Next steps in the development of bi-functional Gas-Diffusion-Electrodes for Zinc-Air-Batteries

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Introduction

Motivation

- **Zinc-Air-Batteries (ZAB) -** a solution for **midterm energy storage systems** due to their cost structure, safety and abundance of materials**.**
- Besides the **Zinc-Anode** limits cyclability, state-of-the-art **gas-diffusion-electrode (GDE)** challenge the economic feasibility due to the sluggish oxygen reactions ($\eta_{RTE} \approx 60\%$) and the use of expensive bi-functional catalysts.
- Additional: **material stability** under oxygen evolution reaction problematic**.**
- ➢ **Existing GDEs need to be optimized for bi-functionality.**

Objective

1. **Identify electrochemical limits of materials**
2. **Optimize pore network** for changing requirements and conditions of oxygen evolution (2-phase-reaction) and oxygen reduction reaction (3-phase-reaction)
3. **Enhance performance by a multi-layer approach**: addition of specialized reaction and gas-diffusion layer.

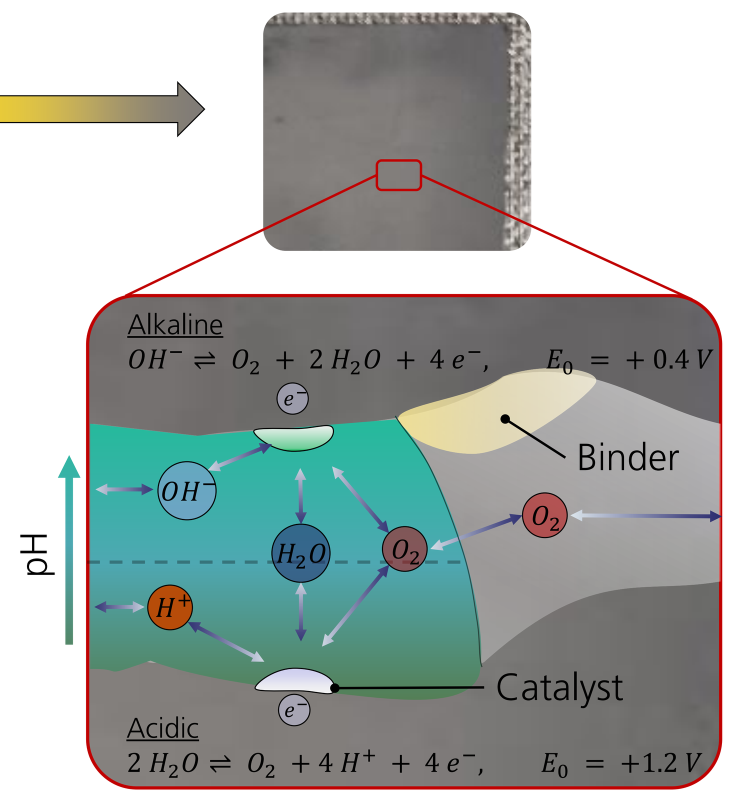
Bi-functional Gas-Diffusion-Electrodes

Manufacturing, Reaction and Transport

Pressing & Heat Treatment
- Pressing
- Melting the binder for mechanical stability

Distribute Powder
1. Glue rubber foam frame to plate
2. Distribute powder evenly
3. Add metal mesh for stability and conductivity

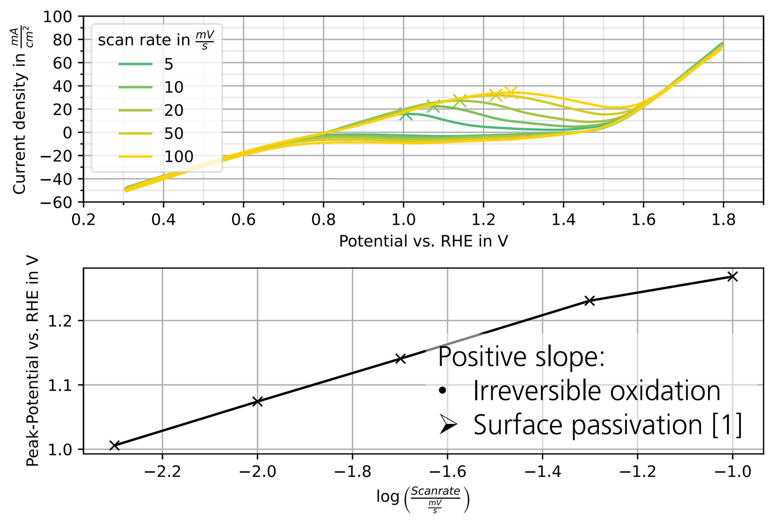
Powder Manufacturing
- Prepare mixture of hydrophilic metal powder, catalyst and hydrophobic binder
- Short milling in double knife mill



