DLFCs:
Activities – Status – Outlook

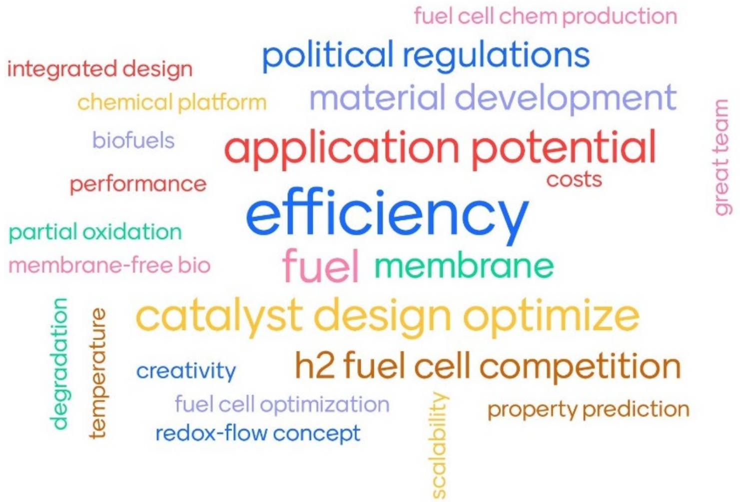
A. K. Mechler

Strategy Meeting 07/06/2023

FSC The Fuel Science Center | AVT Aachener Verfahrenstechnik | LTT Lehrstuhl für Technische Thermodynamik | tme Lehrstuhl für Thermodynamik mobiler Energiewandlungssysteme | RWTH AACHEN UNIVERSITY

Activities in the field of DLFCs

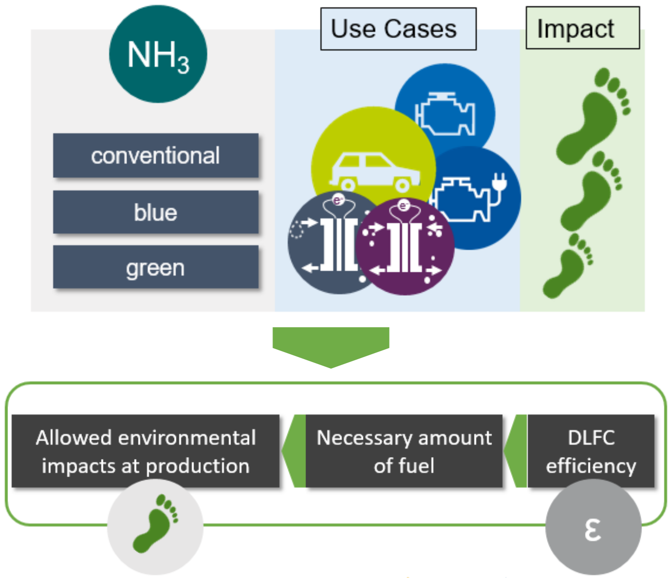
Workshop



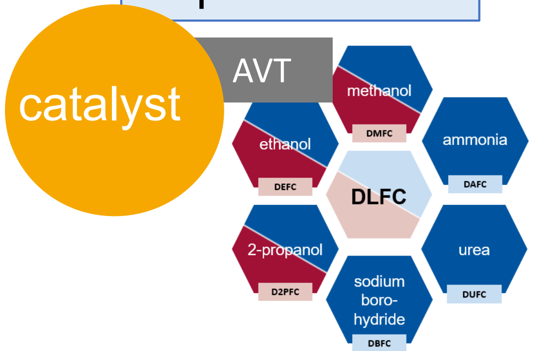
ERS PrepFund (DLFC Part)

Life Cycle Assessment

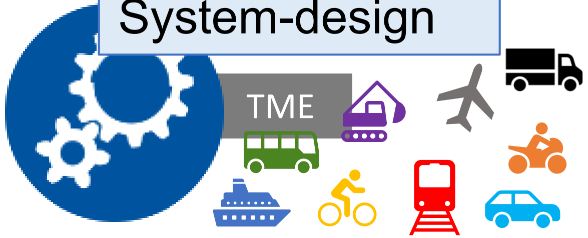
LTT



Experimental



System-design



Potential evaluation

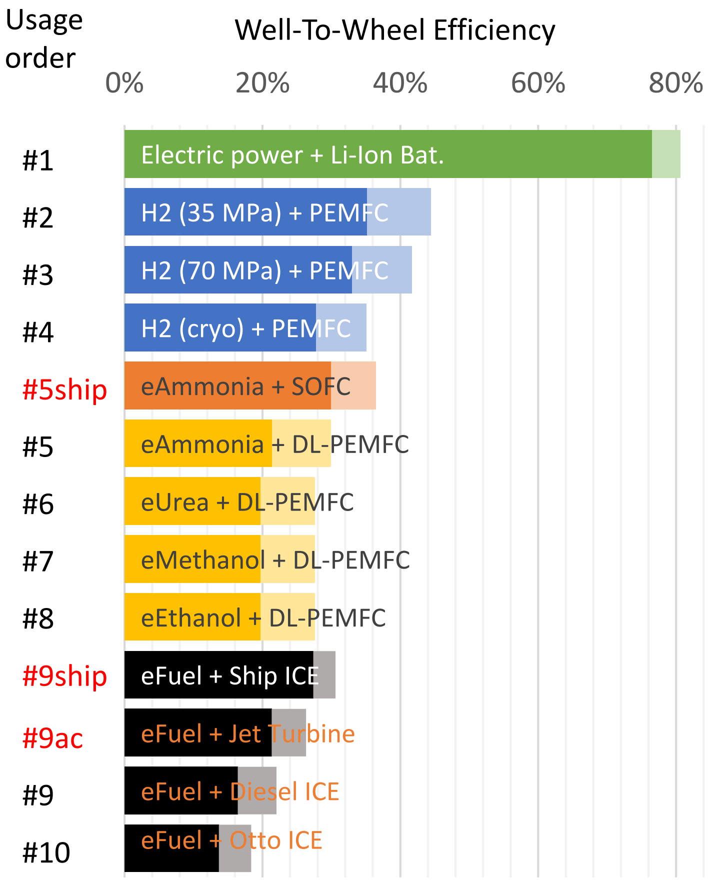
Status - Identification of Potential Applications

