

# Simulation as an enabler

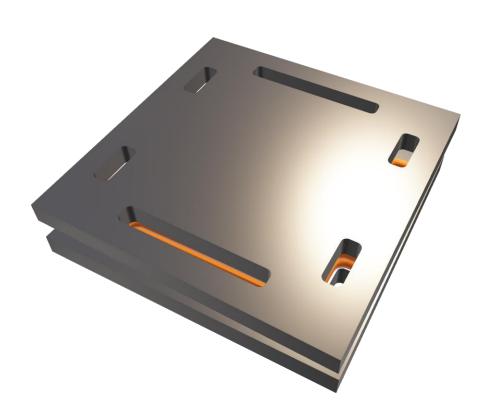
Speaker:

Samuele Cappelli, MSc BSc

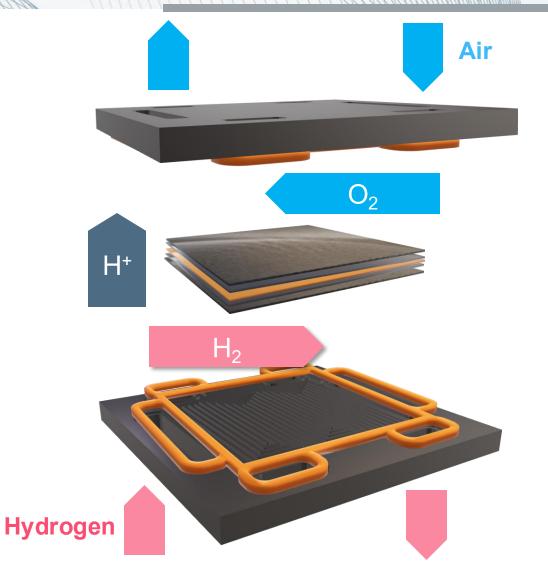


# FC technology









#### **PEMFC** operation

#### **Cathode**

$$1/2 O_2 + 2H^+ + 2e^- \rightleftharpoons H_2O \quad E_{SHE}^0 = 1.229 V$$

#### FC overall reaction

$$H_2 + 1/2 O_2 \rightleftharpoons H_2 O$$

$$E_{SHE}^0 = 1.229 \,\mathrm{V}$$

#### **Anode**

$$H_2 \rightleftharpoons 2H^+ + 2e^-$$

$$E_{SHE}^{0} = 0.000 \text{ V}$$