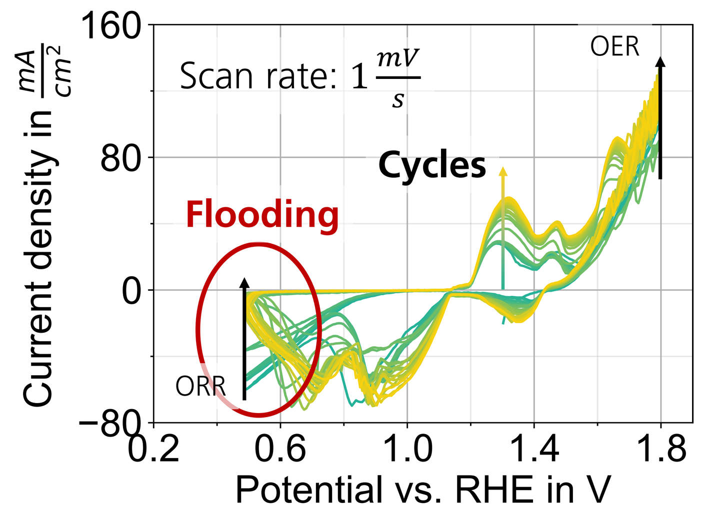
Material Stability

Cyclic-Voltammetry studies in 6M KOH

Nickel GDE
90wt.% Ni – 10 wt.% PTFE



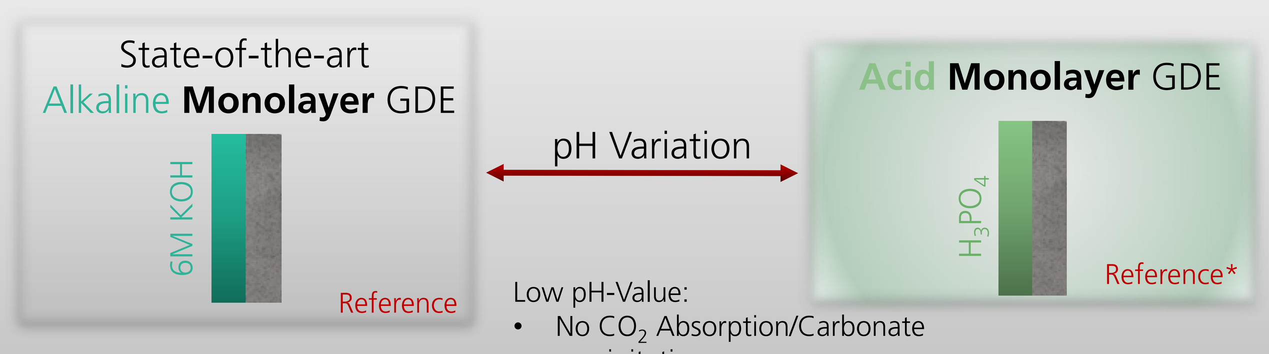
Silver GDE
90wt.% Ag – 10wt.%PTFE



- Potential for OER (U>1V vs. RHE) is demanding for used materials
  - ➢ e.g. typical used Carbon decomposes @ $U > 1.3V$ vs. RHE [2]
- Ni and Ag show good performance without additional catalyst, but also show degradation

Multilayer → **Pore Network**

Architecture Design



Low pH-Value:
- No CO_2 Absorption/Carbonate precipitation
- Better O_2 Solubility
- Material stability

Current

Addition of a **Gas-Diffusion-Layer**:
- No electrolyte breakthrough
- Ensure gas transport

*Partner Advenst

Addition of an acidic **Gel-Polymer-Electrolyte**:
- Electrolyte retention
- Reduce gas crossover
- Enables "bipolar" cell