TME

System Design
- Direct hydrogen FC
- Indirect Hydrogen FC
- Direct Liquid FC

Comparision by
- Energy density
- Conversion efficiency
- Storage efficiency

Future propulsion technology
- Energy power
- Fuel storage capacity

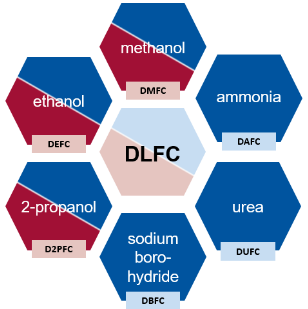


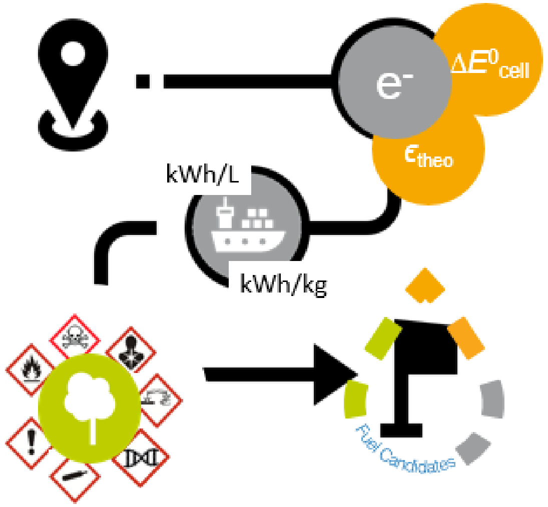
Potential use cases identified

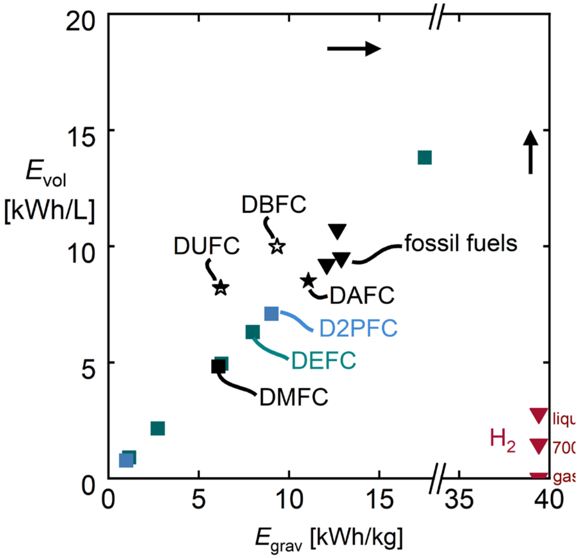
Mobility Segment	Propulsion Technology small ↔ large
Aircrafts	
Ships	
Trains	
Busses	
Commercial Cars	
Passenger Cars	
Construction	
Motorcycles	
Micro Mobility	