# Cathode

Anode

#### **PEMFC** cell structure

Graphite or coated metal BPP
Sealing

Carbon based GDL

PGM based cathode CL

Proton Exchange Membrane

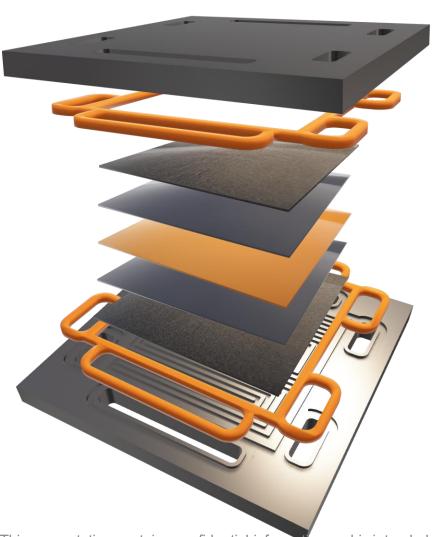
PGM based anode CL

Carbon or nickel-based GDL

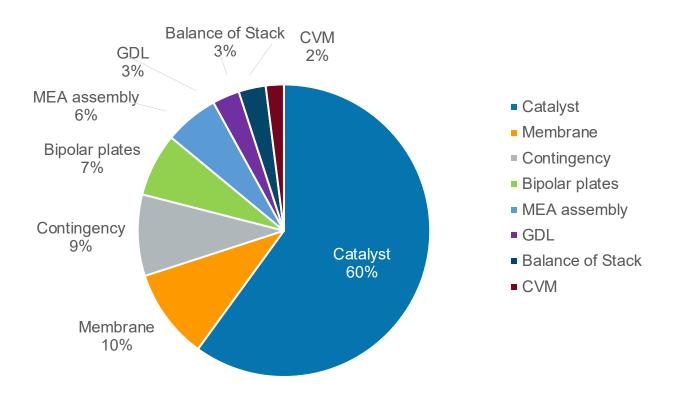
Sealing

Graphite or coated metal BPP



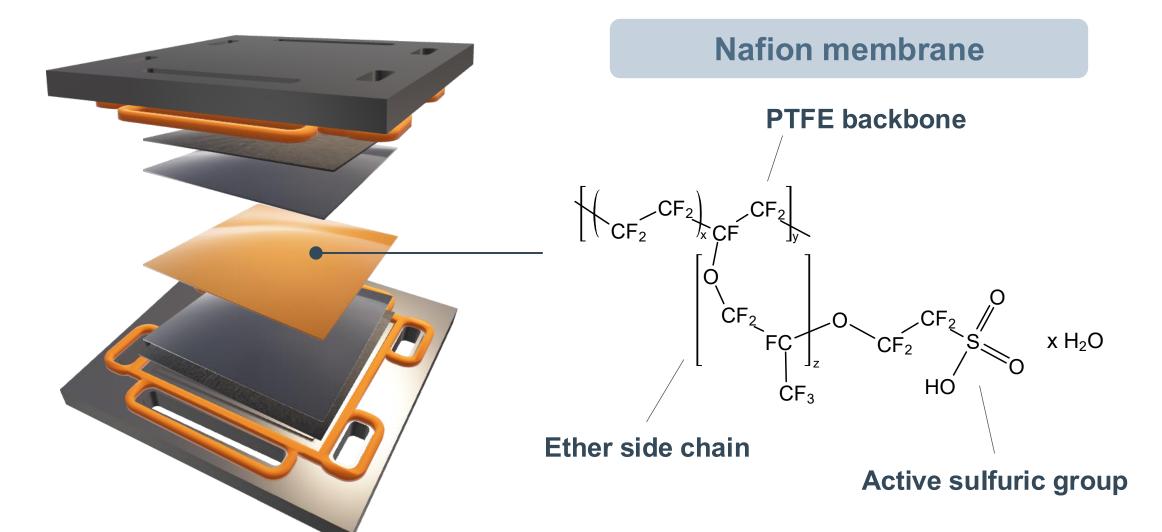


#### PEMFC stack cost breakdown

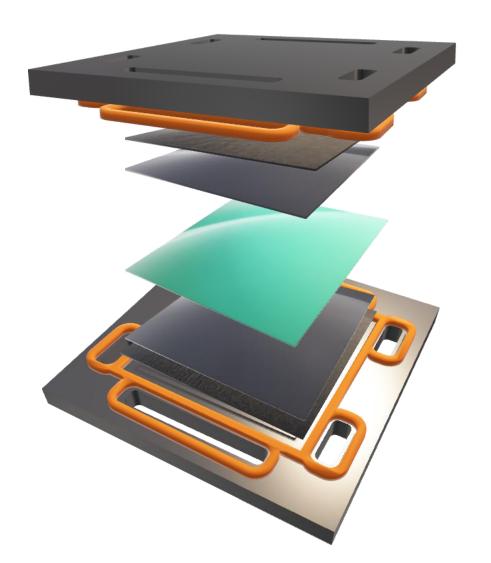


Source: <u>Heavy-Duty Fuel Cell System Cost – 2023</u>



