FURTHER-FC

Further **U**nderstanding **R**elated to **T**ransport limitations at **H**igh current density towards future **E**lect**R**odes for **F**uel **C**ells

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Clean Hydrogen Partnership

Main progress

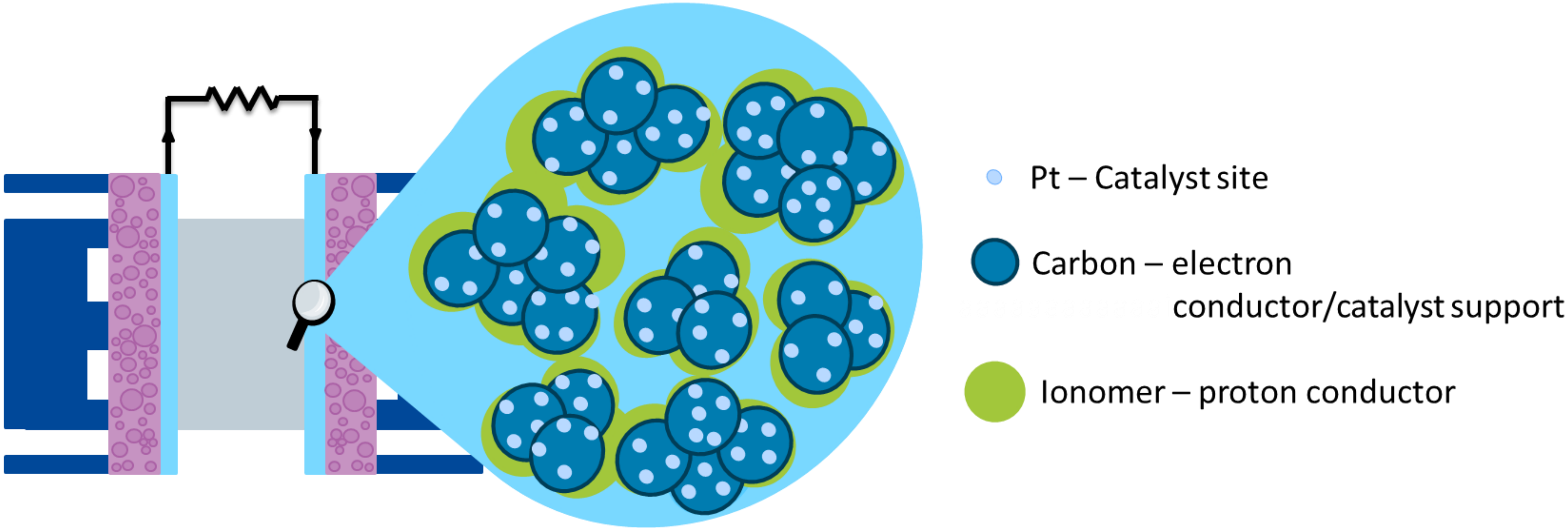
from nanometer scale to cell operation

Approach
From nm to fuel cell operation

Structure, local and effective properties of the CCL from component to layer

→ Characterisation and modeling

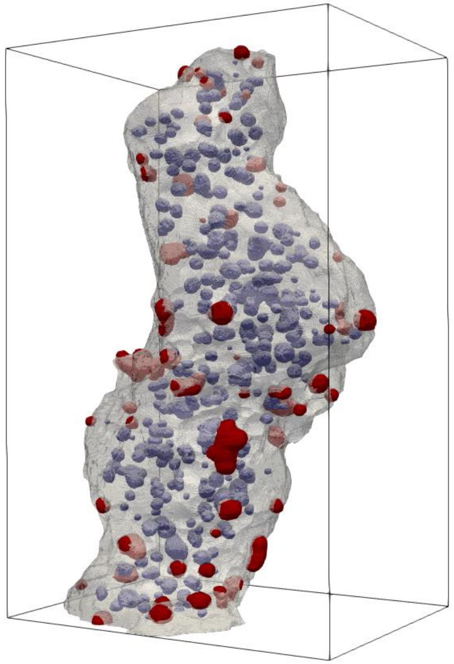
→ Characterisation and simulation of their impact on fuel cell operation



Sub-micrometer structure of CCL
Pt size distribution and ionomer vizualisation

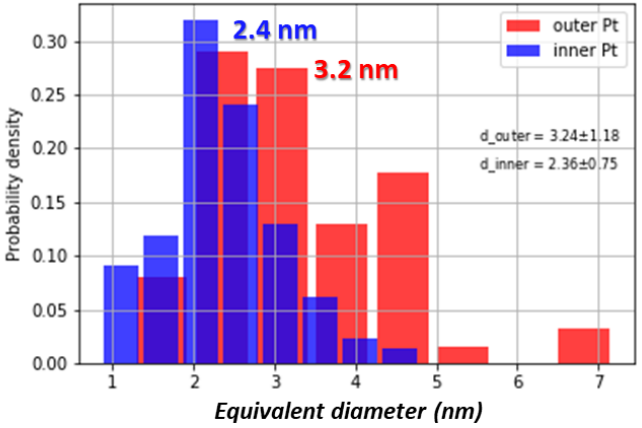
Electron-tomography (TEM)

