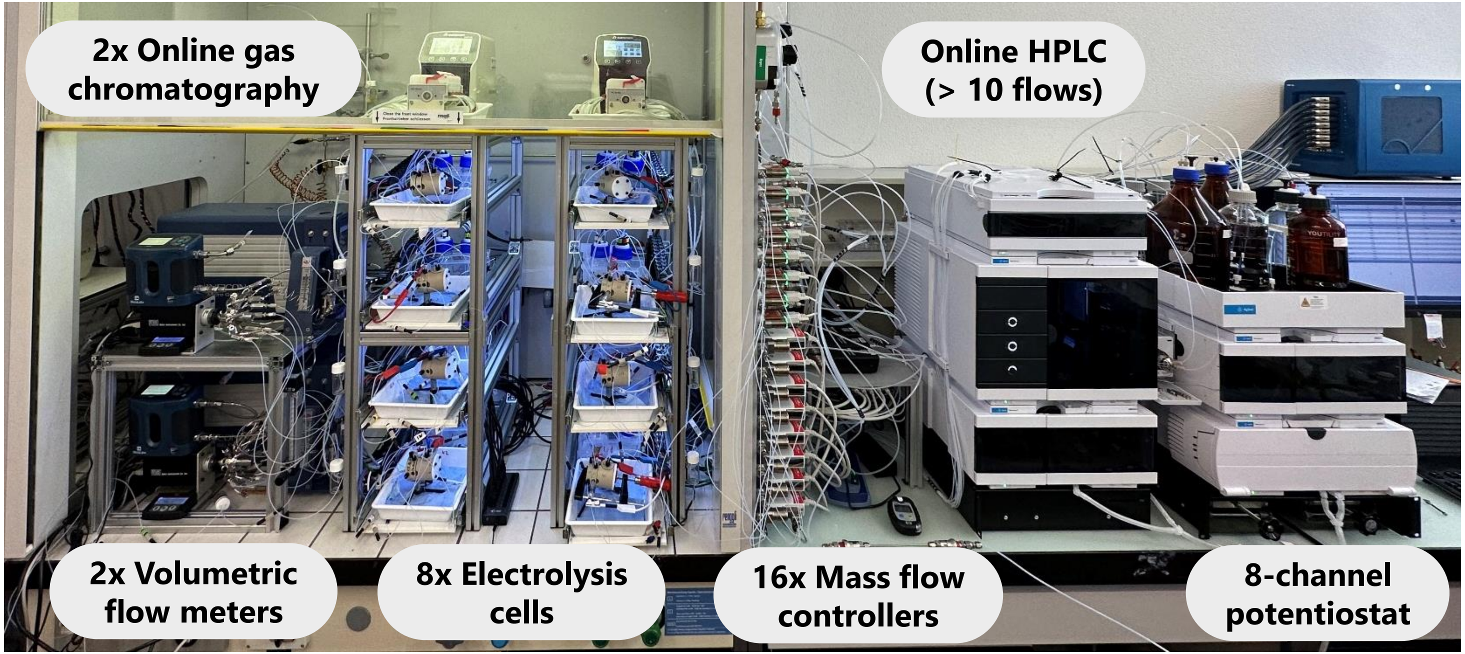


Electrospinning offers precise substrate control and scale-up capabilities.

Bernasconi, Senocrate*, Kraus, Battaglia, *EES Catalysis*, **2023**, *1, 1009.*
Yu, Senocrate*, Bernasconi, Künniger, Müller, Pauer, Battaglia, Wang, *Materials Design* **2023**, 225, 111441.

Parallel analysis of CO_2 conversion products

Empa
Materials Science and Technology

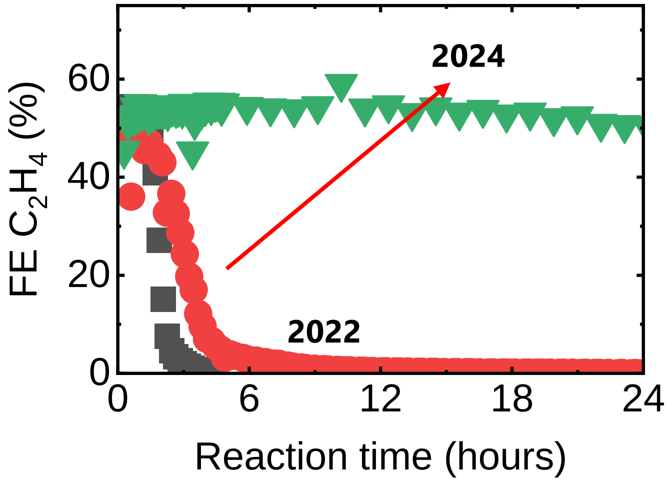


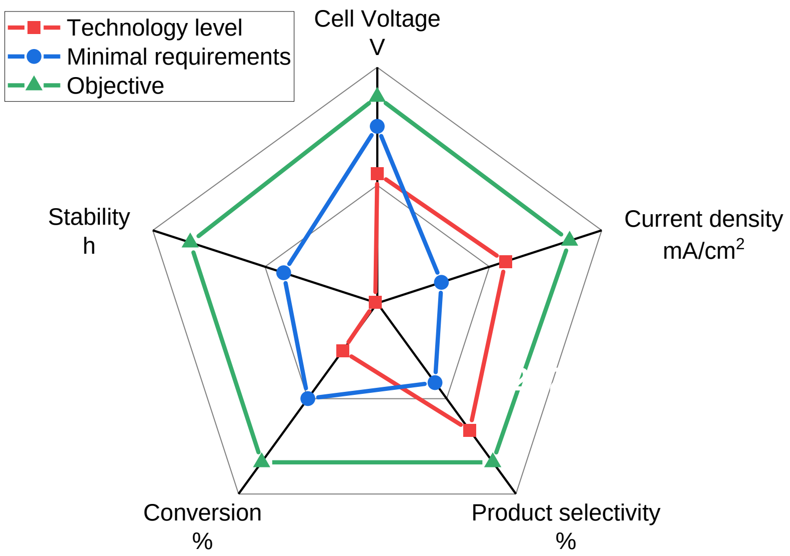
Standardized data handling facilitates implementation of multiple cells.

Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Catal.)*, **2023**.

Technological descriptors for CO_2 conversion

Empa
Materials Science and Technology

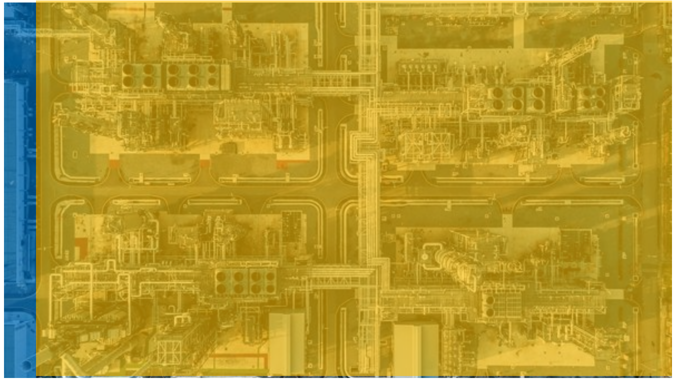




Stability is the main limiting factor for the upscale of the technology

Energy demand for CO_2 conversion

E (kJ/mol)	Collection	Conversion	Separation
Thermodynamics	4-20	1’300	
System level	500-1’000	10’000	1’000



The conversion of CO_2 is the most energy-intense step

https://doi.org/10.1016/j.apenergy.2018.02.144
https://asb-automation.ch/

Practical example: electrify 10% C_2H_4 production

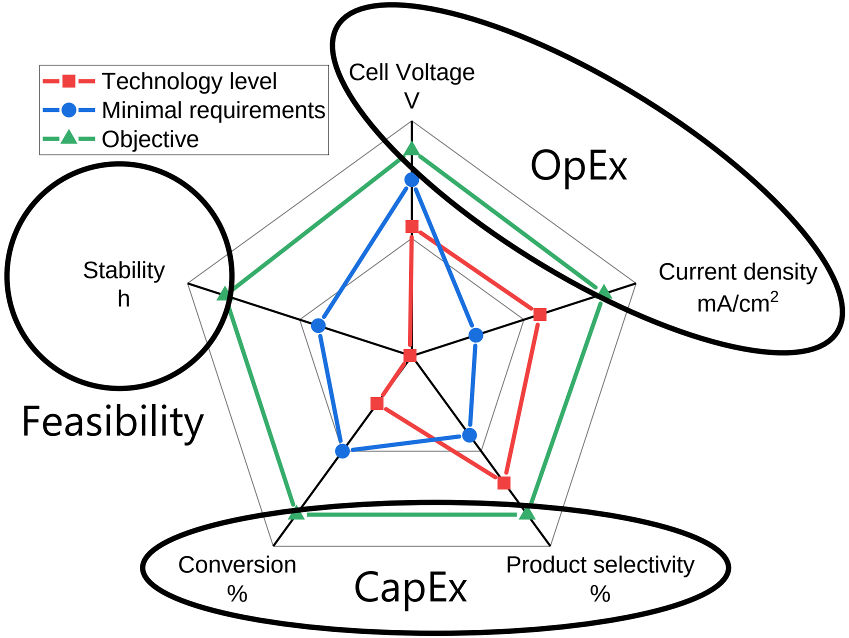
Chemical	Production (Mt/year)
Sulfuric acid	210
Ammonia	180
Ethylene	110
Propylene	80
Methanol	60
Ethylene glycol	60

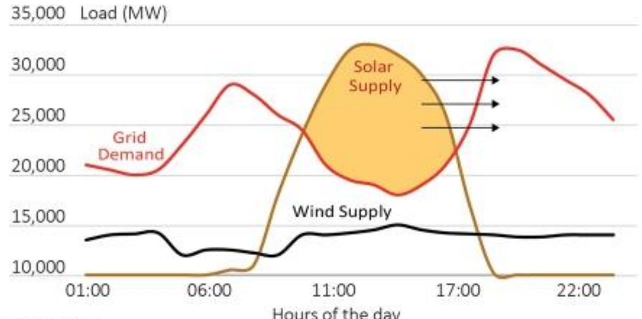
$$CO_2 \xrightarrow{\text{10000 kJ/mol}} C_2H_4 \text{ 11 Mt/year}$$

E ~ 1000 TWh_{year} ~ 2x electricity generated by Germany

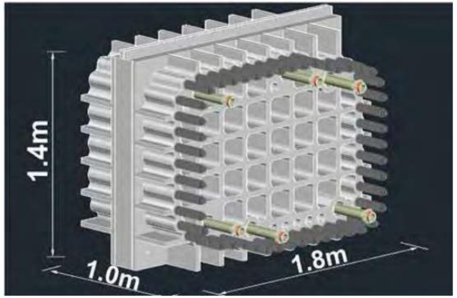
The conversion of CO_2 requires a substantial increase of electricity production

Outlook: challenges and opportunities





Source: QIC



Source: Siemens Enegy

Opportunity to use the electrochemical CO_2 conversion as an electricity sink

Conclusions

Empa
Materials Science and Technology

- The electrochemical CO_2 conversion to platform chemicals is achieved routinely
- Upscale of the technology is promising, catalyst's stability is the main limitation
- Substantial increase in electricification is required to use CO_2 as a feedstock chemical

ETH BOARD
NCCR Catalysis
sweet swiss energy research for the energy transition
FNSNF Swiss National Science Foundation
ESRF
u^b
Agilent