Outlook: Comparative Cost Analysis of Sustainable Propulsion Technologies

Status - Fuel selection





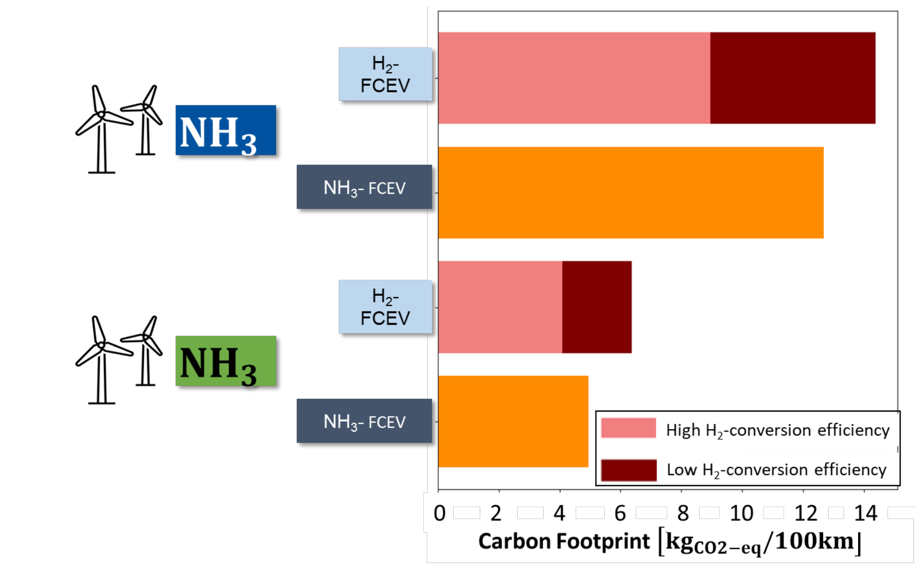


	acidic	E_{cell}/V		alkaline	E_{cell}/V
			93%	DEGFC-O_2 (4*)	0.87
95%	DEFC-O_2 (2*)	0.98	95%	DEFC-O_2 (2*)	0.98
98%	D2PFC-O_2 (2*)	1.10	98%	D2PFC-O_2 (2*)	1.10
97%	D2PFC-O_2 (18)	1.12			
97%	D1PFC-O_2 (18)	1.13			
97%	DEFC-O_2 (12)	1.14	97%	DEFC-O_2 (12)	1.14
92%	DEFC-O_2 (4*)	1.17	84%	DUFC-O_2 (10)	1.16
95%	DDEFC-O_2 (12)	1.20	89%	DAFC-O_2 (6)	1.17
97%	DMFC-O_2 (6)	1.21	97%	DMFC-O_2 (6)	1.21
99%	DEGFC-O_2 (10)	1.22			
83%	PEM-O_2 (2)	1.23	83%	AFC-O_2 (2)	1.23
96%	DDMFC-O_2 (16)	1.23	94%	DEGFC-O_2 (8*)	1.27
102%	DTFC-O_2 (12)	1.34	59%	DGFC-O_2 (12)	1.31
106%	DFAFC-O_2 (2)	1.40	93%	DEFC-O_2 (4*)	1.33
94%	DHzFC-O_2 (4)	1.51	93%	DBFC-O_2 (8)	1.65

- Easy handling, transport and storage
- Promising theoretical energy densities
- Systems with higher ΔE^0_{cell} than H_2
- Highest ΔE^0_{cell} for DBFC-O_2

Status - Ammonia's carbon footprint in respect to Synthesis routes & propulsion systems

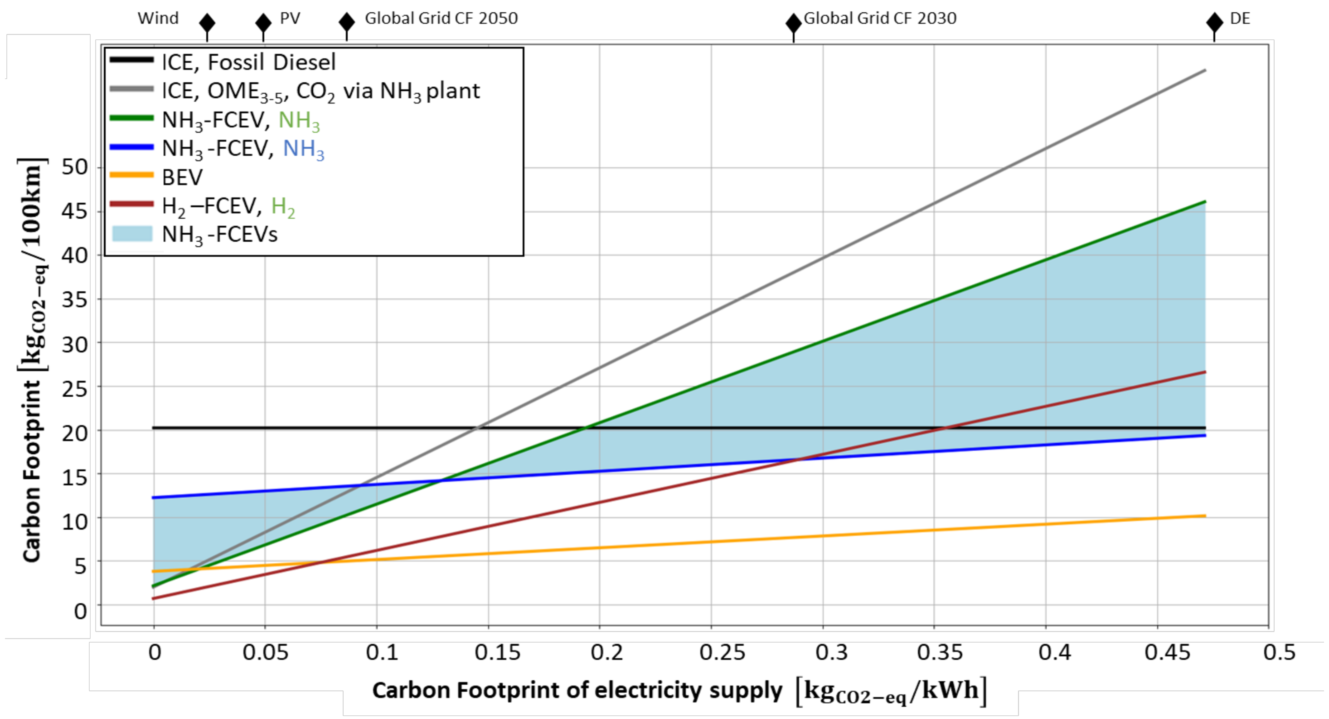
LTT



✓ Usage of NH_3 in fuel cells can reduce CF more than usage of NH_3 as a transport vector

- Depends on conversion efficiency of NH_3 splitting and system efficiency of NH_3 fuel cell

✓ NH_3–FCEVs have lower CF than fossil Diesel-ICE and comparable CF to other low-carbon options!



