

GEFÖRDERT VOM



Bundesministerium  
für Bildung  
und Forschung

# CARBON2CHEM®

A Contribution to Sustainable Industries  
Selected Results (2016 – 2020)



# Chemie Ingenieur Technik

Verfahrenstechnik · Technische Chemie · Apparatewesen · Biotechnologie

**10 | 2020**

**Themenheft:**  
Carbon2Chem®  
Teil 2

GEFÖRDERT VOM



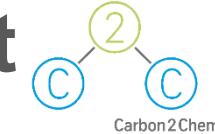
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Görgen Deerberg  
Markus Oles  
Robert Schlägl

**Herausgeber:**  
DECHEMA  
GDCh  
VDI-GVC

**WILEY-VCH**



# Acknowledgement



**Grundlagenforschung**  
Max-Planck-Gesellschaft  
Erforschung der Prinzipien

**Anwendungsorientierte  
Forschung**  
Fraunhofer-Gesellschaft  
Transferforschung

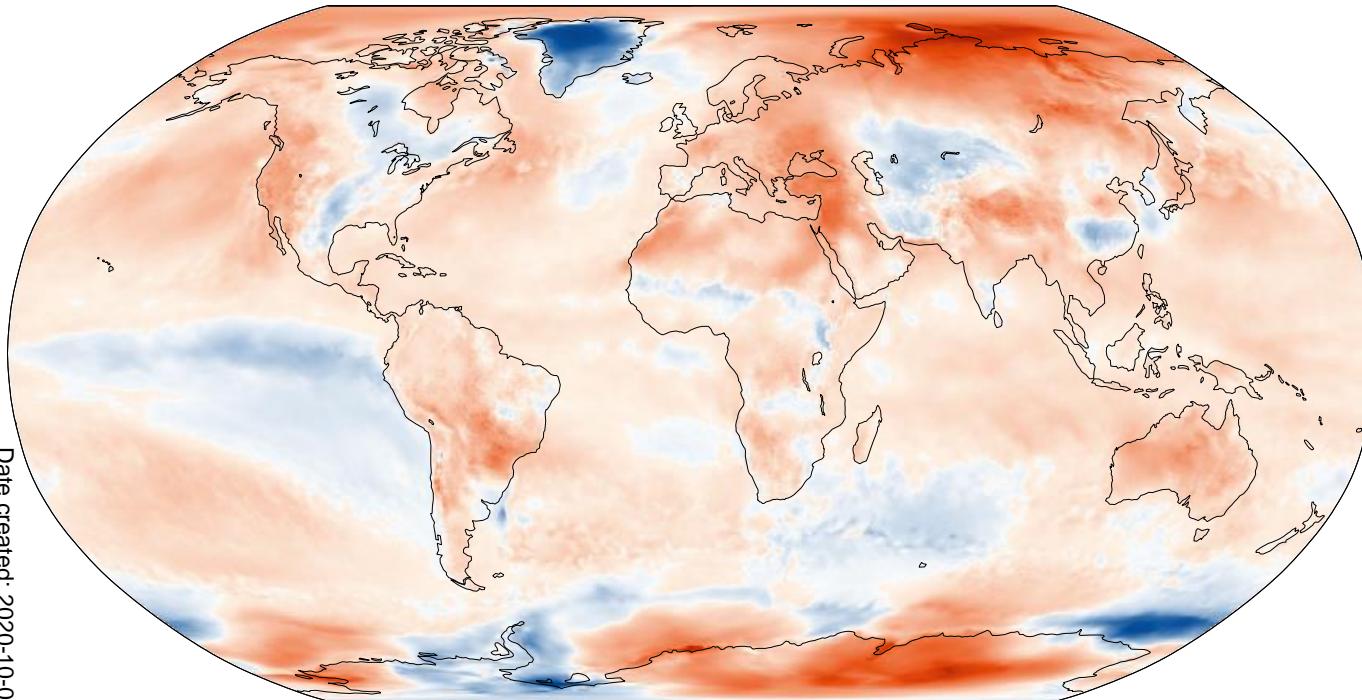


C2C practices with over 250 participants  
the collaboration between science  
organisations, science disciplines and  
across industry sectors on relevant  
scales of dimension and effort.

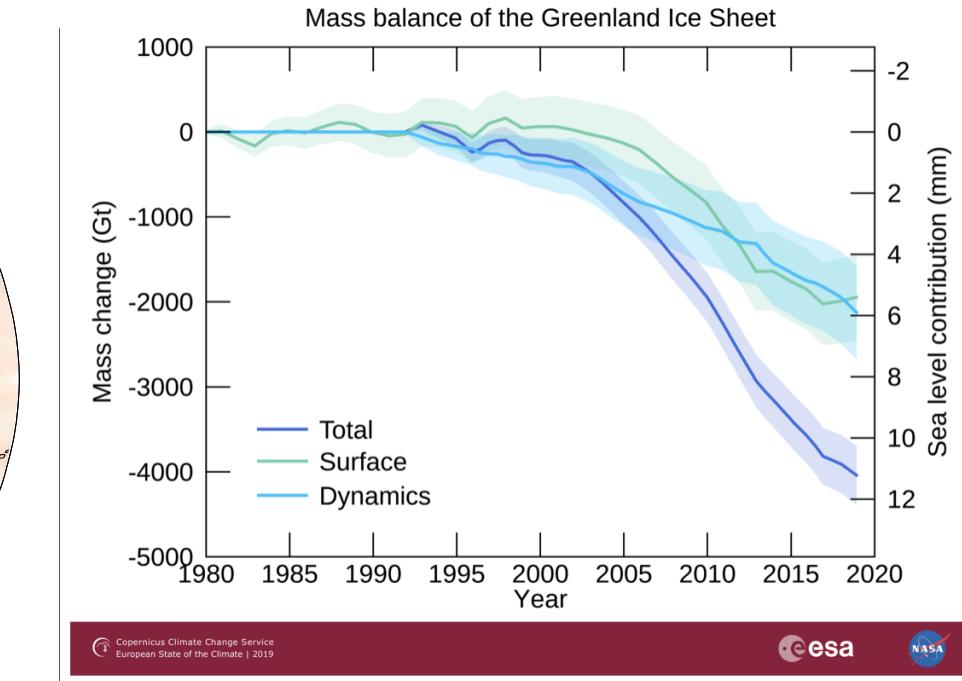
# Stop this now!



## Surface air temperature anomaly for September 2020



(Data: ERA5. Reference period: 1981-2010. Credit:

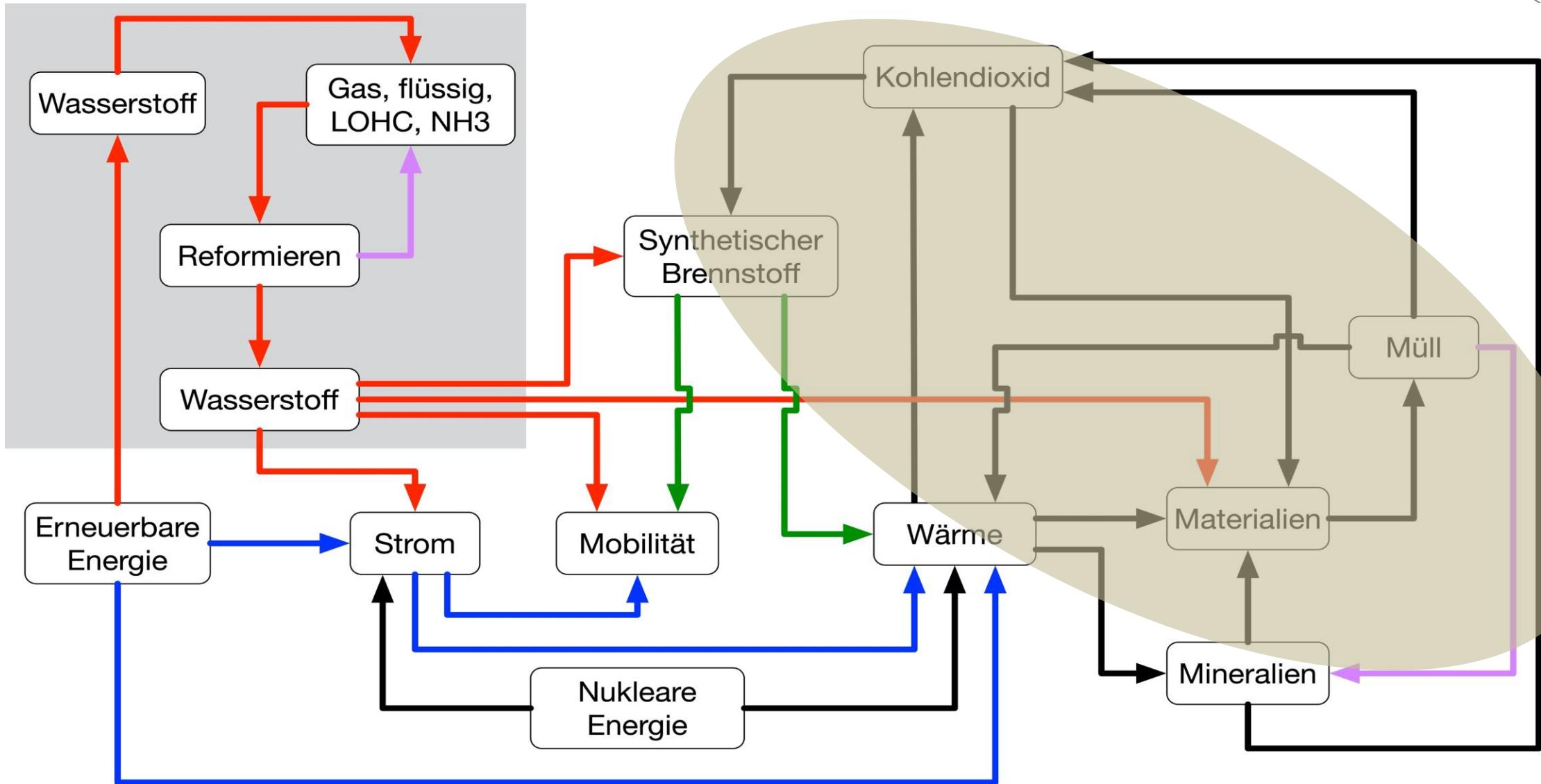


Total cumulative Greenland ice sheet mass change, partitioned into surface and dynamics components. Change relative to 1992. Data source: IMBIE (Shepherd et al., 2020), Credit: IMBIE/ESA/NASA.

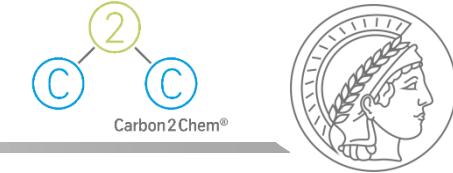


GHG levels rise with 2.5 ppm/a

# A sustainable energy system



# C2C: Put carbon in a loop



Steelmaking in DE

43 Mt/a

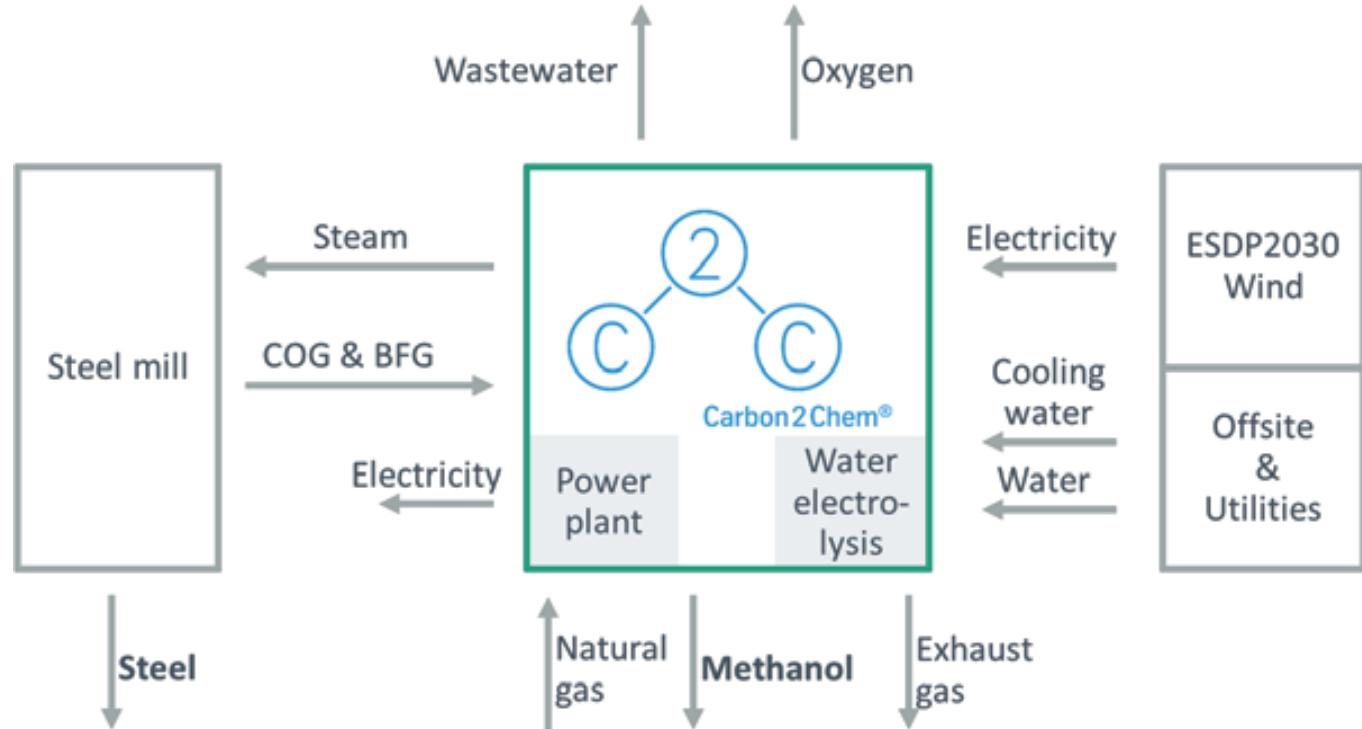
167 TWh Energy

58 Mt CO<sub>2</sub>

0,35 Mt/TWh

(Power DE 0,48 Mt/TWh)

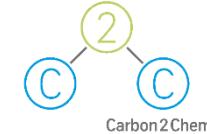
| Final energy<br>2018 | Energy<br>(TWh) | Emission<br>(Mt) |
|----------------------|-----------------|------------------|
| <b>Total</b>         | <b>2492</b>     | <b>704</b>       |
| Industry             | 1085            | 467 (0,43)       |
| Mobility             | 642             | 126 (0,20)       |
| Domestic             | 645             | 83 (0,13)        |
| Air/marine           | 121             | 36 (0,30)        |



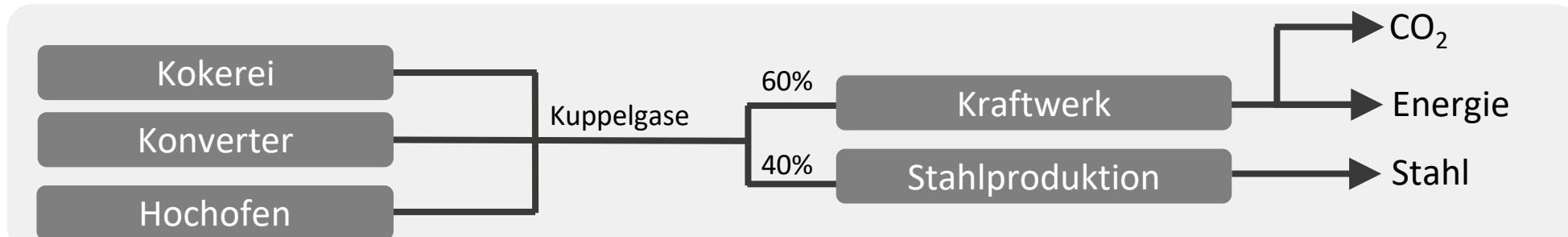
C2C engages further in the synthesis of urea and of selected other chemicals

C2C operates in a system-oriented fashion and knowledge-based.

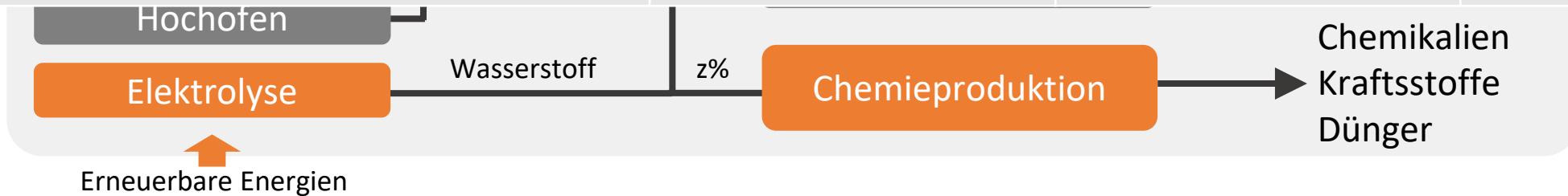
# The tasks



## Aktuell: Integrierte Hütte

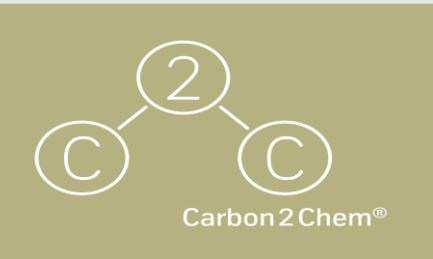


| Komponenten                          | Koksofengas               | Hochofengas                 | Konvertergas              |
|--------------------------------------|---------------------------|-----------------------------|---------------------------|
| Stickstoff (N <sub>2</sub> )         | 5%                        | 49%                         | 14%                       |
| Wasserstoff (H <sub>2</sub> )        | 61%                       | 4%                          | 4%                        |
| Kohlenstoffmonoxid (CO)              | 6%                        | 25%                         | 65%                       |
| Kohlenstoffdioxid (CO <sub>2</sub> ) | 2%                        | 23%                         | 17%                       |
| Menge (Bsp. Hütte Duisburg)          | 180 000 m <sup>3</sup> /h | 2 000 000 m <sup>3</sup> /h | 100 000 m <sup>3</sup> /h |