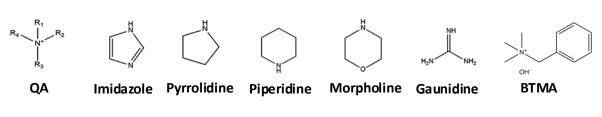






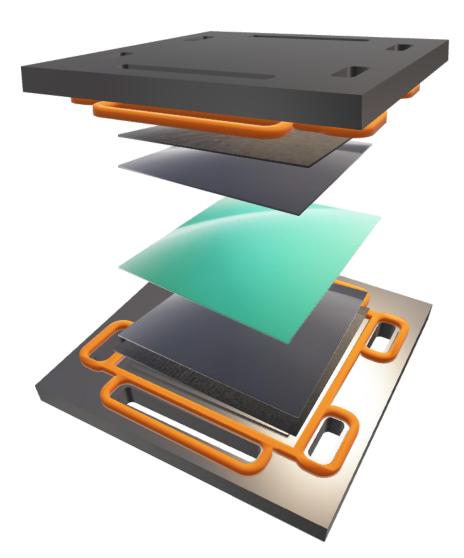
#### **Anion Exchange Membrane**

#### **Polymeric backbones**



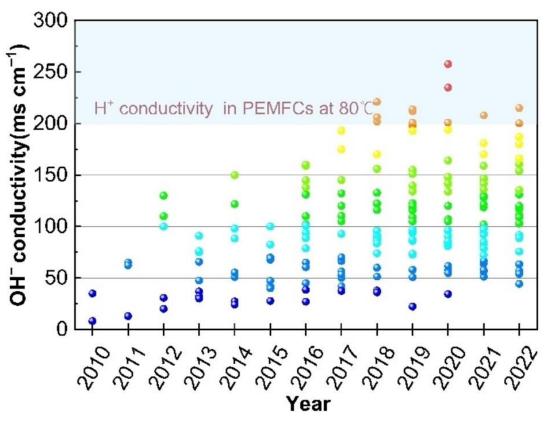
**Functional groups** 





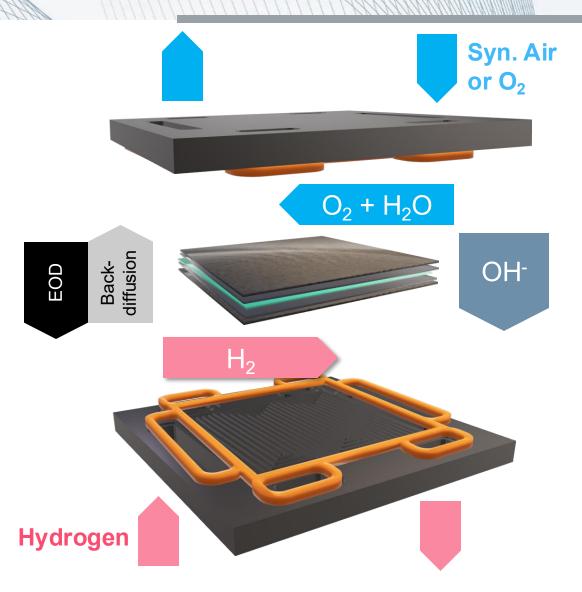
#### **Anion Exchange Membrane**

High ion conductivity (>200 mS cm-1 @ 80°C)



Source: Recent Development of Anion Exchange Membrane Fuel Cells and Performance Optimization Strategies: A Review