H_2: hydrogen, NH_3 : ammonia, HB: Haber-Bosch, CCS: Carbon capture and storage, FCEV: Fuel cell electric vehicle, ICE: Internal Combustion Engine, BEV: Battery-Electric Vehicle, CF: Carbon Footprint

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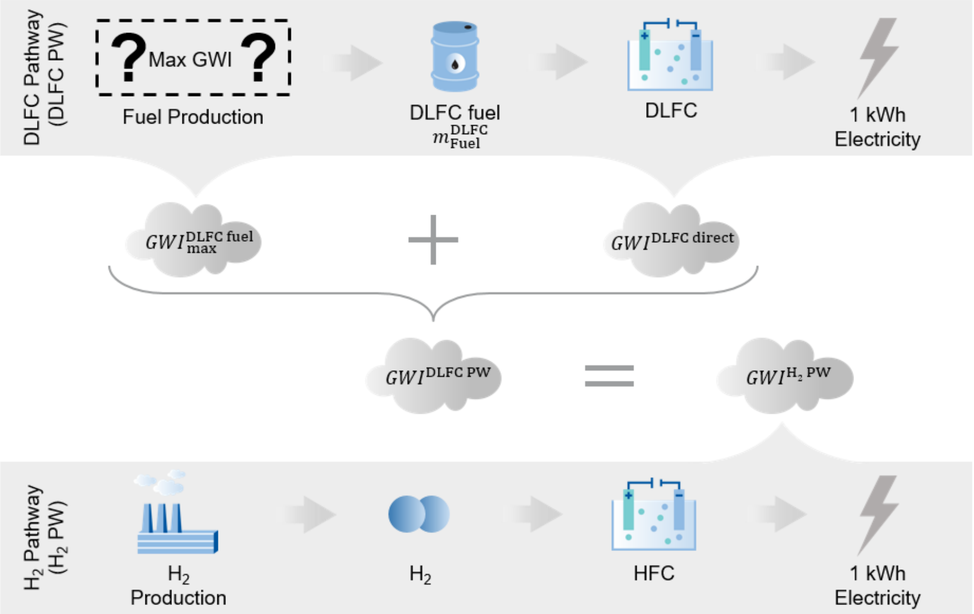
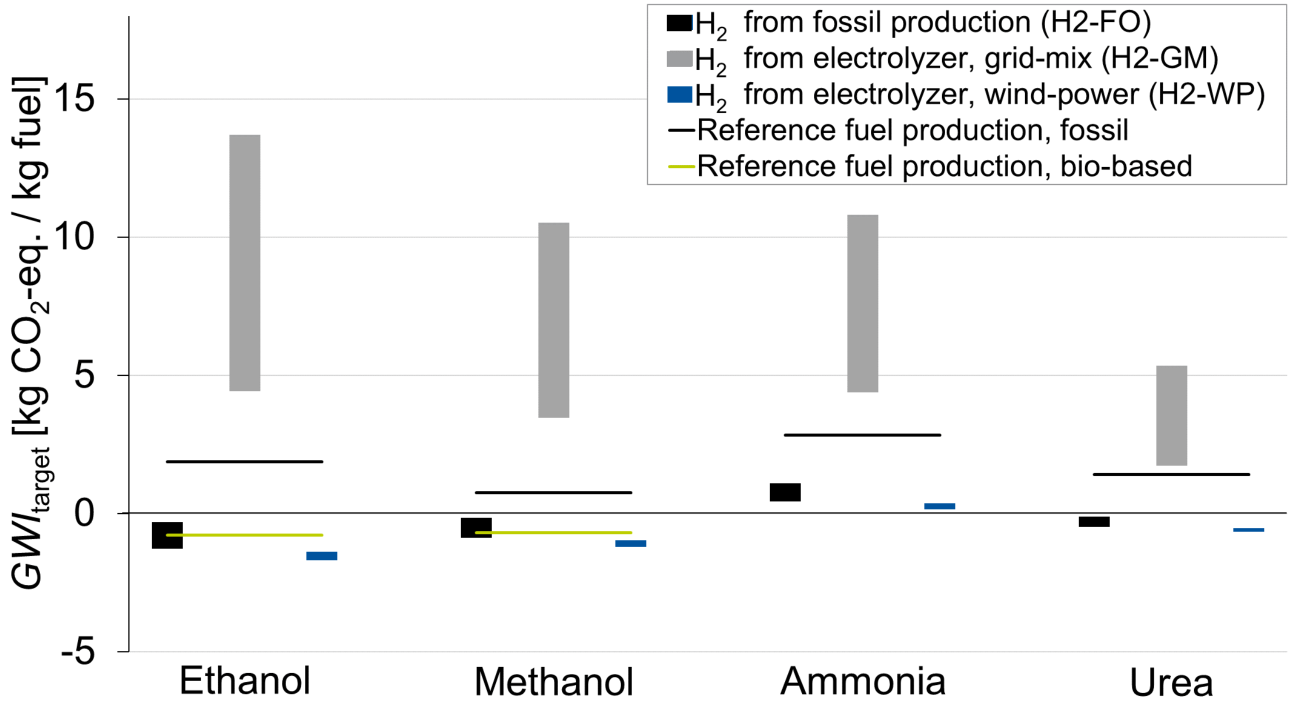
Status - Carbon footprints evaluation for different potential fuels

LTT





DLFCs can be a climate-friendly alternative to HFCs.

- H2-GM: Fossil fuel production routes meet their targets.
- H2-FO and H2-WP: Negative GWI for production of Ethanol, Methanol and Urea necessary.
- State-of-the-art HFC with fossil H_2: Bio-based ethanol and methanol productions meet their targets.