# Project Coordination

Prof. Dr.-Ing. Görge Deerberg, Fraunhofer UMSICHT  
Dr. Markus Oles, thyssenkrupp  
Prof. Dr. Robert Schlögl, MPI-CEC



## L-KK

### Coordination and Communication

Fraunhofer UMSICHT  
MPI-CEC



## L-O

### System-Integration

thyssenkrupp

Fraunhofer UMSICHT | MPI-CEC | Siemens AG | Siemens Gas and Power

## L-I

### CO<sub>2</sub>-Sources

thyssenkrupp  
  
Fraunhofer UMSICHT  
Lhoist Rheinkalk Germany  
Remondis  
Thyssen  
Vermögensverwaltung

## L-II

### Methanol

Nouryon  
  
Clariant  
Fraunhofer ISE  
Fraunhofer UMSICHT  
Ruhr-Universität Bochum  
thyssenkrupp

## L-III

### Synthesis Gas

Linde  
  
Clariant  
Fraunhofer UMSICHT  
Ruhr-Universität Bochum  
thyssenkrupp

## L-IV

### Higher Alcohols

Evonik  
  
Fraunhofer UMSICHT  
Ruhr-Universität Bochum  
RWTH Aachen  
thyssenkrupp Industrial Solutions

## L-V

### Carbon2Polymers

Covestro  
  
MPI-KoFo  
RWTH Aachen

## L-VI

### Synthetic Fuels

N.N.

## Carbon2Chem® laboratory

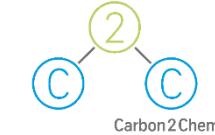
Fraunhofer UMSICHT | MPI-CEC

## Carbon2Chem® technical shop

thyssenkrupp

Organizational chart Carbon2Chem®

# Alternative Industrial CO<sub>x</sub> Sources



## Steel making

Alternative Processes

Direct reduction with CO/H<sub>2</sub>

Direct reduction with H<sub>2</sub> (future)

In each process like in the blast furnace process tail gasses result in substantial quantities with albeit greatly varying composition.

Use the modular C2C technology train to deal with them in a systemically most effective manner.

## Unavoidable point sources

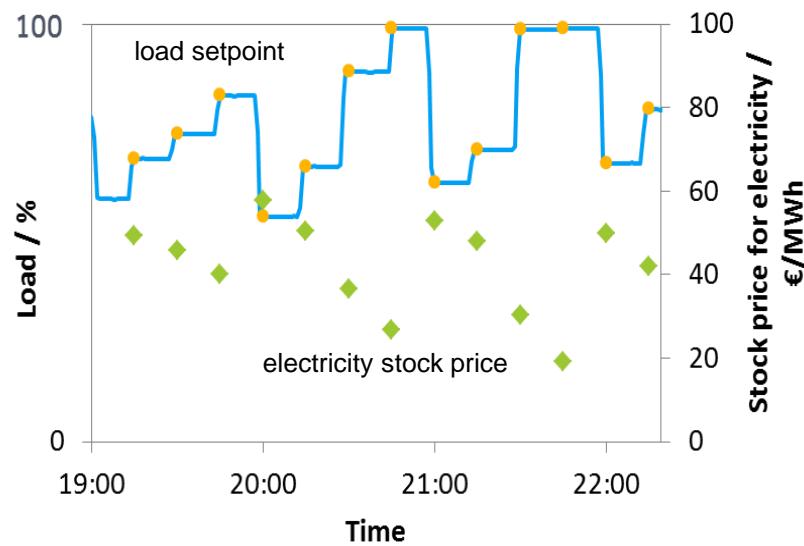
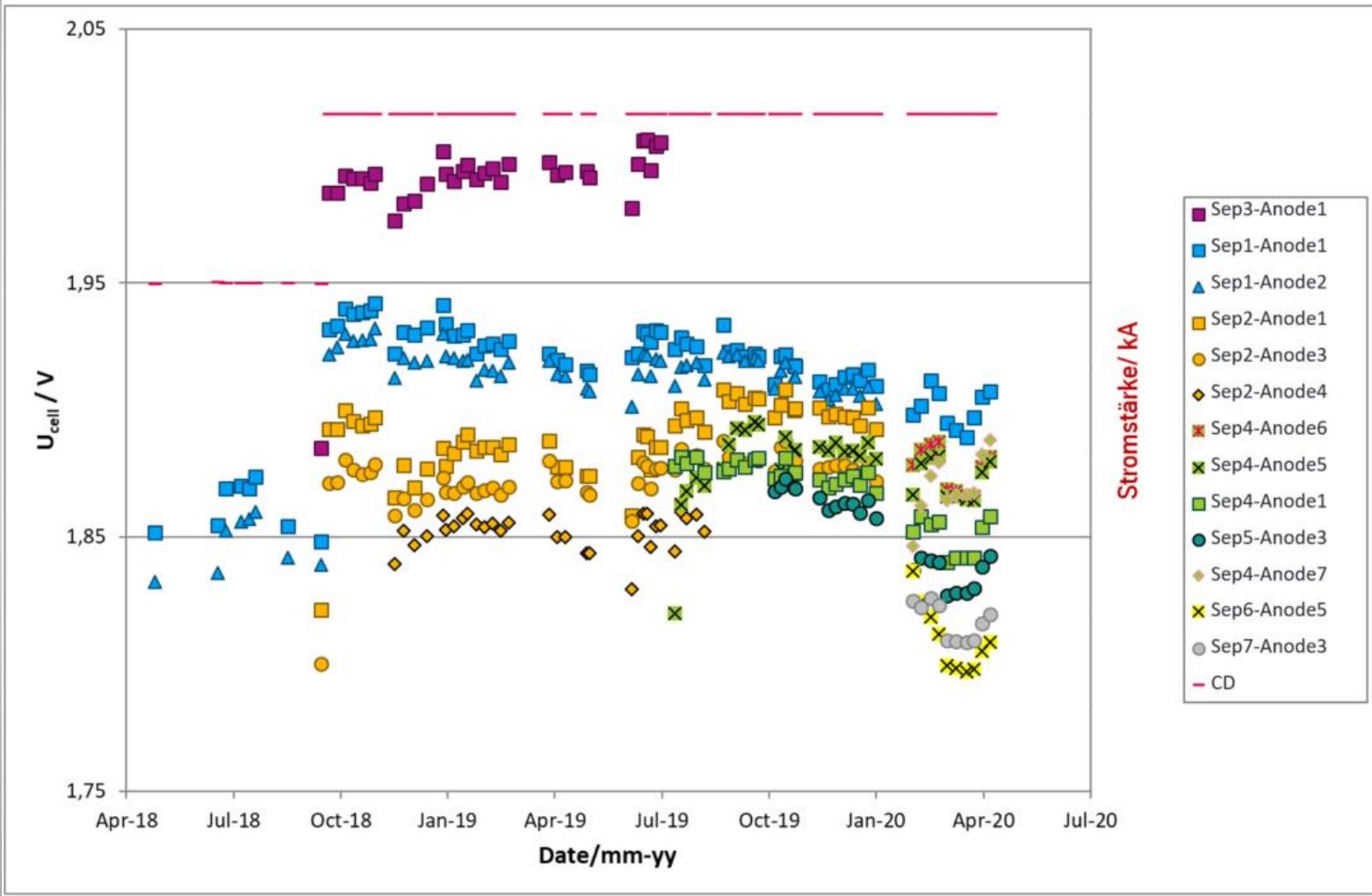
Cement/ lime production

Waste incineration.

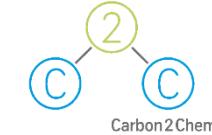
Use the modular C2C technology train to synthesize e-kerosene und *Syn Fuels* for heavy duty applications.