Alessandro Senocrate


Francesco Bernasconi


Nukorn Plainpan

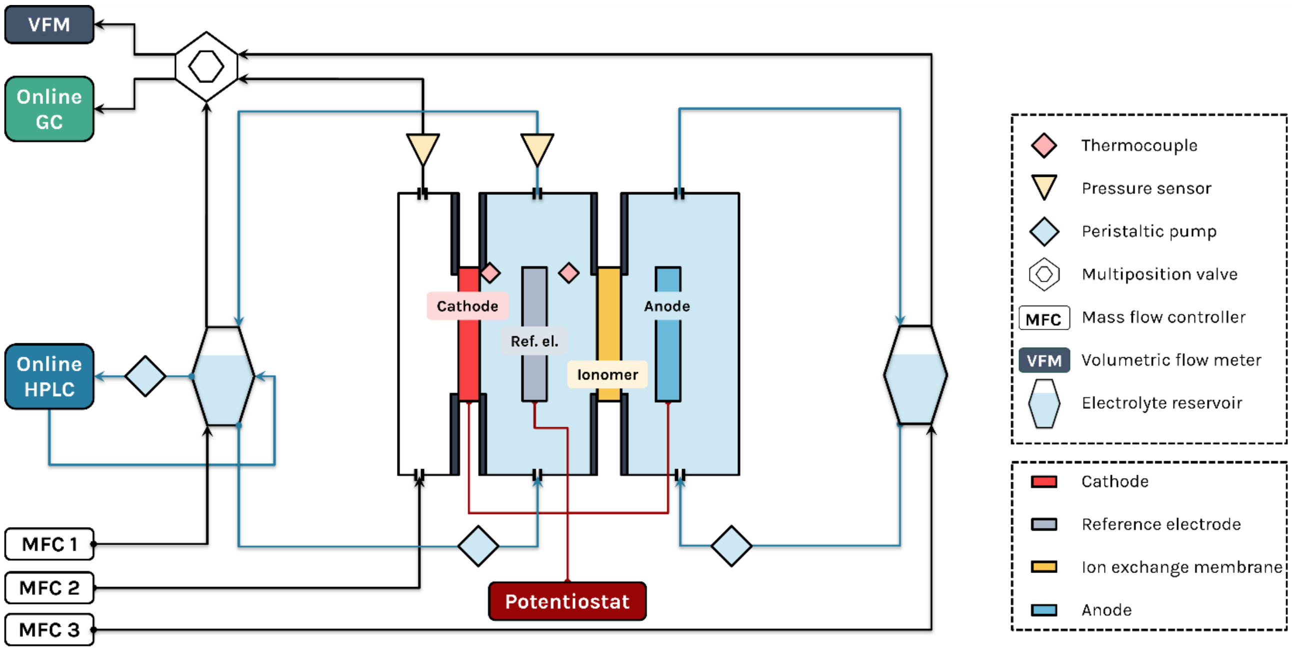

Peter Kraus


Corsin Battaglia

Thank you for your attention!

Extras

Comprehensive analysis system for CO_2 reduction

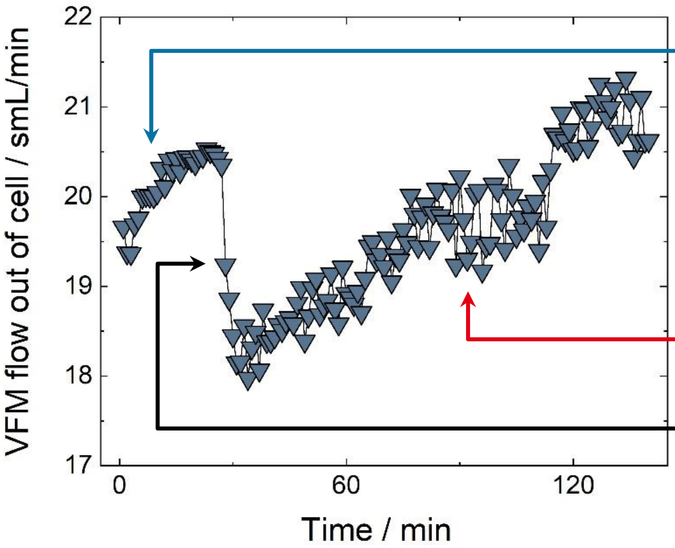


Electrocatalytic performance depends on a huge variety of parameters.

Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.)*, **2023**.

Issue: CO_2 flow variations during experiment

Empa
Materials Science and Technology



CO_2 saturates electrolyte (50 mL KCl)

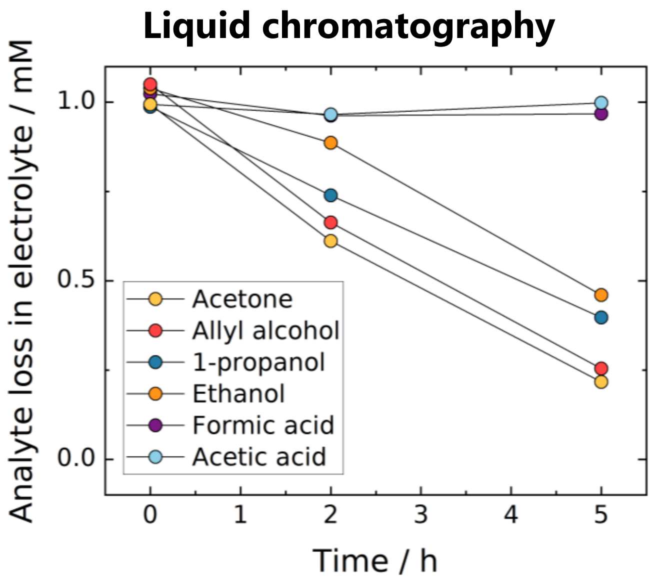
H_2 evolution (Cu at 200 mA/cm²)