More detailed modelling of both pathways necessary:

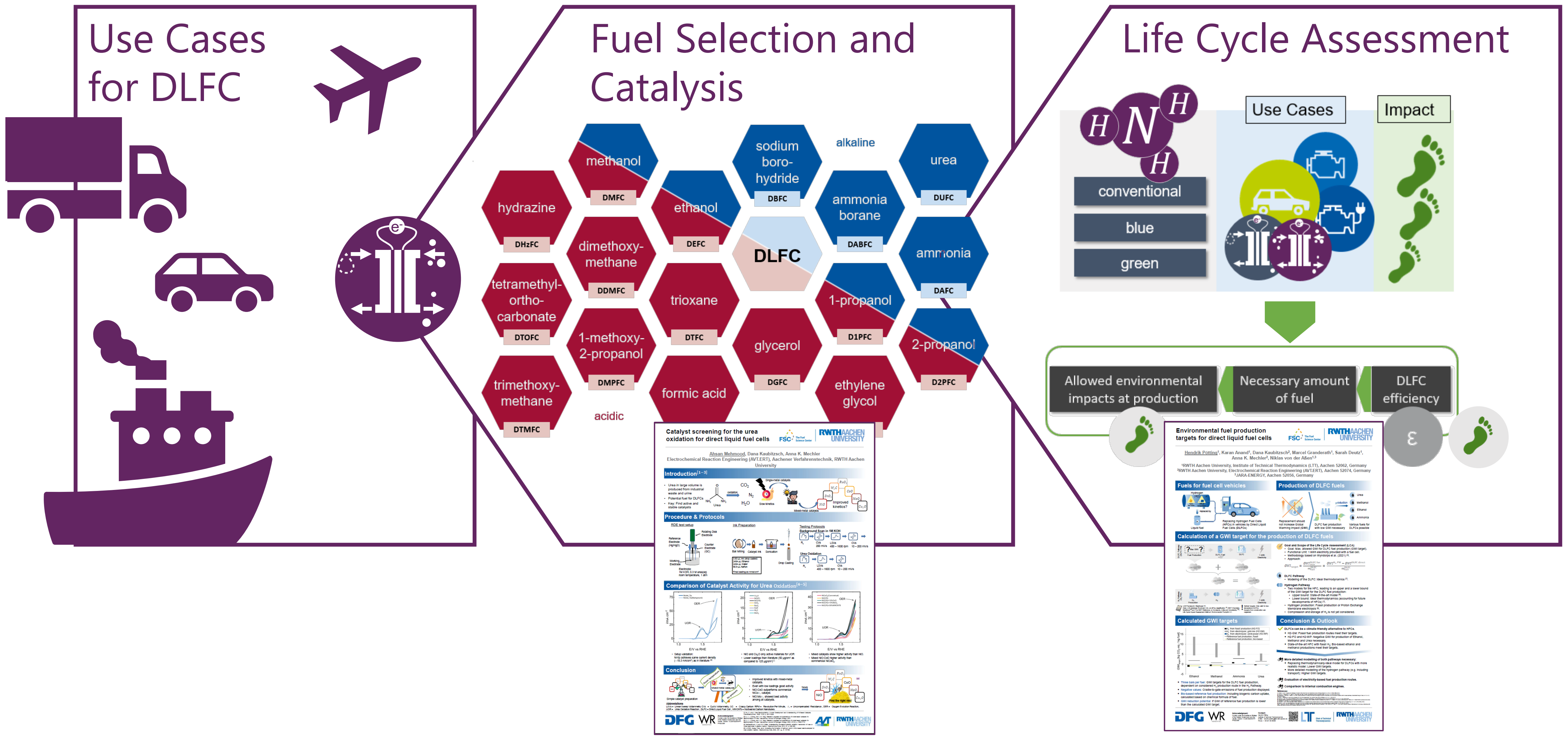
- Replacing thermodynamically-ideal model for DLFCs with more realistic model: Lower GWI targets.
- More detailed modelling of the hydrogen pathway (e.g. including transport): Higher GWI targets.