**C2C sets up prototypical circular economies with carbon**

# The Electrolyzer (AEL)



# Cost of Hydrogen for Industry



| Production costs AEL 2030 (€ t <sup>-1</sup> H <sub>2</sub> ), CAPEX 450 € kW <sup>-1</sup> |       |       |       |       |       |       |
|---|-------|-------|-------|-------|-------|-------|
| Load factor   | 25 %  | 40 %  | 50 %  | 60 %  | 75 %  | 90 %  |
| 25 €/MWh  | 3,600 | 2,800 | 2,500 | 2,300 | 2,100 | 2,000 |
| 40 €/MWh  | 4,400 | 3,500 | 3,200 | 3,000 | 2,800 | 2,700 |
| 50 €/MWh  | 4,800 | 4,000 | 3,700 | 3,500 | 3,300 | 3,200 |
| 60 €/MWh  | 5,300 | 4,500 | 4,200 | 4,000 | 3,800 | 3,700 |
| 75 €/MWh  | 6,100 | 5,200 | 5,000 | 4,800 | 4,600 | 4,400 |
| 100 €/MWh   | 7,300 | 6,500 | 6,200 | 6,000 | 5,800 | 5,700 |
| 125 €/MWh   | 8,600 | 7,700 | 7,400 | 7,200 | 7,000 | 6,900 |

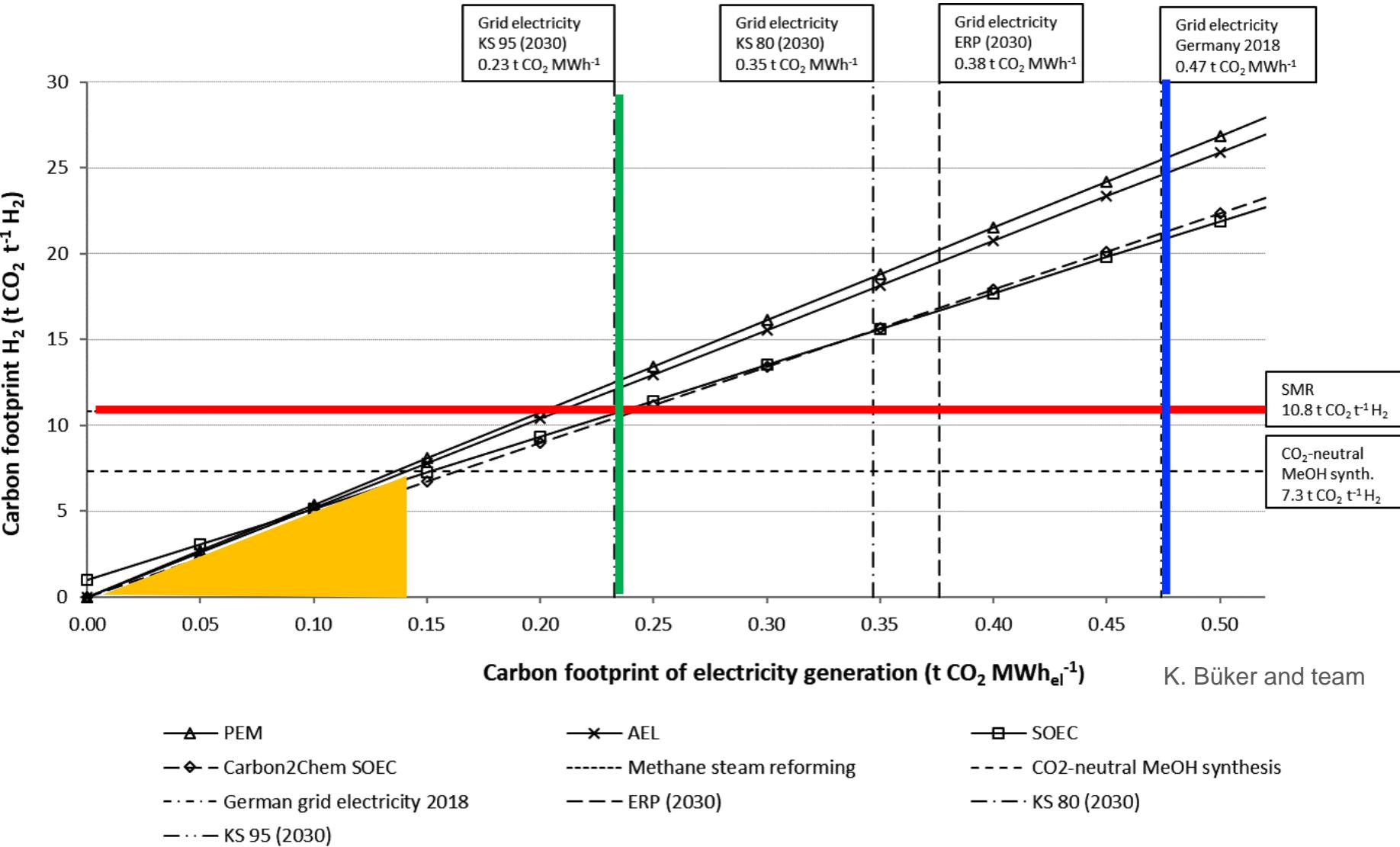
| Production costs PEM 2030 (€ t <sup>-1</sup> H <sub>2</sub> ), CAPEX 810 € kW <sup>-1</sup> |        |       |       |       |       |       |
|---|--------|-------|-------|-------|-------|-------|
| Load factor   | 25 %   | 40 %  | 50 %  | 60 %  | 75 %  | 90 %  |
| 25 €/MWh  | 5,300  | 4,000 | 3,500 | 3,200 | 2,900 | 2,700 |
| 40 €/MWh  | 6,200  | 4,800 | 4,400 | 4,100 | 3,800 | 3,600 |
| 50 €/MWh  | 6,700  | 5,400 | 4,900 | 4,600 | 4,300 | 4,100 |
| 60 €/MWh  | 7,300  | 5,900 | 5,500 | 5,200 | 4,900 | 4,600 |
| 75 €/MWh  | 8,100  | 6,700 | 6,300 | 6,000 | 5,700 | 5,500 |
| 100 €/MWh   | 9,400  | 8,100 | 7,600 | 7,300 | 7,000 | 6,800 |
| 125 €/MWh   | 10,800 | 9,500 | 9,000 | 8,700 | 8,400 | 8,200 |

K. Büker and team

Cost depends critically on power price (political) and on load factor. CAPEX is an additional factor that can be improved by industrial manufacturing.

In DE today barely possible to generate economically green hydrogen (different in other European countries): DE has a critical disadvantage here.

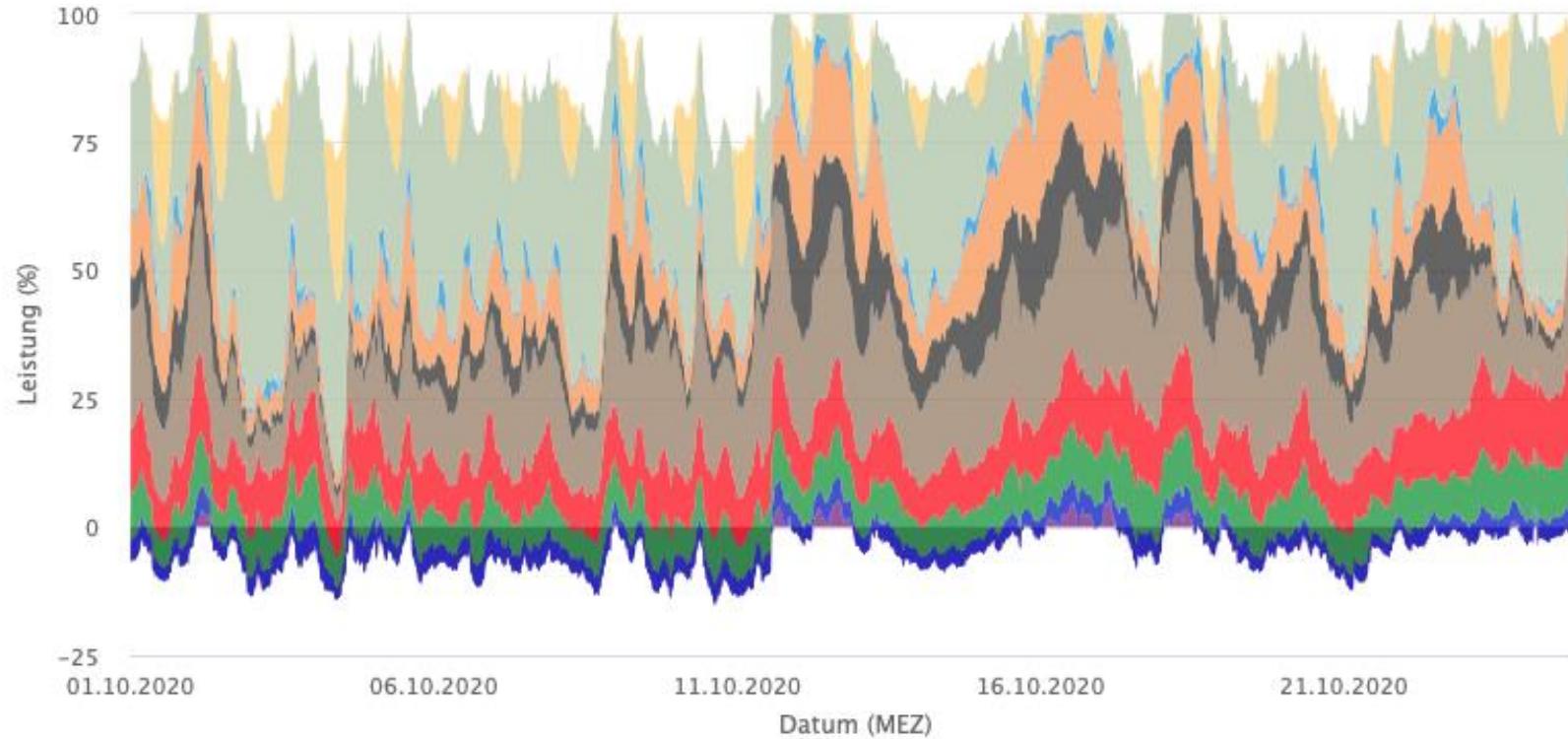
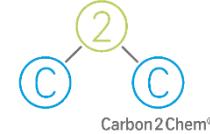
# Electrolysis and Power Mix



Water splitting for „green“ hydrogen is within the coming decade not feasible in DE.