*Partner Politecnico di Torino

Multilayer GDE
GDE+**GDL**
Alkaline or Acid

Multilayer GDE
GDE+ **Acidic GPE**

Addition of an alkaline **Gel-Polymer-Electrolyte**:
- Zn-Electrode needs alkaline conditions
- Leads to "bipolar-cell"

*Partner CIC energiGUNE

Multilayer GDE
GDE+ **Bi-layer GPE**

- Improved η_{RTE}
- Electrochemical stable in conditions of secondary ZABs
- Optimal wetting for OER and ORR conditions

Goal

Use optimized monolayer GDE

Optimize pore network

① Model development

First step towards an informed GDE Design

GDE production & FIB-SEM characterization

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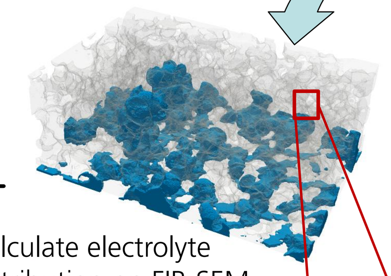
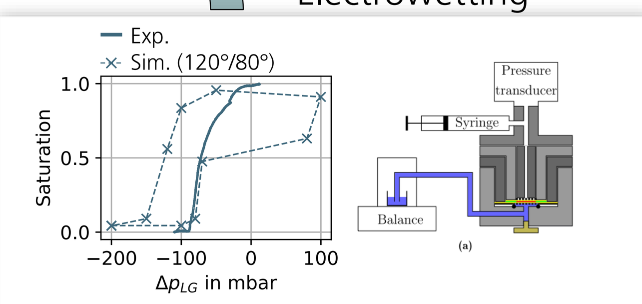
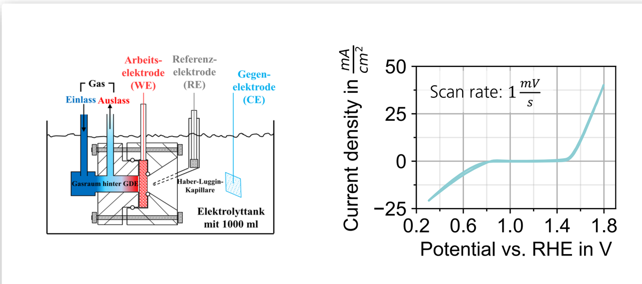


Calculate electrolyte distribution on FIB-SEM picture with **Pore morphology method (PMM)**

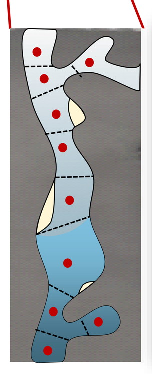
Parametrize change of contact angle due to:
- Inner surface roughness
- Electrowetting



Validation of wetting behavior



Validation of performance



Calculate GDE performance by transport/reaction model
1D Discretization along pore path (e.g. maximum ball algorithm)
- Phase distribution from PMM model and FIB-SEM
- $\frac{\partial c_i}{\partial t} = -\nabla J_i + r_i$
- Solubility, mass transfer and diffusion coefficients from experimental data
- Reaction model: Butler-Volmer

② Virtual microstructure design

Optimize performance

Train
Predict
Confirm

- via experimental results
- optimal production parameters using developed Model
- machine learning tool with GDE FIB-SEM pictures (different production parameters)

Machine Learning tool to
- **Reconstruct** 3D FIB-SEM picture from 2D slice
- **Predict FIB-SEM** picture depending on production parameters

*Partner IREC

References

(1) Cano, Z. P., et al. (2018). "New Interpretation of the Performance of Nickel-Based Air Electrodes for Rechargeable Zinc–Air Batteries." The Journal of Physical Chemistry C 122(35): 20153-20166.

(2) Yi, Y., et al. (2017). "Electrochemical corrosion of a glassy carbon electrode." Catalysis Today 295: 32-40.

Summary

- To achieve a economical viable ZAB for midterm storage state-of-the-art electrodes need to be improved to overcome their shortcomings: low η_{RTE} & material stability.
- In the HIPERZAB project first steps are done to follow two approaches:
  1. Use model based insides to improve the monolayer GDE
  2. Extend the monolayer architecture

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