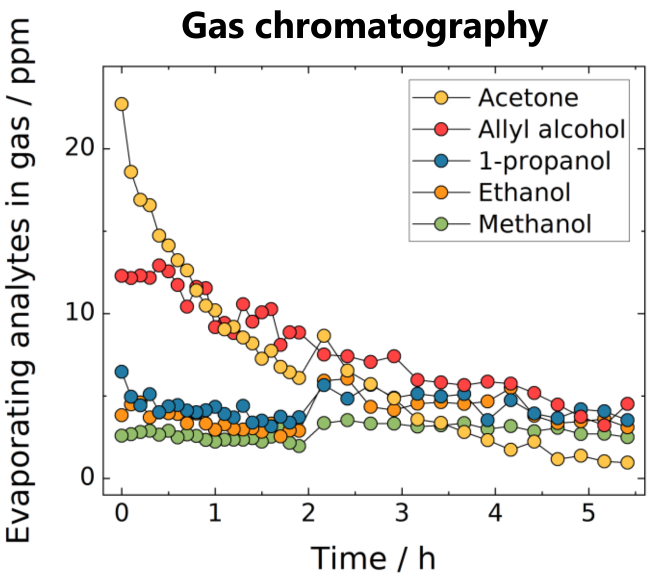
CO_2 consumed (Cu at 200 mA/cm²)

The flow varies strongly due to H_2 evolution, CO_2 dissolution, product formation.
A volumetric flow meter is key to capture the variations and reach accurate FEs.

Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.)*, **2023**.

Issue: evaporating liquid products

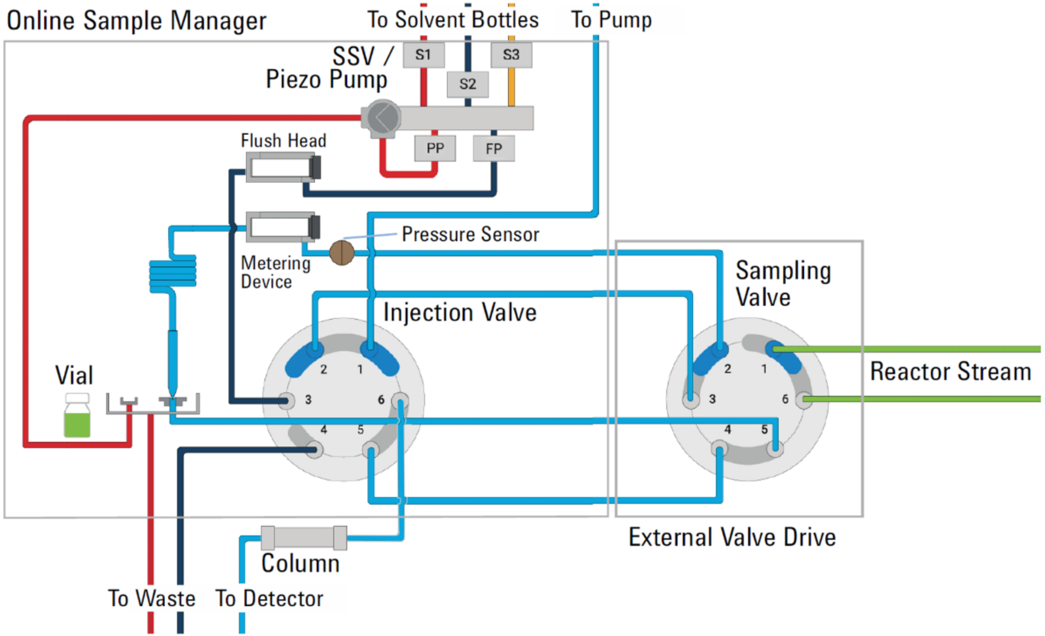




Significant loss of liquid products evaporating in the gas stream.
Electrolyte must be collected immediately and stored sealed.

Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.)*, **2023**.

Online liquid sampling and analysis

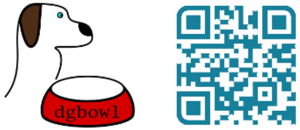


Online sampling extracts and stores liquids from the electrochemical cell/reactor.

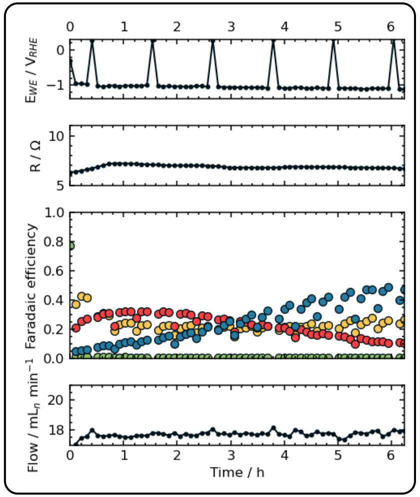
Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.)*, **2023**.