#### **AEMFC** operation

#### Cathode

$$O_2 + 2H_2O + 4e^- \rightleftharpoons 4OH^ E_{SHE}^0 = 0.4010 \text{ V}$$

Advantage: high ORR activity in alkaline environment

$$H_2 + 1/2 O_2 \rightleftharpoons H_2 O$$

$$E_{SHE}^0 = 1.2291 \,\mathrm{V}$$

**Challenge**: difficult water management due to water consumption at cathode and high EOD

#### Anode

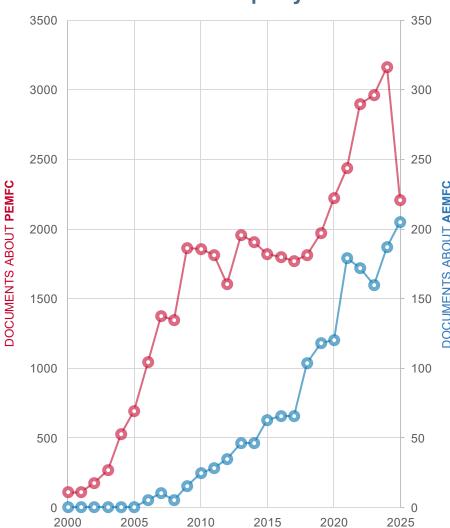
$$H_2 + 20H^- \rightleftharpoons 2H_2O + 2e^ E_{SHE}^0 = -0.8281 \text{ V}$$

Advantage: wide range of available fuels

### AEMFC - Current R&D efforts

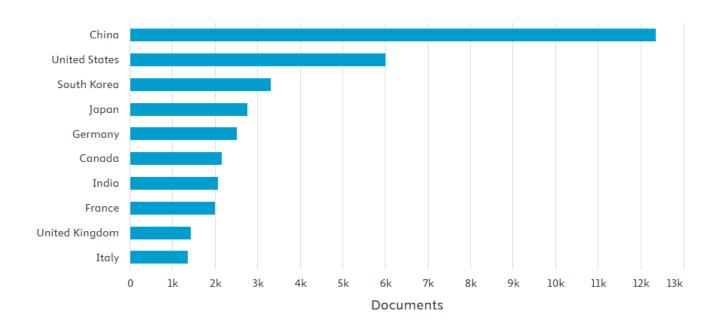


#### **Documents per year**



#### **Documents by country or territory**

Compare the document counts for up to 15 countries/territories



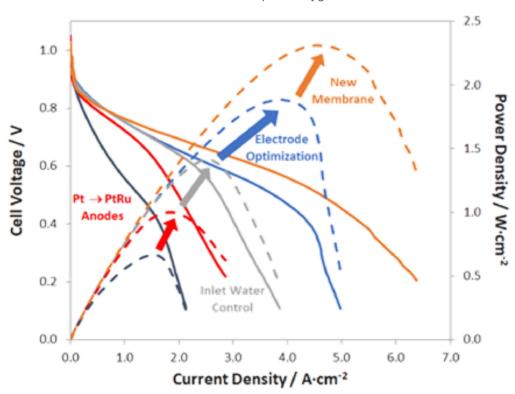
Chronology of publications about PEMFC and AEMFC. Source: <a href="http://www.scopus.com">http://www.scopus.com</a>; search settings: 1) pemfc 2) aemfc, anion exchange membrane fuel cell, alkaline membrane fuel cell, hydroxide exchange membrane fuel cell; limited to Article, Review, Conference Paper (accessed November 2025).

### AEMFC - Present R&D trends



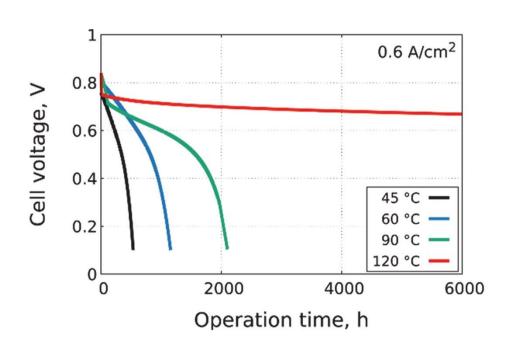
#### **Specific performances**

Performances with pure oxygen feed



#### **Durability / Lifetime**

Galvanostatic stability



Source: Understanding how high-performance anion exchange membrane fuel cells were achieved: Component, interfacial, and cell-level factors William E. Mustain, 2018, <a href="https://doi.org/10.1016/j.coelec.2018.11.010">https://doi.org/10.1016/j.coelec.2018.11.010</a>