Taking coal out of the power system is of utmost priority far more than agreed in legislation.

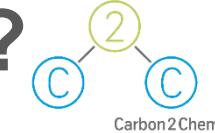
# Volatility and RES expansion in the German Power System



Quelle:  
Fraunhofer ISE  
Energy Charts  
Oktober 2020

The present power system in DE reaches its limits in dealing with volatile RES. More RES could allow some hydrogen generation (planned 5GW) but only when grid infrastructure and pipelines are suitably interconnected and upgraded now.

# Where from will we get sufficient hydrogen?

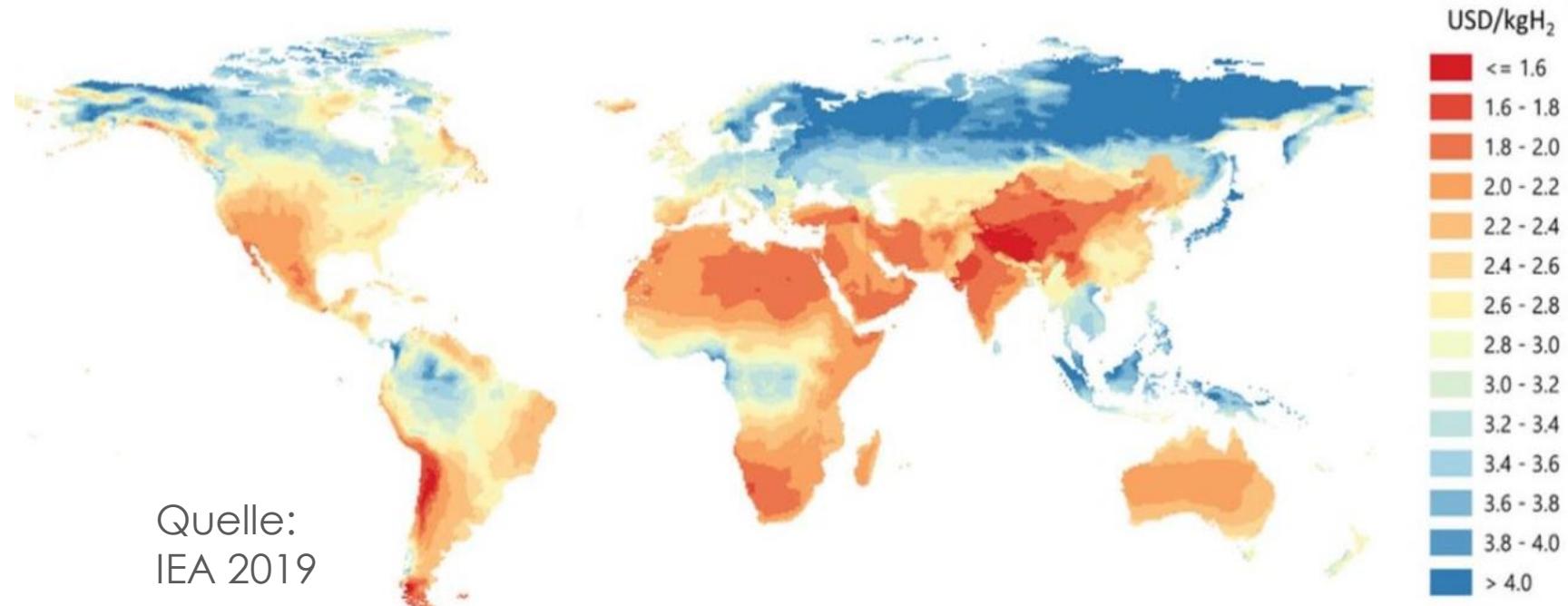


Transport of hydrogen through derivatives (e-fuels) is a small contribution to cost.

Transport forms induce substantial energy losses.

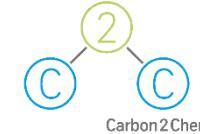
Tolerable by the vast excess of available energy and improved processes.

Mind non-technical consequences of this global technology.



Science and Technology are needed now

# Chemistry in C2C



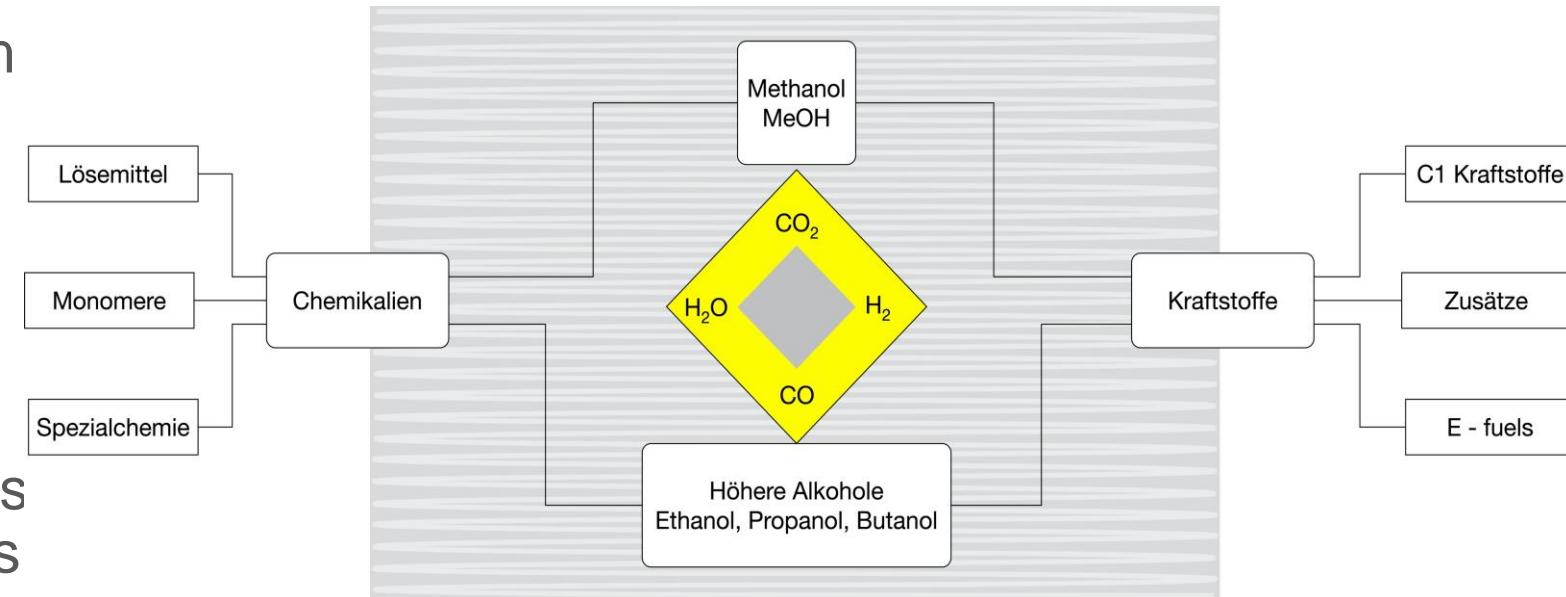
Alcohols are versatile platform molecules for future and changing markets.

They are well accessible from CO<sub>2</sub> and hydrogen.

MeOH is today a 80Mt/a commodity chemical.

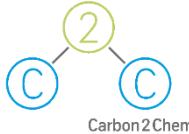
Higher alcohols from synthesis gas /MeOH by heterogeneous catalysis are novel products on technical scales. C2C contributes substantially to this endeavour.

In the Franco-German sister project CatVic novel concepts of olefin synthesis from CO<sub>2</sub> at a chemical parc are being explored.

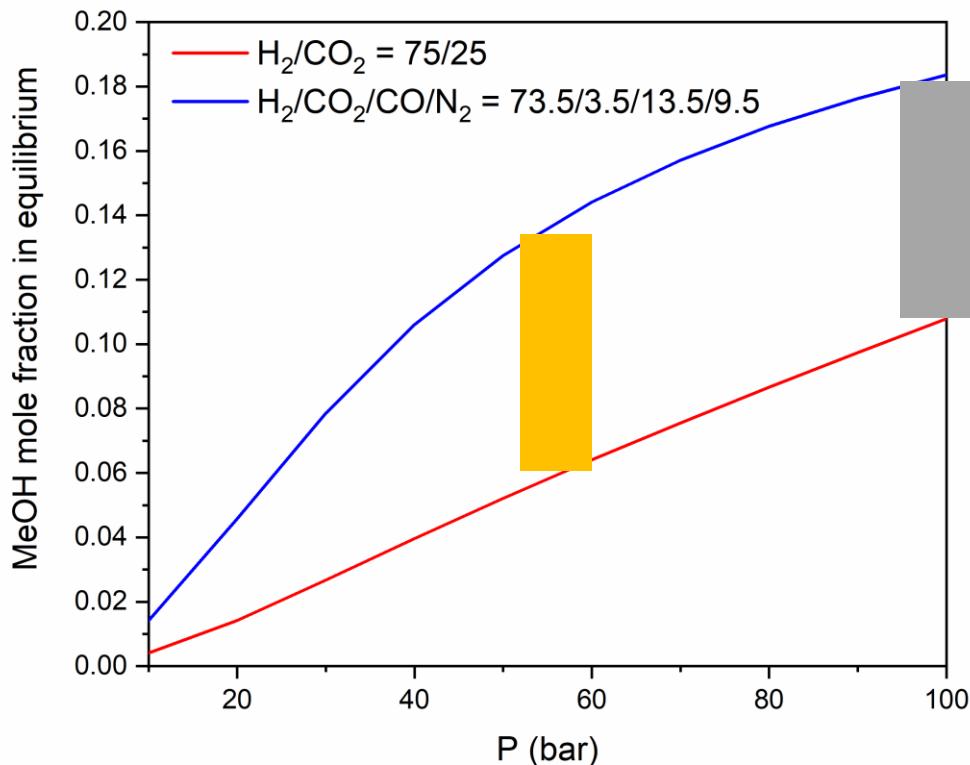


In addition, C2C deals with various pathways to urea, the synthesis of monomers for polymers and with the exploration of innovative process concepts using molecular catalysis.