The need for a standard data pipeline

Raw data — *Schema* → **FAIR data** — *Recipe(s)* → **Results**



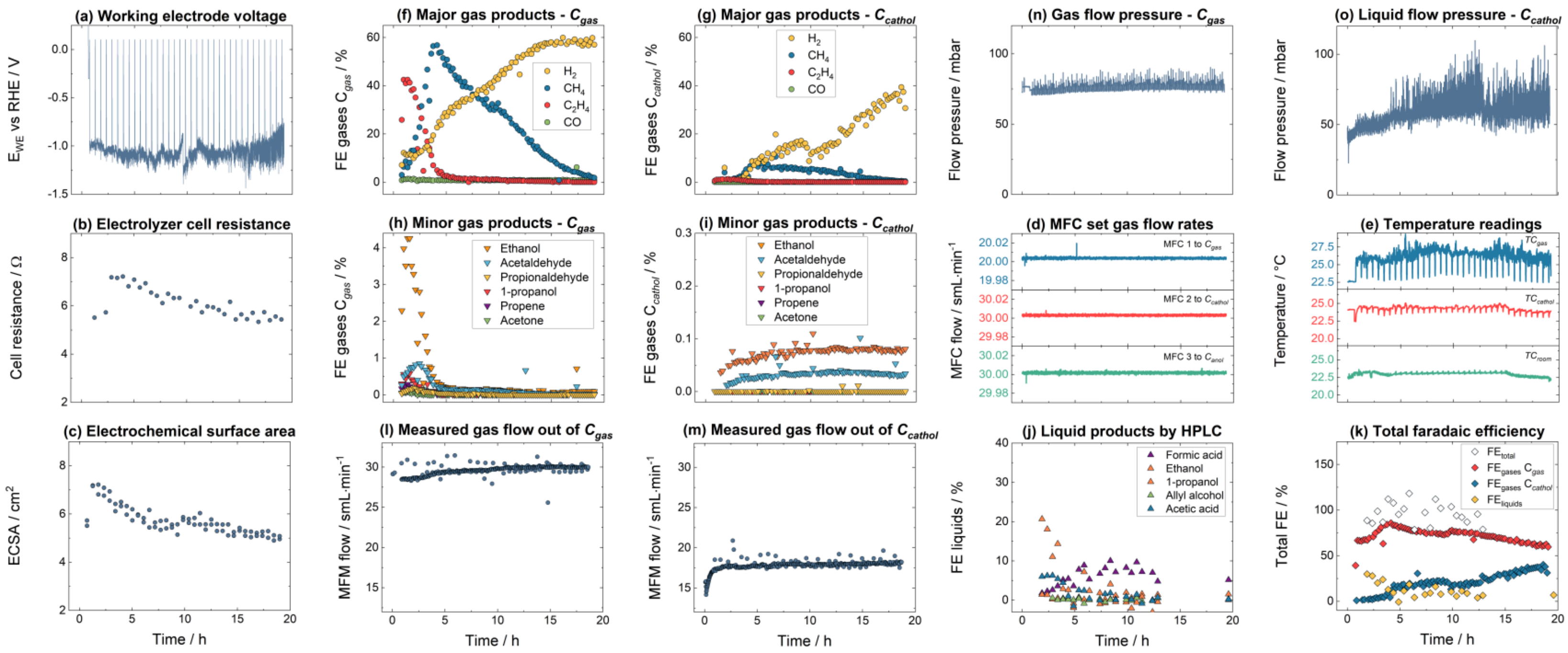
https://dgbowl.github.io



Automatic parsing and processing of complex, heterogeneous datasets.

Kraus, Vetsch, Battaglia, *J. Open Source Softw.* **2022**, 7, 4166.

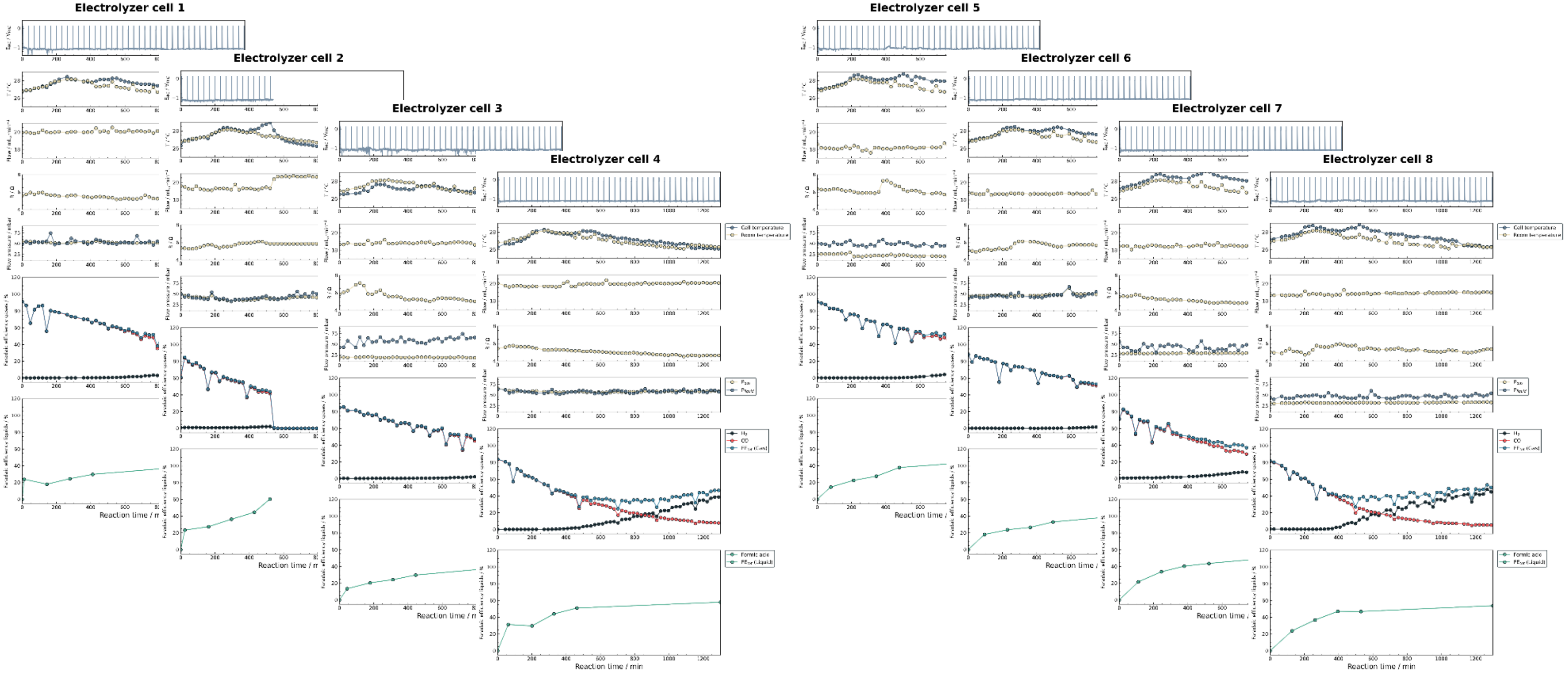
Comprehensive dataset on Cu GDEs



Catalyst, electrode and electrolyzer parameters form a complex but rich dataset.