Source: A surprising relation between operating temperature and stability of anion exchange membrane fuel cells Karam Yassin et al., 2021, <a href="https://doi.org/10.1016/j.powera.2021.100066">https://doi.org/10.1016/j.powera.2021.100066</a>



# COMET Project GAMBIT



Goal: Assessment of AEMFC technology potential for the application in the mobility sector (heavy-duty, rail, maritime)

#### Focus on:

- HC-based membrane
- Zero or extremely low PGM loading
- Multi-fuel capability (e.g. ammonia, methanol)
- Power density optimization
- Hygrothermal management
- Degradation mitigation strategies

#### **Methodology:**

- Simulation in virtual environments
- Experimental analysis

















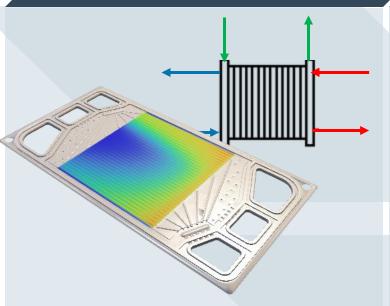
### Simulation as enabler



#### **Simulation**

#### **Implementation**

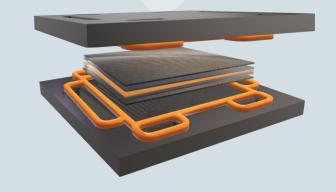
#### **Validation**

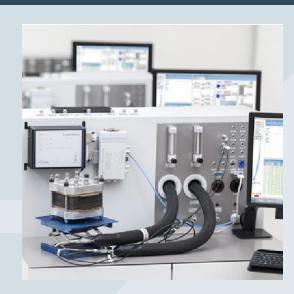


- Research on AEMFC
- Simulation 0D, 1D, 3D



No commercially available AEMFC
 Model

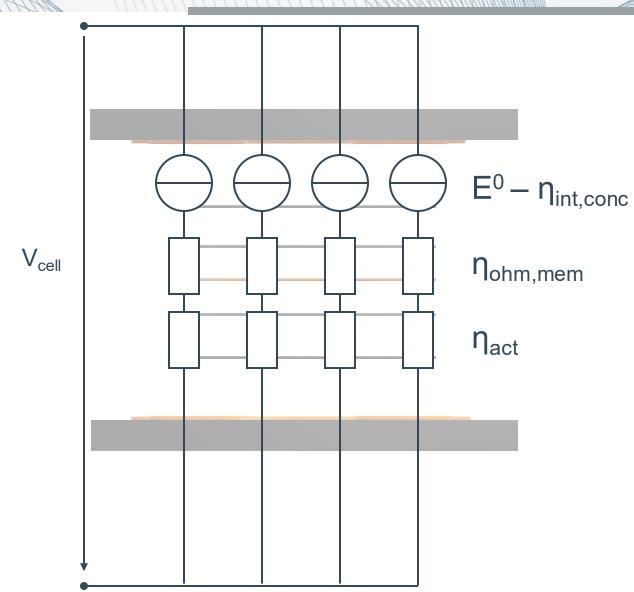




Single-cell testing

### Along-the-channel AEMFC model





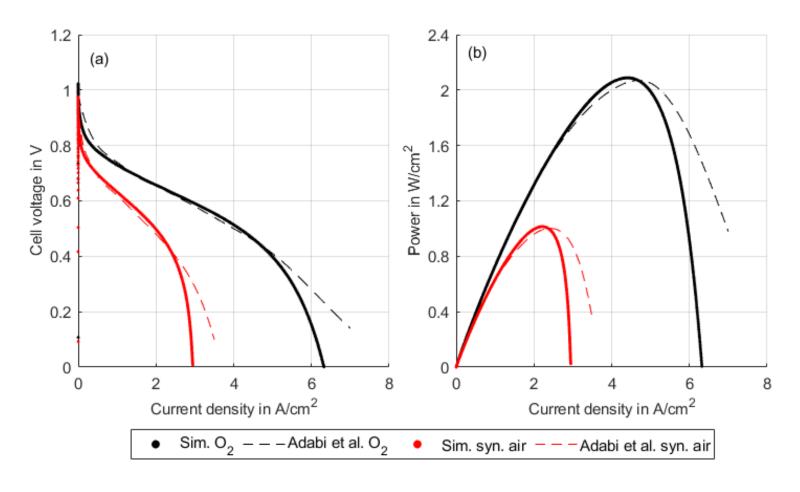
#### Voltage model

- Cell discretized along the Gas Flow Channel (GFC) leading to a so-called pseudo-1D model