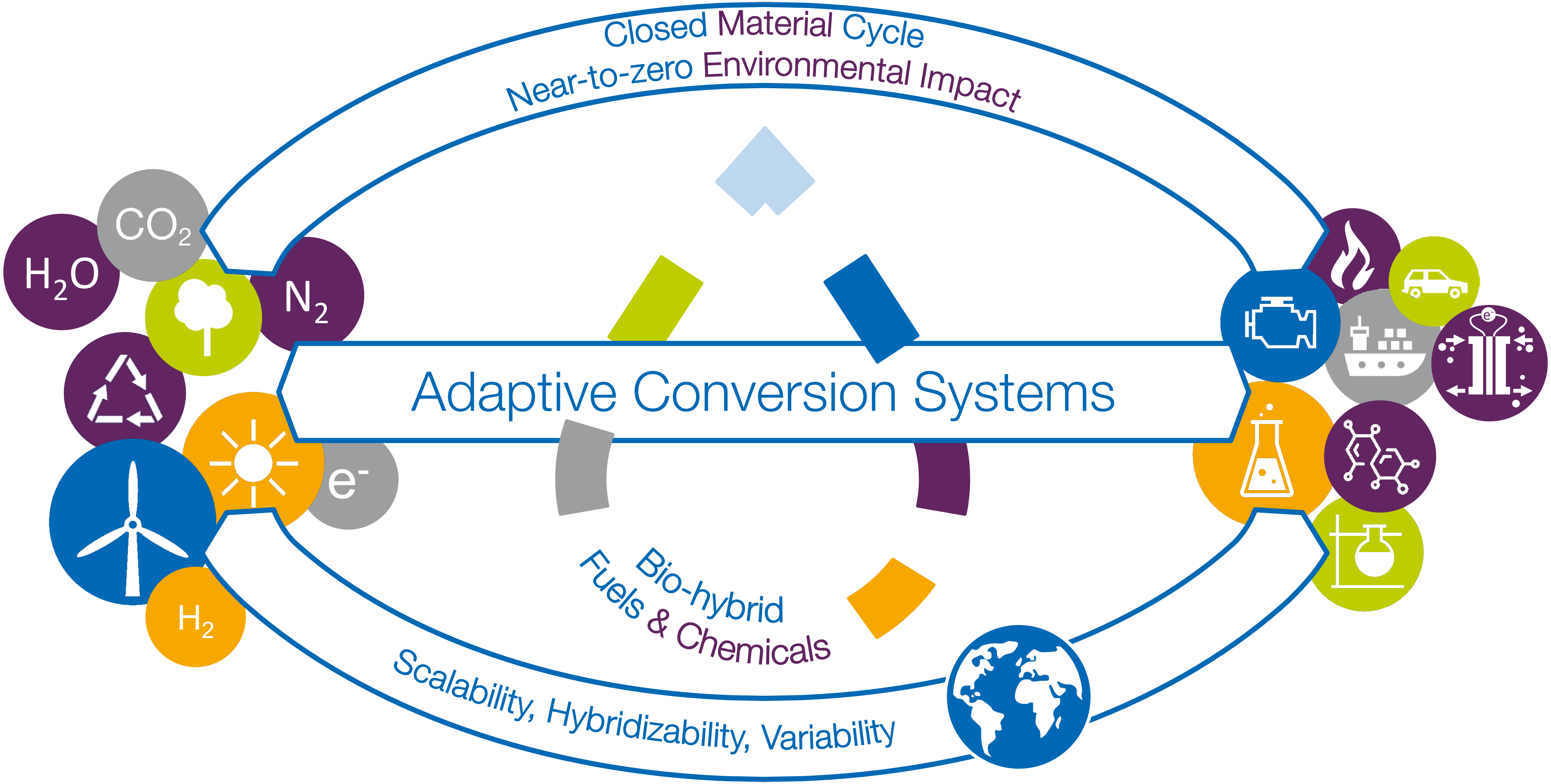
Evaluation of electricity-based fuel production routes.

Comparison to internal combustion engines.

Status - Recap of the latest results presented at the FSC conference

3 presentations and 2 posters




Closed Material Cycle
Near-to-zero Environmental Impact
H_2O
CO_2
N_2
e^-
H_2
Adaptive Conversion Systems
Bio-hybrid
Fuels & Chemicals
Scalability, Hybridizability, Variability

Outlook - Driving factors for developing DLFCs now!

Additive manufacturing methods

Membrane development

Sustainable fuel availability

Demand to import sustainable energy-carrying molecules

Decreasing acceptance of fossil fuels

Changing regulatory

Local shortage of green H_2

Outlook - Why were DLFCs neglected after the period of 1990-2000?
What is different today?

Problematic membranes:
Low stability
High fuel crossover

Catalysts…
Pt-based
Stability
Scalability of synthesis

High costs:
Low staibility of membranes

Catalyst materials + synthesis
Overall low efficiency

Missing regulations

Improved synthesis methods

New materials

Better mechanistic understanding

Improved Anion-Exchange membranes for alkaline media

Catalyst materials improved (multi-metallic, non Pt) but not enough

In-Situ investigations to identify reaction mechanisms

DFT calculations to understand limiting steps

Sustainable production routes for fuel candidates

DLFCs have development potential in the knowledge areas of FSC PI's

Outlook - How to develop efficient DLFCs applying FSC core know-how?

DLFC'S ARE NOT EFFICIENT ENOUGH TODAY, TO COMPETE WITH HYDROGEN FC'S

Anna Mechler

Catalyst Design

- New catalyst materials
- RDE & cell testing
- DFT-calculations
- In-situ characterization
- Ex situ characterization

Process Design

- Membrane development
- Cell design
- CFD simulations
- Additive manufacturing
- Scalability concepts

Stefan Pischinger, Niklas von der Aßen

System Design

- Stack testing
- Use cases
- CFD simulations
- LCA assessment
- Cost analysis

CREATE AN UNDERSTANDING OF SUB-LAYING PROCESSES AND TRANSFER IT INTO ADAPTIVE, SCALABLE, SUSTAINABLE MOBILITY CONCEPTS FOR THE FUTURE

Mirijam Zobel, Regina Palkovits, Karl J. J. Mayrhofer, Rüdiger-A. Eichel, Matthias Wessling, Reinhold Kneer, Heinz Pitsch, Kai Leonhard, Alexander Mitsos, Ulrich Simon, Lars Blank, Lars Lauterbach