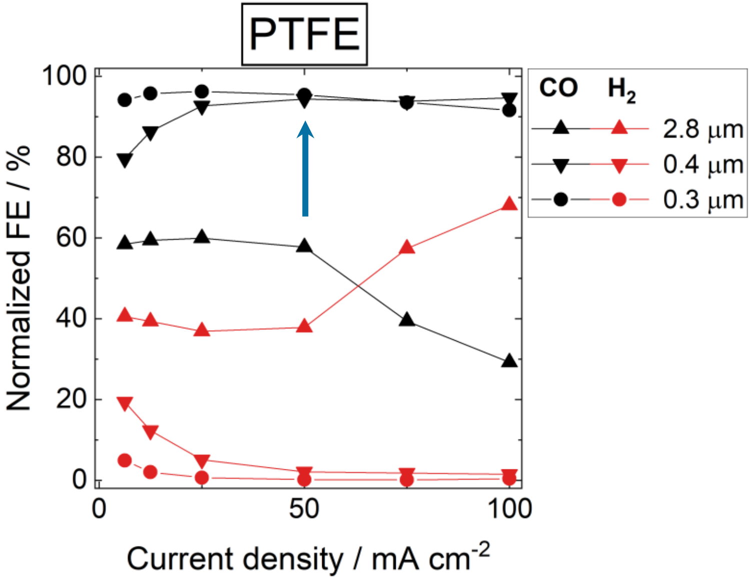
Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.)*, **2023**.

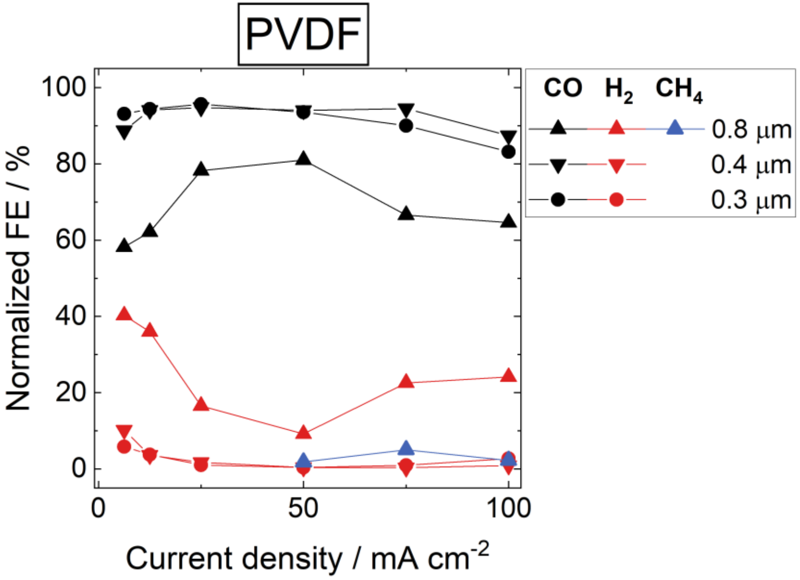
Example of 8 parallel datasets on Ag GDEs



Senocrate*, Bernasconi, Kraus Plainpan, Trafkovski, Tolle, Weber, Battaglia, *accepted (Nat. Cat.),* **2023**.

Ag GDEs: wetting behavior influences selectivity



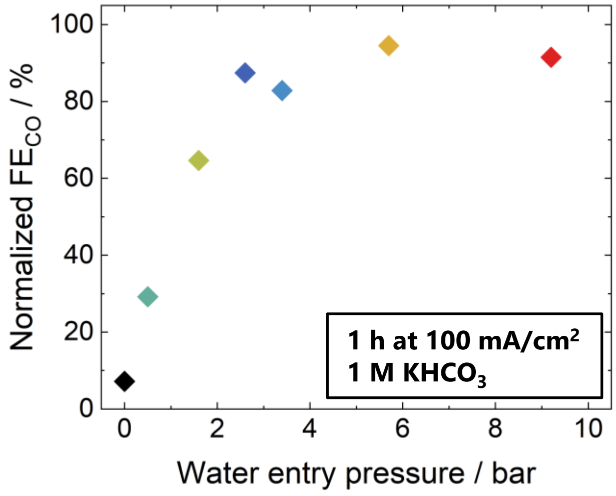


FE_{CO} strongly increases when decreasing substrate pore size

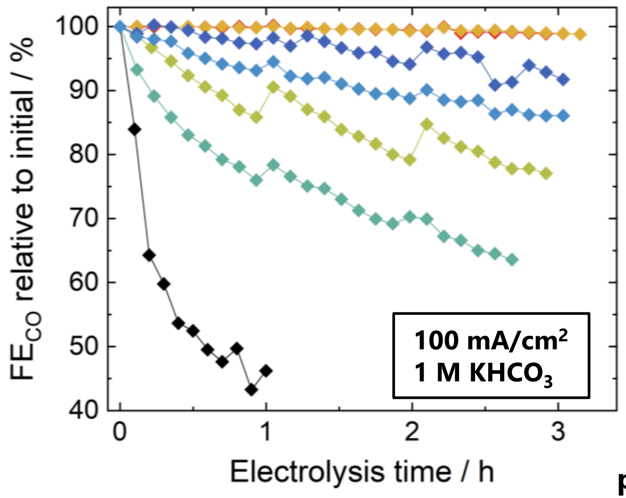
Senocrate*, Bernasconi, Rentsch, Kraft, Trottmann, Wichser, Bleiner, Battaglia, *ACS Appl. En. Mat.*, **2022**, 5, 14504.