- Segments connected in parallel
- Possibility to further discretize each segment across the MEA to reach a pseudo-2D model
- Cell voltage equal to the reversible cell potential minus all overvoltages
- Segment current calculated via explicit finite difference equations
- Coded in Matlab/Simulink

### Model validation vs. literature



AEMFC (a) **polarization curve** and (b) **power curve** with simulation results feeding pure oxygen (O<sub>2</sub>) and synthetic air (syn. air.) from this work and experimental results adapted from Adabi et al.



#### **Simulation inputs**:

- 20 μm membrane thickness
- inlet temperature for all media at 80°C
- 250 cm2 active area
- RH cathode/anode 75%/25%
- Operating pressure steady at 2.0bar(a) on both anode and cathode

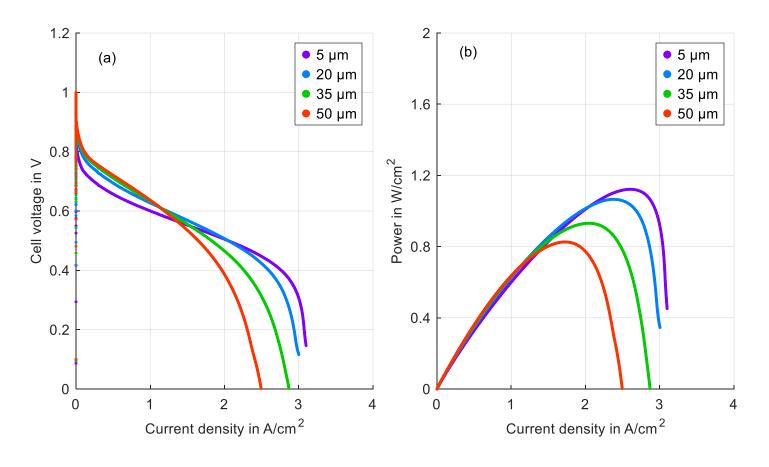
#### Experimental reference:

H. Adabi et al., "High-performing commercial Fe–N–C cathode electrocatalyst for anion-exchange membrane fuel cells," Nature energy, vol. 6, pp. 834-843, 2021.

### Membrane thickness variation



AEMFC (a) **polarization curve** and (b) **power curve** with simulation results feeding synthetic air to cells parametrised with varying **membrane thickness** 



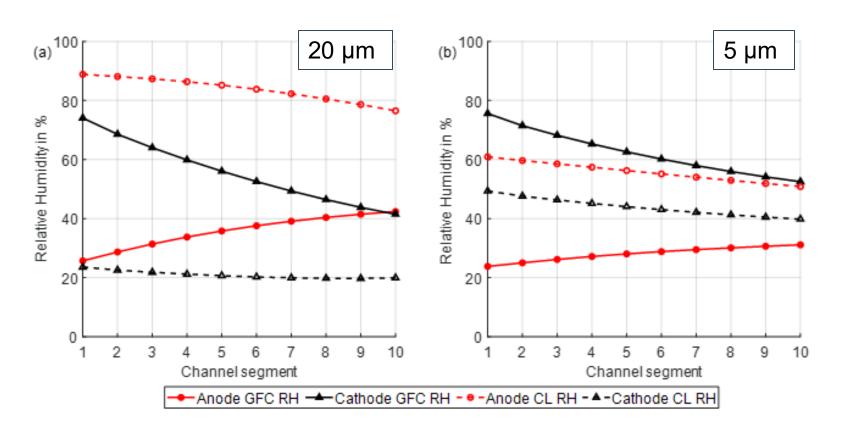
#### **Simulation inputs**:

- membrane thickness variation between 5 and 50 µm
- cathode fed with synthetic air
- inlet temperature for all media at 80°C
- 250 cm2 active area
- RH cathode/anode 80%/25%
- Operating pressure steady at 2.0bar(a) on both anode and cathode

### Along-the-channel AEMFC model



Sensitivity analysis of membrane thickness on water management. RH is plot for both anode and cathode with (a) 20 µm and (b) 5 µm thick membrane, at GFC and CL

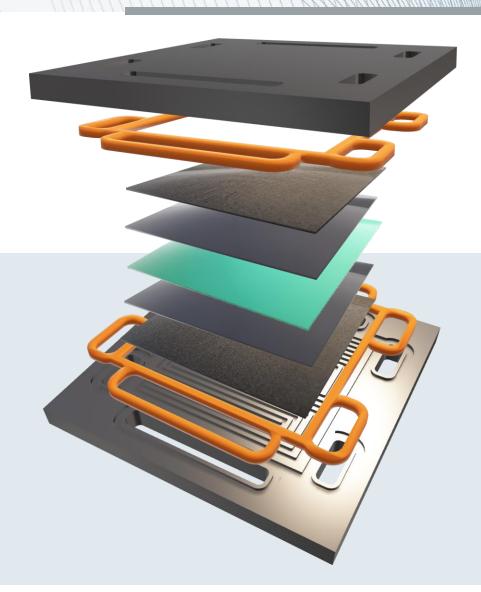


#### **Simulation inputs:**

- H2/syn.air on Anode/Cathode
- Inlet temperature for all media at 80°C
- 250 cm<sup>2</sup> active area
- RH cathode/anode 90% / 20%
- Current density at 2 A/cm<sup>2</sup>

### Along-the-channel AEMFC model





#### **Advantages**

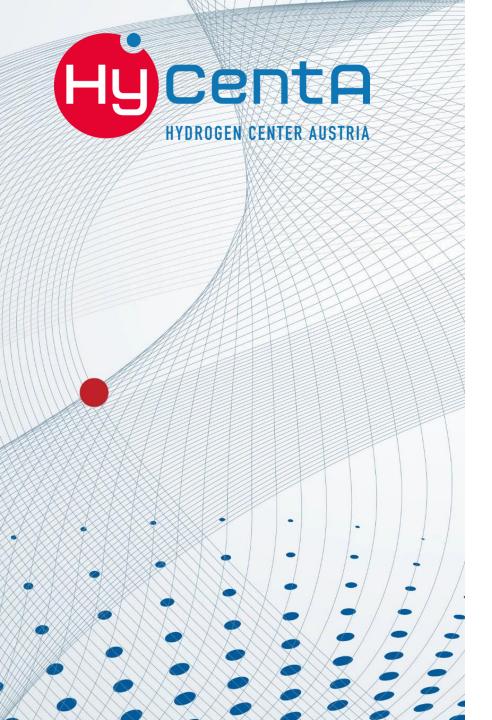
- Use of non-precious metal catalysts
- Cost effectiveness
- high ORR activity in alkaline environment
- wide range of available fuels

#### **Challenges:**

- Water management
- Carbonation
- Upscaling

#### **COMET Phase 2**

Further catalysts, stack



#### Join us in shaping the future of hydrogen technology!

#### **HyCentA Research GmbH**

Inffeldgasse 15

A-8010 Graz

• Phone: +43 316 873 9500

- office@hycenta.at
- www.hycenta.at



















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