The Fuel Science Center

FSC The Fuel Science Center

AVT Aachener Verfahrenstechnik

LTT Lehrstuhl für Technische Thermodynan

tme Lehrstuhl für Thermodynamik mobiler Energie-wandlungssysteme

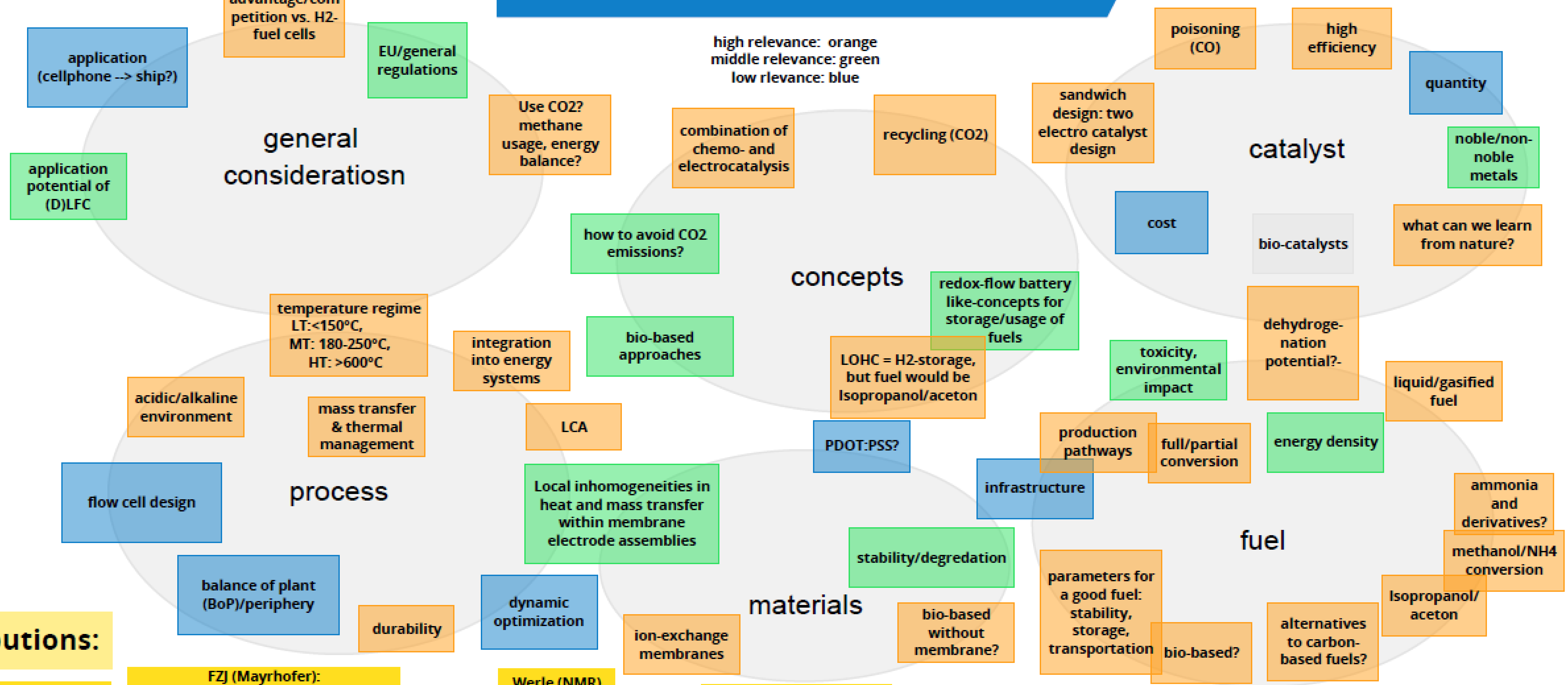
DFG Deutsche Forschungsgemeinschaft

German Research Foundation

WR WISSENSCHAFTSRAT

(Direct) Liquid Fuel Cells

high relevance: orange
middle relevance: green
low rlevance: blue



Contributions:

FZJ (Mayrhofer):
- online-evaluation of reaction

Werle (NMR)

durability

optimization

ion-exchange membranes

bio-based without membrane?

stability, storage, transportation

bio-based?

alternatives to carbon-based fuels?

aceton

Contributions:

IAC:
- electrochemical characterization
- TEM with electrochemical cell (under development)
- inorganic material synthesis and characterization
- FTIR- quantitative gas-analysis

IfK Zobel:
- X-ray and neutron scattering, XRD, PDF, QENS, SAXS/SANS to indentify short-long-range structures and diffusion dynamicx of H-containing molecules

FZJ (Mayrhofer):
- online-evaluation of reaction products with coupled analytics
- time-resolved measurement of selectivity of reactions and stability of electrode materials
- previous knowledge in liquid fuel ells

ITMC:
- electro catalyst design
- reaction mechanims (at electrodes)
- heterogenious catalysis
- (porous) membrane materials

ITV:
- quantum chemical calculations
- multi-phase transport phenomena

HGD:
- quantum chemical calculations

Werle (NMR)

IEK-9 (FZJ): NMR for degradation/reaction studies, catalyst & membrane combinations

ERT:
- evaluation on cell level
- reaction parameters
- safety assesment of fuel (together with TME)
- catalyst evaluation/poisoning

CVT:
- ion-exchange membrane materials
- PEDOT:PSS?
- additive manufacturing (junior research group Linkhorst)
- flow cell desing and scale-up

TME:
- system design and simulation
- identification of possible use-cases
- testing cells and stacks
-flow field, cell and stack design
- CFD simulation incl. water transport and simplified electrochemistry