Ag GDEs: wetting behavior influences selectivity

Empa
Materials Science and Technology



Electrolyte penetration: High → Low



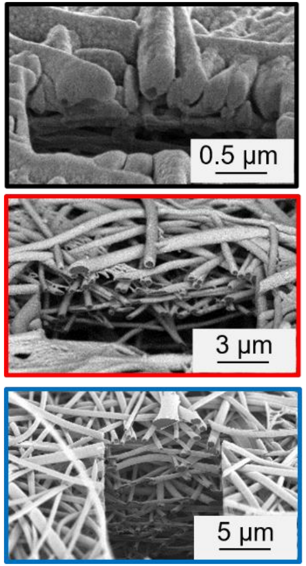
Low ↓ High

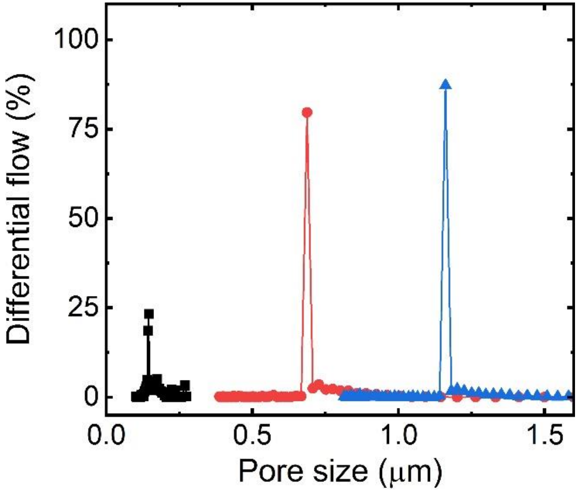
Electrolyte penetration

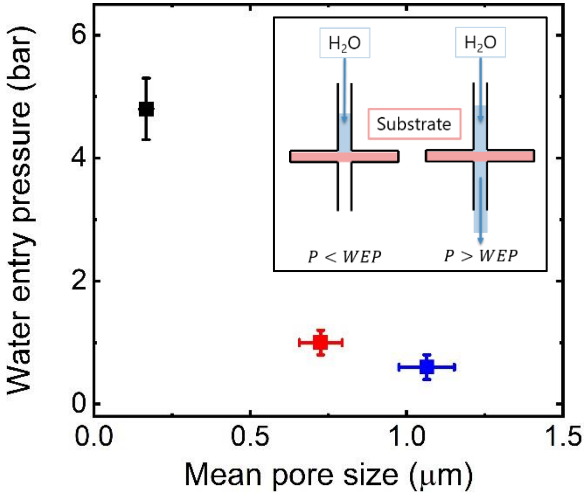
Lower electrolyte penetration leads to higher FE_{CO} and higher stability

Senocrate*, Bernasconi, Rentsch, Kraft, Trottmann, Wichser, Bleiner, Battaglia, *ACS Appl. En. Mat.*, **2022**, 5, 14504.

Substrate pore size and wetting behavior





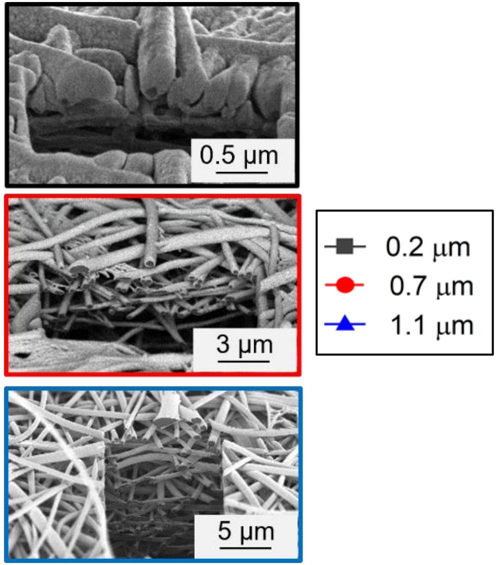


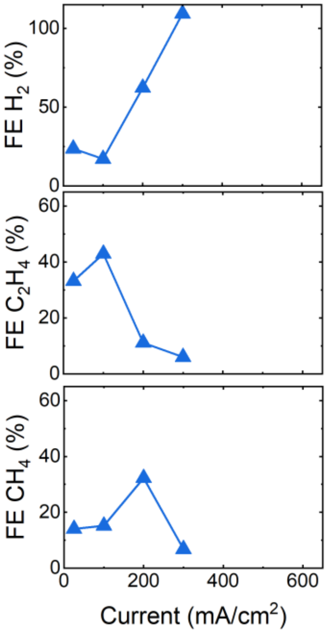
High water entry pressure means lower electrolyte penetration.

Senocrate*, Bernasconi, Rentsch, Kraft, Trottmann, Wichser, Bleiner, Battaglia, *ACS Appl. En. Mat.*, **2022**, 5, 14504.
Bernasconi, Senocrate*, Kraus, Battaglia, *EES Catalysis*, **2023**, 1, 1009.