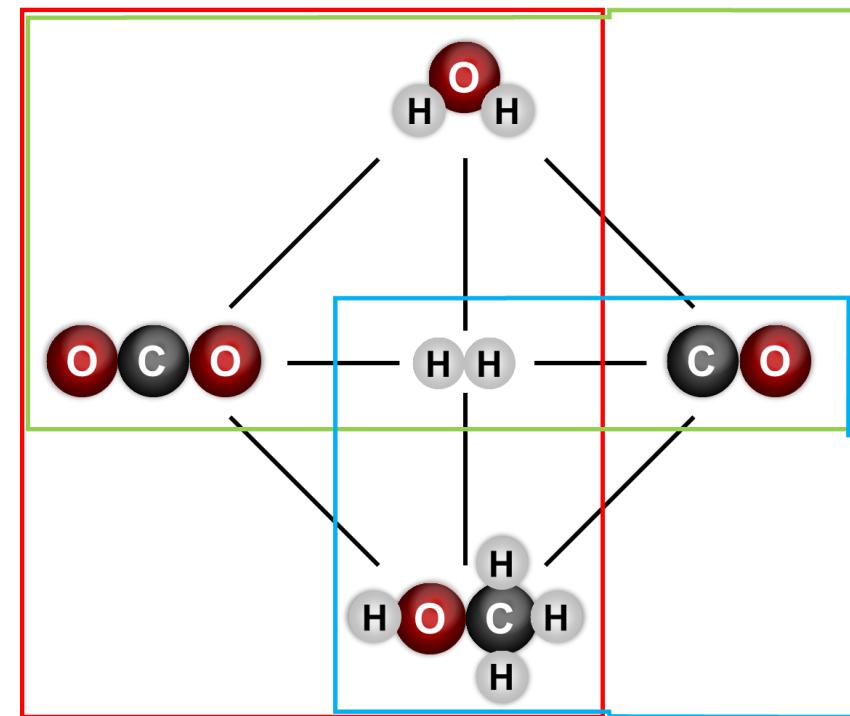
# Methanol Synthesis: Opportunity and Limitation



Synthesis of MeOH requires for thermodynamic reasons a recycle strategy (breakthrough alternatives are searched in the C2C lab). Critical are usage of hydrogen and accumulation of inerts and catalyst poisons.



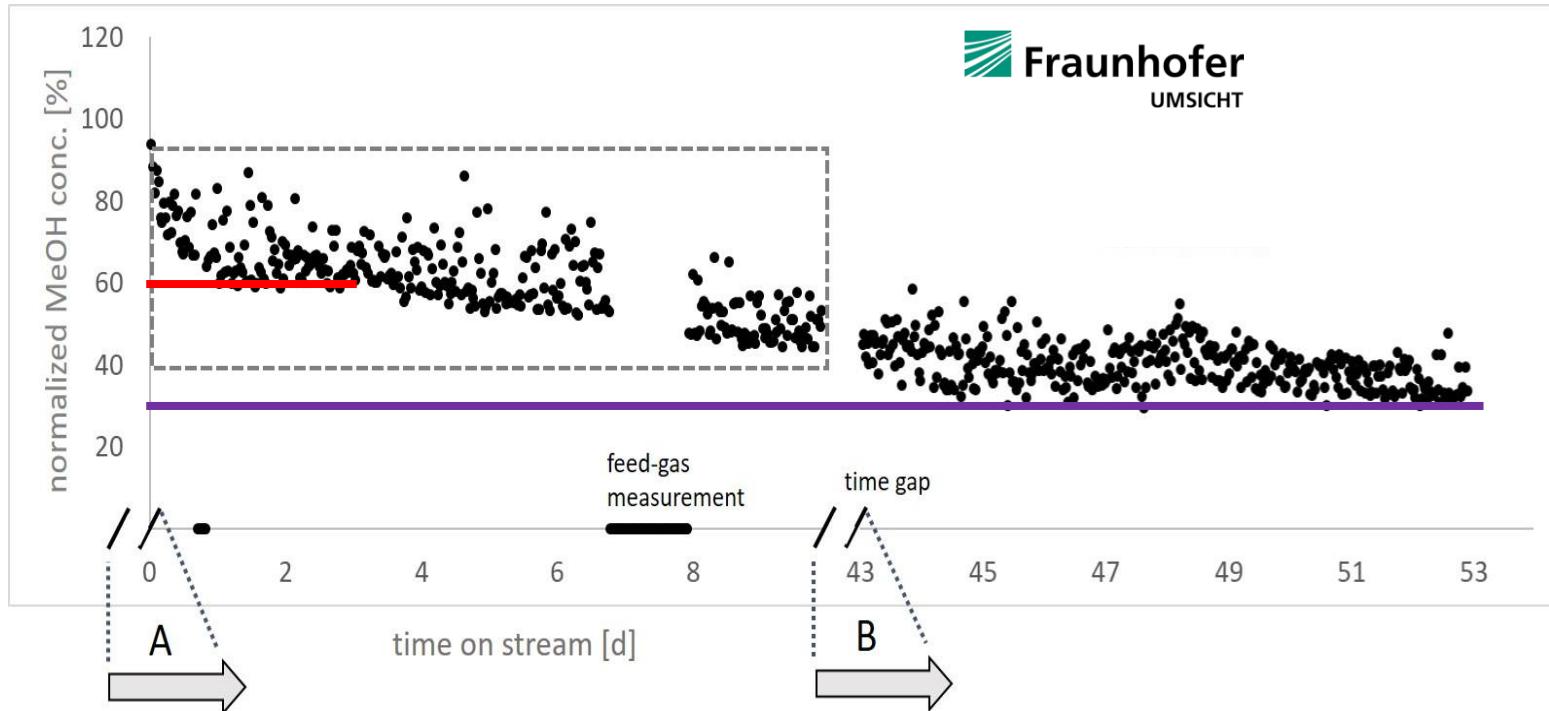
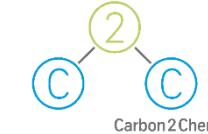
Complex optimization of pressure, recycle scheme and gas cleaning strategy to achieve stable and cost-effective process.



Case 1: H<sub>2</sub>:CO<sub>2</sub> = 3:1, T = 250°C, P = 10-100 bar

Case 2: 13.5% CO, 3.5% CO<sub>2</sub>, 73.5% H<sub>2</sub>, 9.5% N<sub>2</sub>, T = 250°C, P = 10-100 bar

# Methanol Synthesis: Beware of Unsuitable Conditions



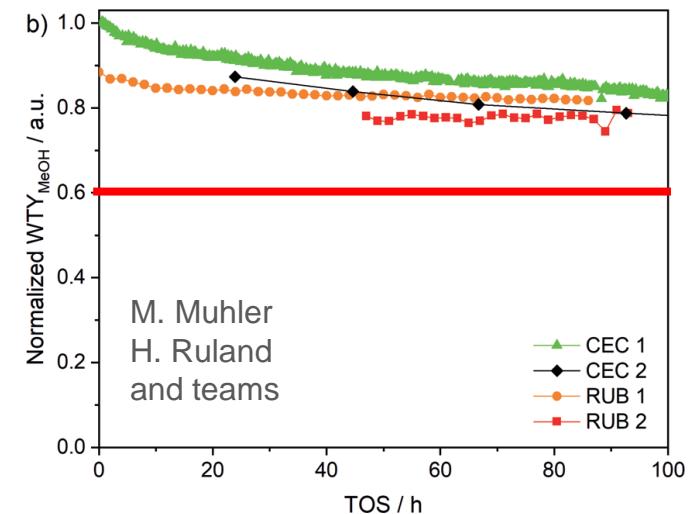
A:

- 1) 4 days reference-gas test
- 2) 2 days down-time
- 3) 1 day reference-gas test