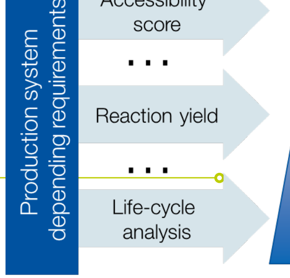
WSA:
- IR Thermography; mass spectrometer; FTIR; Visualization techniques
- test bench for determination of transient temperature fields and contact heat transfer coefficients
- profile sensor for characterization of liquid structures within the boundary layer
- cavity-ring down spectrometer for line-of-sight determination of multi-species concentration within the boundary layer of a flat plate

LTT(KL):
- degradation studies (with ERT)
- simulation or reactions on catalysts
-CAMD for fuel cells (with SVT)
- integrated design/optimization of fuels and production
LTT (NVDA):
- LCA & process integration

SVT:
- optimization frameworks for integrated design
- CFD simulations
- computer aided screening of reactions, materials, catalysts
- screening of production pathways (with LTT (NVDA))
- predictive models of properties
- previous work on fuel cells, flow batteries and H2 generation an dpower 2x

iAMB:
- engineering of biocatalysts for LFC
- nuclear resonance vibrational spectroscopy for evalutaion of iron containing (bio-)catalysts
- design of biological membrane-free LFC
- understanding of catalytic mechanism of biocatalysts with biochemical methods for learning from nature

Why were DLFCs neglected after the period of 1990-2000?



Low efficiency due to:

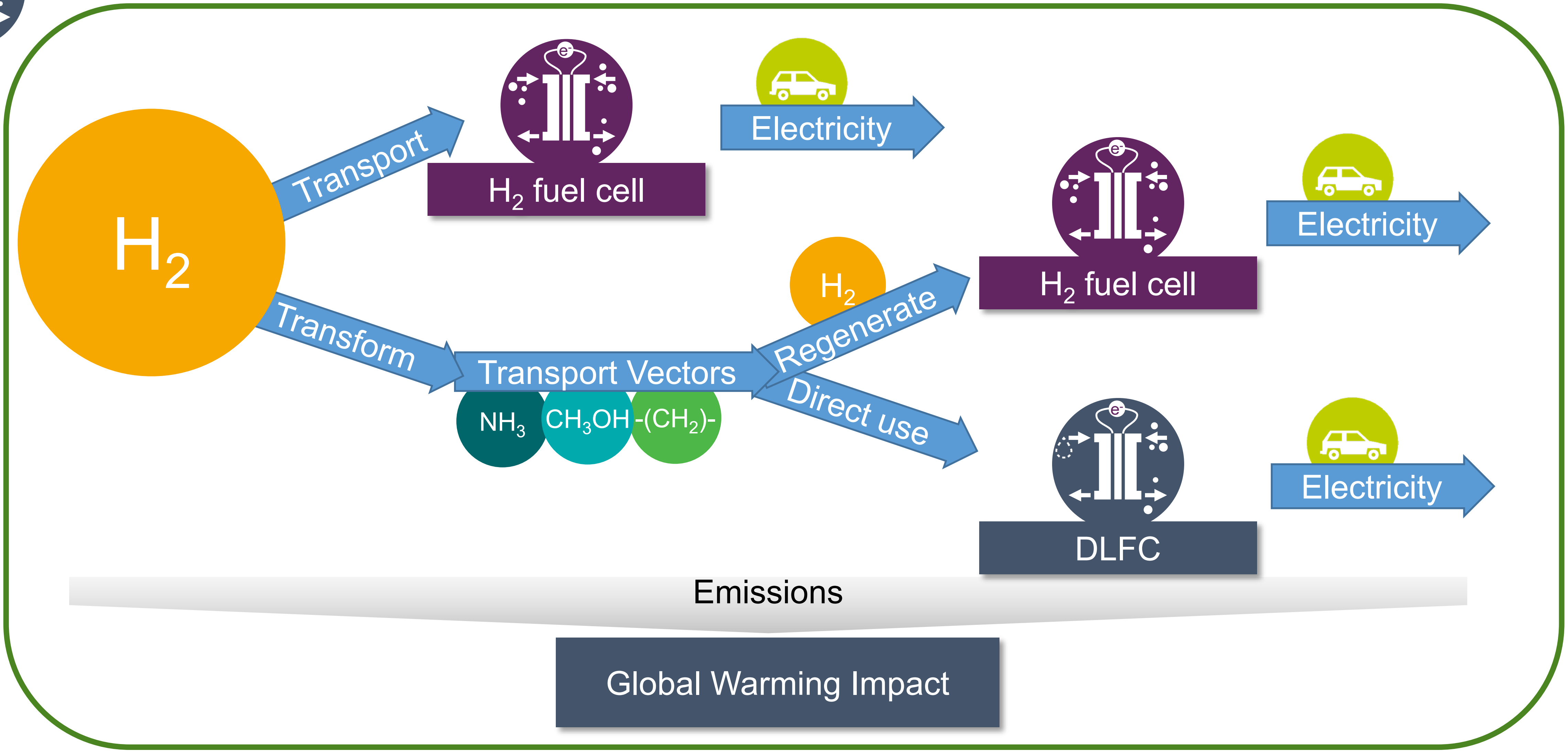
- Low stability of membranes
- High fuel crossover

Low catalyst activity:

- High loadings
- Only Pt
- Stability

→ High prices approx. 41% on catalyst material + synthesis

Benchmark



H_2
Transport
H_2 fuel cell
Electricity
Transform
Transport Vectors
NH_3
CH_3OH
$-(CH_2)-$
H_2
Regenerate
Direct use
H_2 fuel cell
Electricity
DLFC
Electricity
Emissions
Global Warming Impact