Cu GDEs: small pore sizes increase $C_{\geq 2}$ production

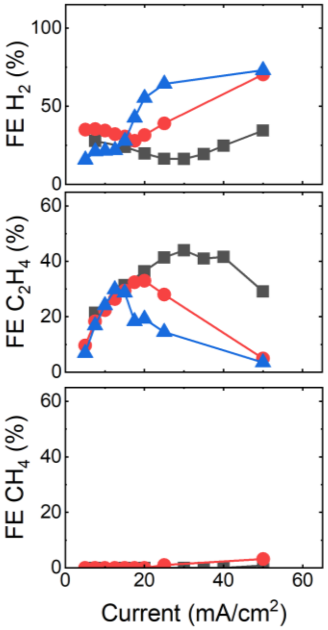
Empa
Materials Science and Technology





eCO$_2$R

1 M KCl
0.5 h avg



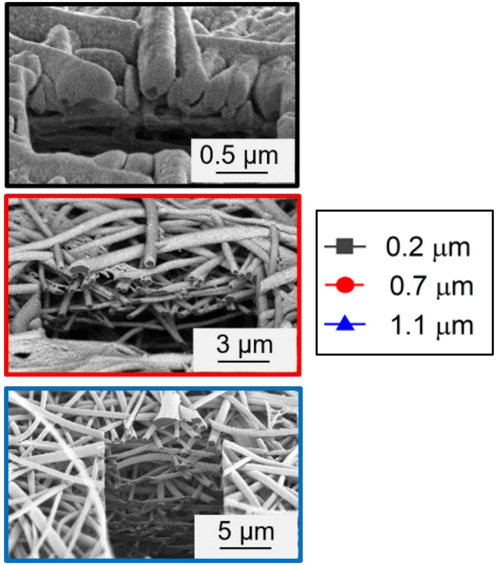
eCOR

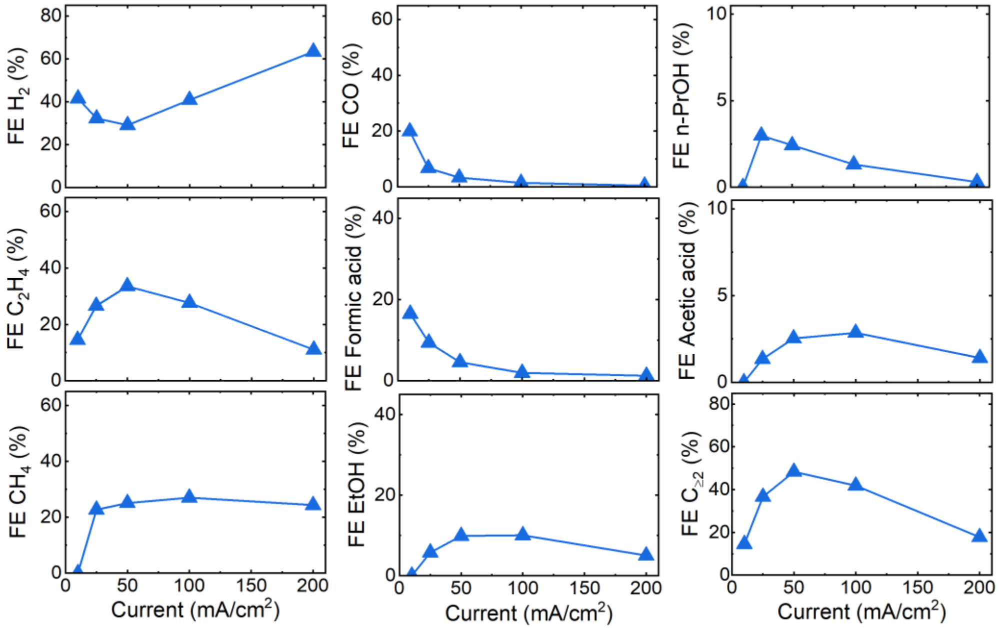
1 M KCl
1 h avg

Cu GDEs with small pore sizes show high $FE_{C\geq 2}$. FE for C_2H_4 exceeds 55 %.

Senocrate*, Bernasconi, Rentsch, Kraft, Trottmann, Wichser, Bleiner, Battaglia, *ACS Appl. En. Mat.*, **2022**, 5, 14504.
Bernasconi, Senocrate*, Kraus, Battaglia, *EES Catalysis*, **2023**, 1, 1009.

Cu GDEs: small pore sizes increase $C_{\geq 2}$ production



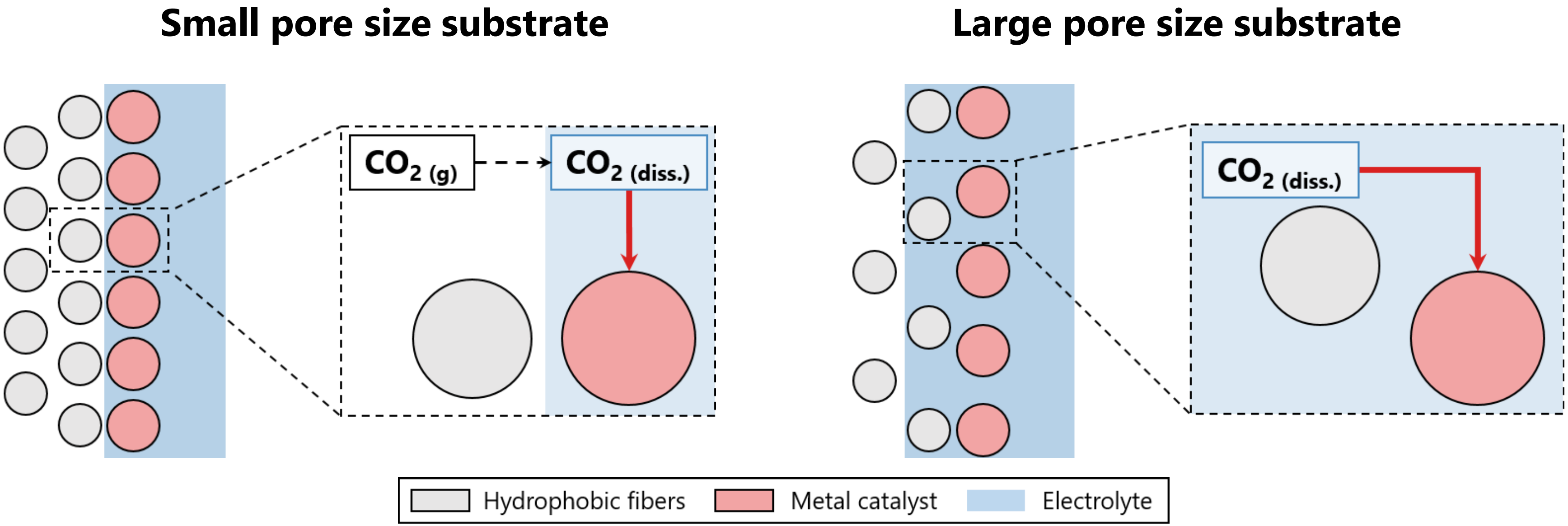


Cu GDEs with small pore sizes show high $FE_{C\geq 2}$. Ag GDE show high FE_{CO}.

Senocrate*, Bernasconi, Rentsch, Kraft, Trottmann, Wichser, Bleiner, Battaglia, *ACS Appl. En. Mat.*, **2022**, 5, 14504.
Bernasconi, Senocrate*, Kraus, Battaglia, *EES Catalysis*, **2023**, 1, 1009.

Proposed mechanism

Empa
Materials Science and Technology



Electrolyte layer thickness controls local CO_2 availability and its mass transport.

Vesztergom, Senocrate*, Kong, Kolivoška, Bernasconi, Zboray, Battaglia, Broekmann, *Chimia*, **2023**, 77, 3.