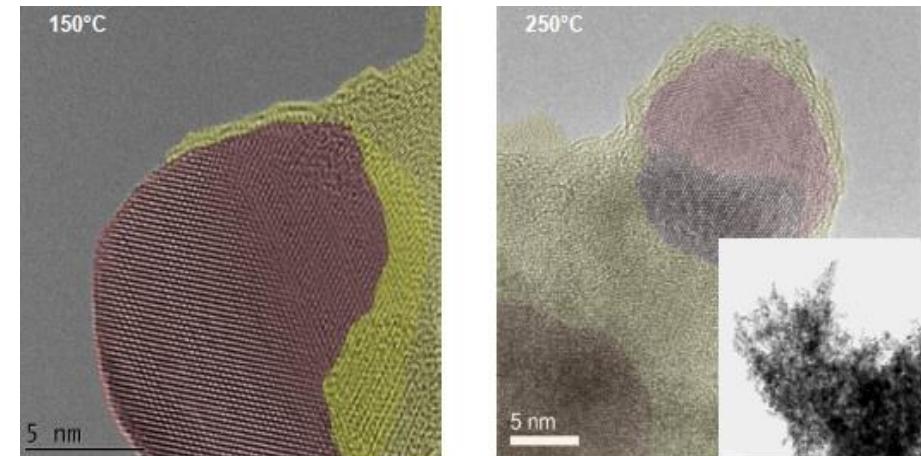
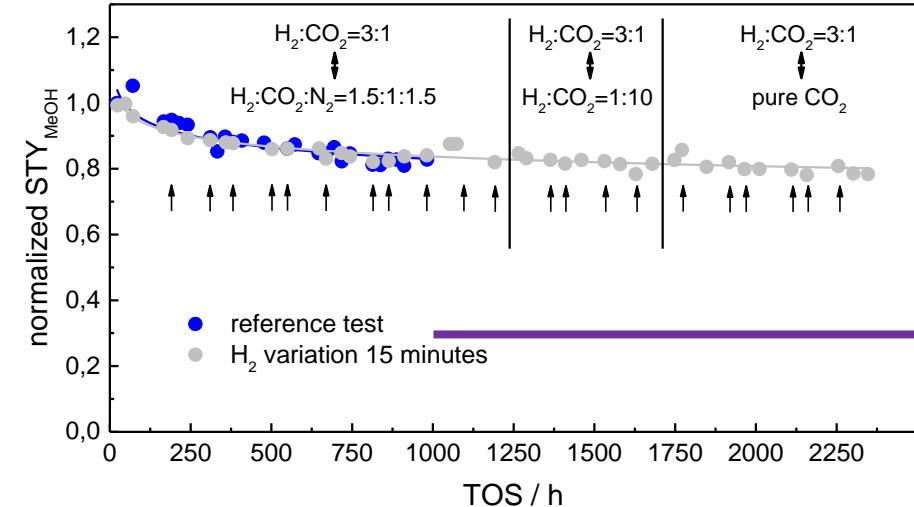
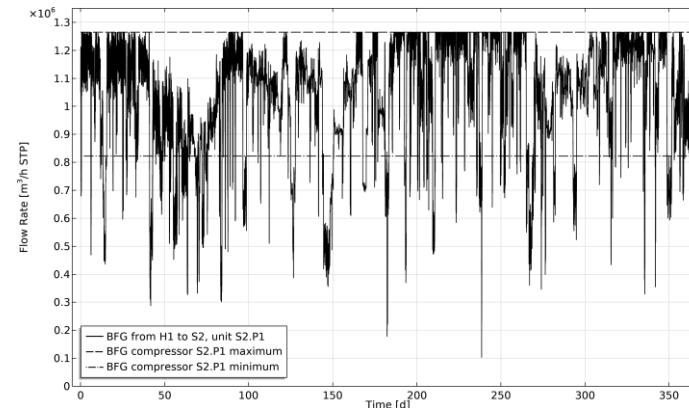
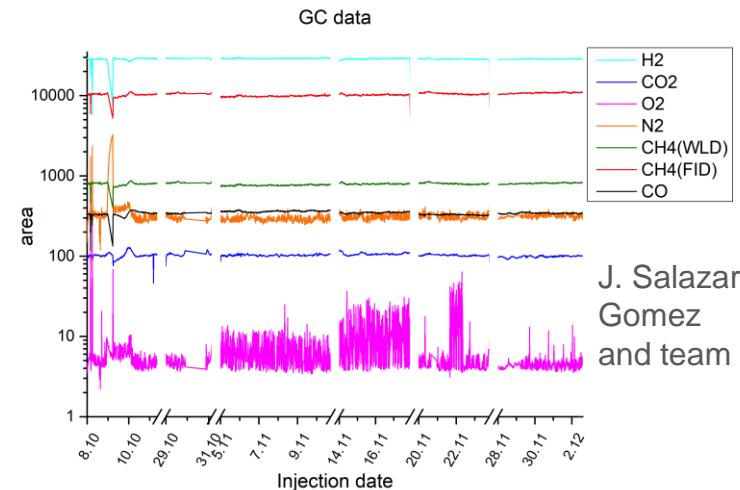
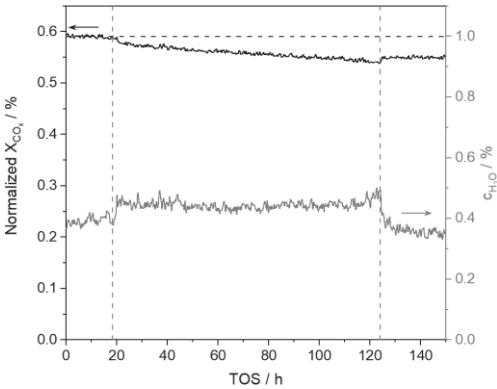
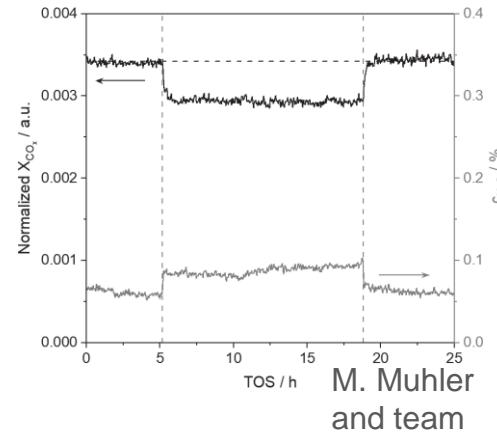
B:

- 1) 4 days reference-gas test
- 2) 2 days synthetic H<sub>2</sub>-enriched Blast-Furnace-Gas
- 3) 27 days down-time

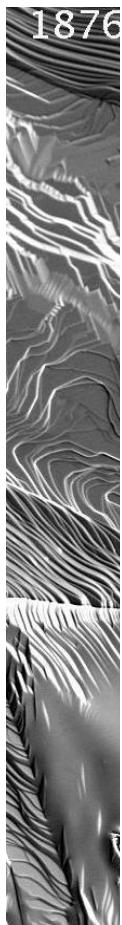
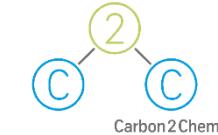
BFG enriched with additional H<sub>2</sub>, S<sub>N</sub>=2.4  
 10.3% CO, 9.5% CO<sub>2</sub>, 58.6% H<sub>2</sub>, 23.4% N<sub>2</sub>, T = 250°C, P = 84 bar



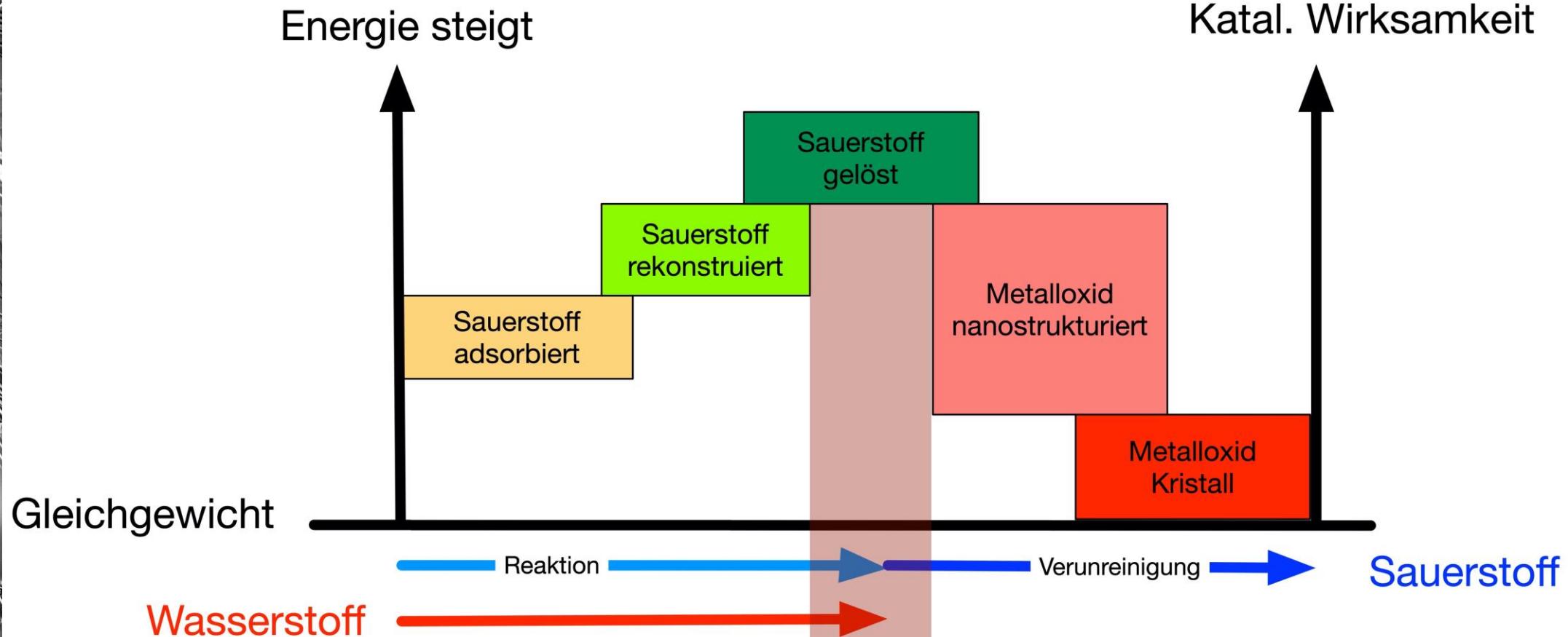
# MeOH Synthesis: Dynamics and Deactivation



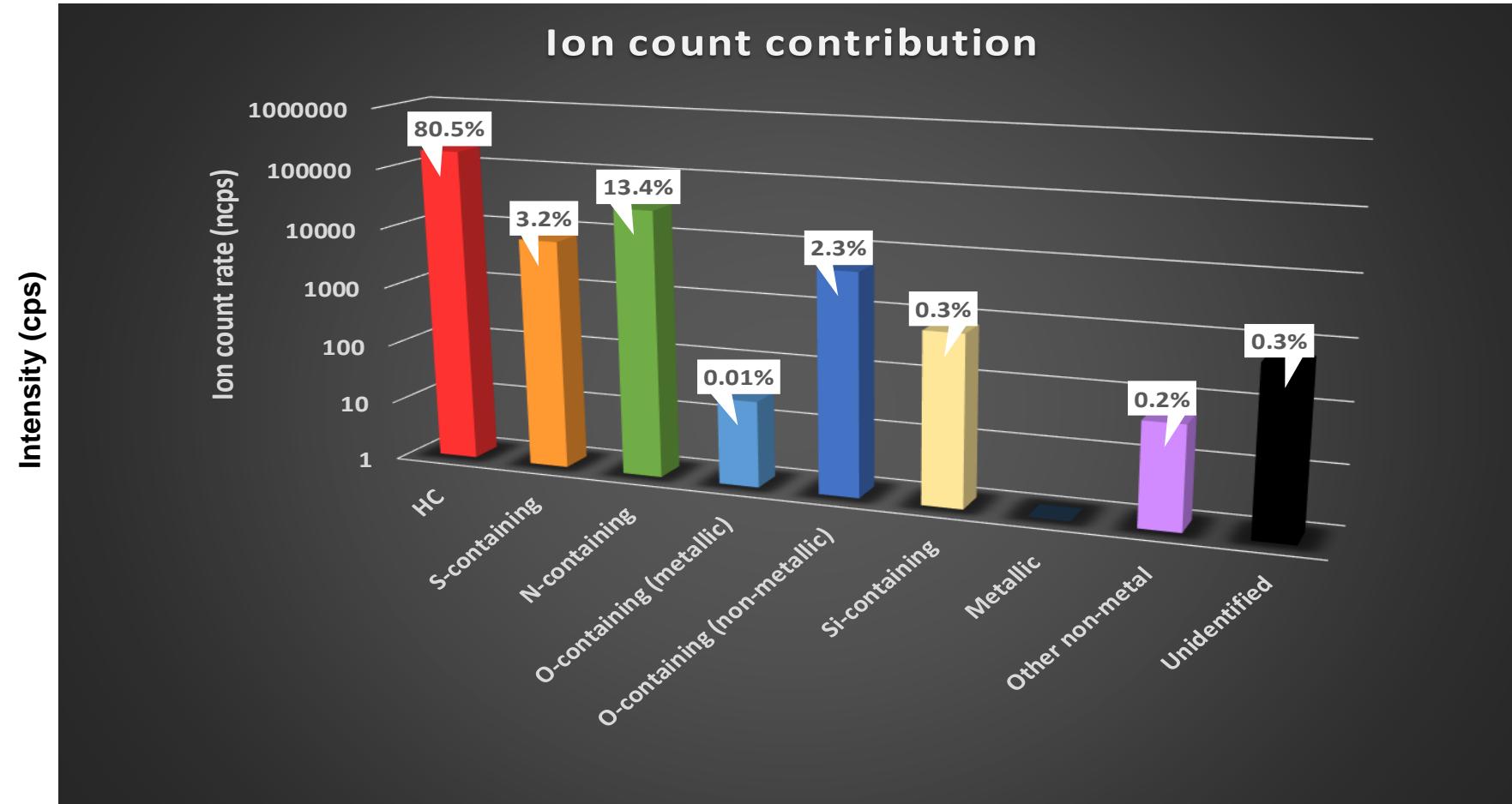
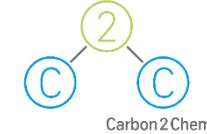
# The Dynamical Catalyst ( $\text{Cu}, \text{H}_2, \text{O}_2, 673 \text{ K}$ )



1876



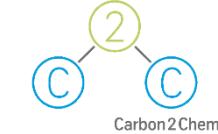
# Trace gas analysis



Design and validation of a multi-component ultra-sensitive on-line probing instrumentation based upon the PTR-MS-TOF technique. More than 540 components were identified and mapped in their compositional dynamics.

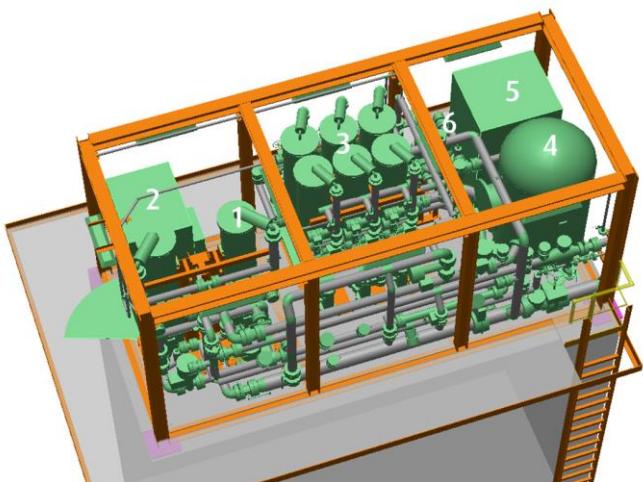
# Gas cleaning (Linde)

## Scaling of MeOH synthesis (Fraunhofer)



Gas cleaning has to purify the dynamical gas flows to an optimum between cost and stability of downstream processing.

Innovative process designs and electrostatic desorption are tested and plasma technologies are validated.

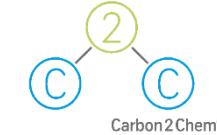


- Voradsorber<sup>1</sup>
- Schaltschrank<sup>2</sup>
- DWA<sup>3</sup> (6 Adsorber)
- Restgaspuffer<sup>4</sup>
- Analysenschrank<sup>5</sup>
- DeOxo (Produkt)<sup>6</sup>

Re-vamping and validation of a MeOH synthesis pilot plant demonstrating industrial production concepts. It includes closing all material streams and implements industrial energy flow patterns. Connection of its performance to laboratory experiments (downscaled version by MPI for dynamic operation testing). Real feed gas early next year.



# Summary C2C



Defossilising steel making creates large demands for RES that will need import and exchange of hydrogen within Europe.

The scientific and systemic basis for C2C in the steel industry and in related applications is verified leading now to process design.

Present RES availability in Germany impedes scaled roll out of any „green“ steel technology without imports.

The C2C technology basis is sound and firm; challenges in dynamic operation and in unusual feed compositions were addressed and solved.

The C2C technology is generic for steelmaking and other industries with unavoidable carbon emissions.

Implementation of larger demonstrators for different usage scenarios should be started now; different energy systems throughout the EU call for collaborative action in critical dimensions ( $10^4$  t/a). C2C is ready for that!

Only then the closure of the carbon circular economy can be demonstrated with downstream processing of platform chemicals to materials and fuels.



1. Understand that CCU is an element of future energy systems; implement technology-openness (REDII!).
2. Implement now circular economy for carbon; close the loop for mobility without double counting.
3. A CO<sub>2</sub> pricing mechanism is needed for carbon in all energy sectors EU wide.
4. A reliable and long-term stable price is needed for industrial power.
5. Large quantities (5000 TWh) of certified hydrogen with free exchange within the EU need to be available.
6. Create now a trans-European infrastructure with high availability and maximal operational safety as critical first step.

Albert Einstein

There is no fundamental law requiring simplicity in natural processes



We cannot solve our problems with the same thinking we used when we created them

Thank You