Pt/C (HSA) catalyst powder

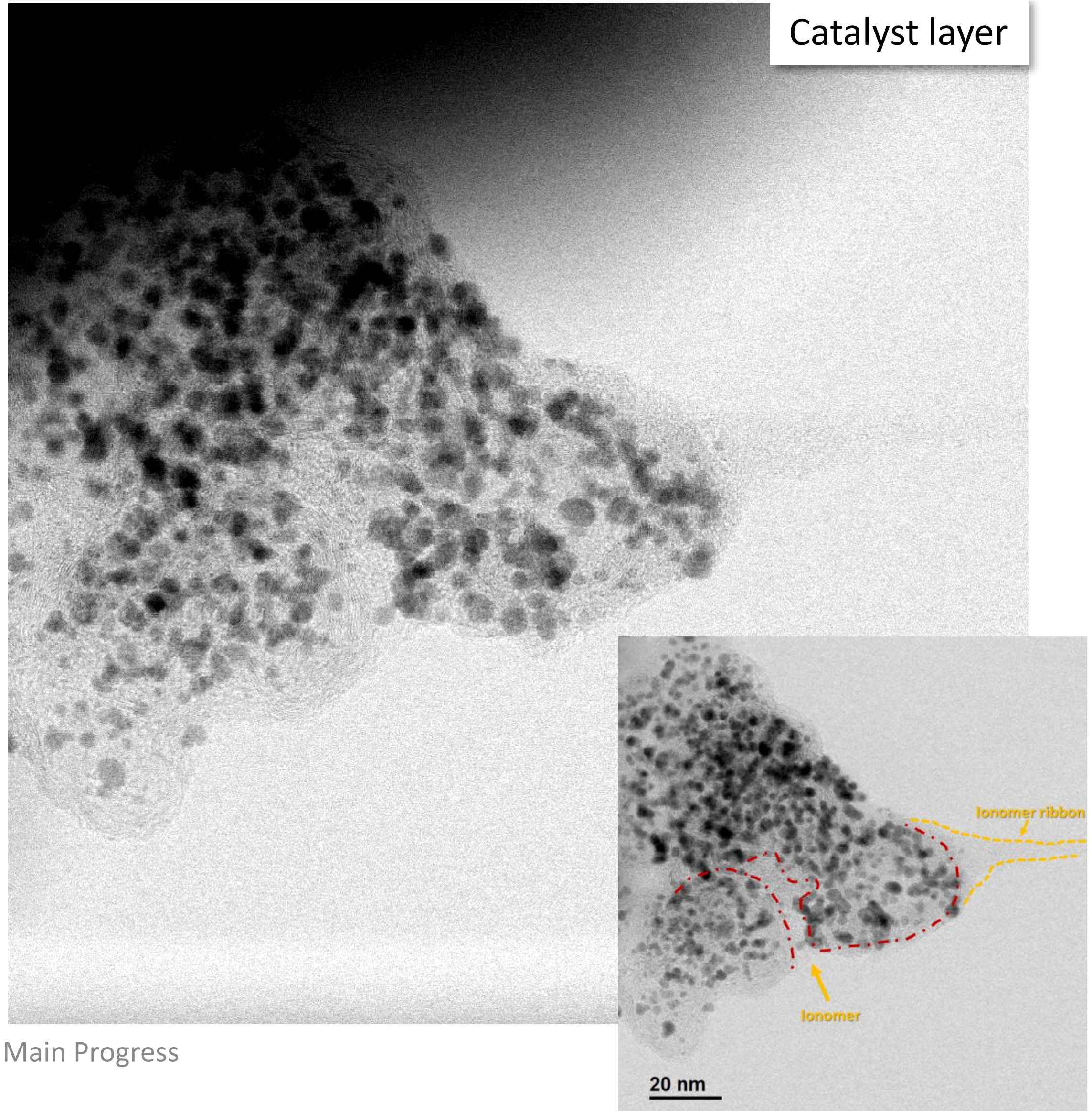


Outer Pt
Inner Pt
Carbon

356 Pt NPs = 294 Inner Pt NPs + 62 Outer Pt NPs



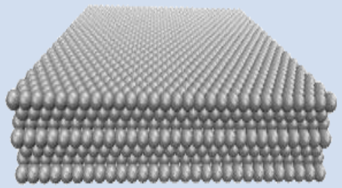
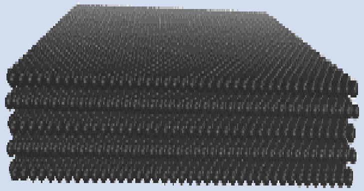
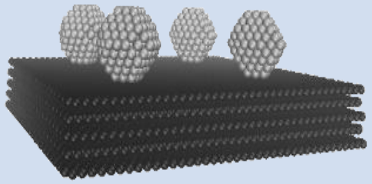
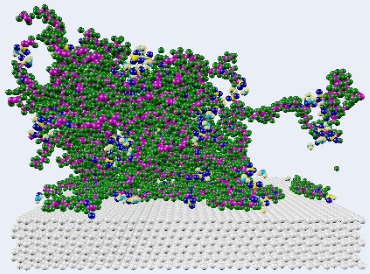
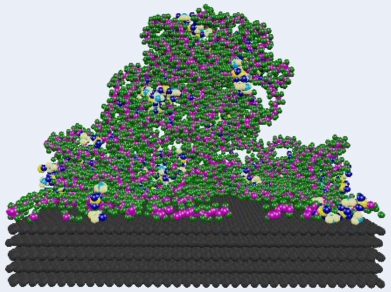
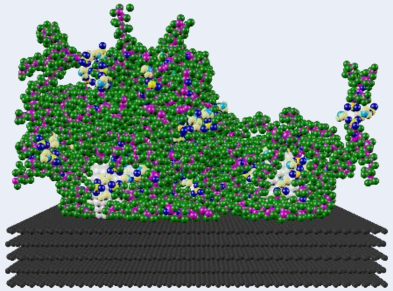
Catalyst layer



Different types of catalyst (HSA, Graphitized)

Sub-micrometer structure of CCL
Simulation of ionomer structure and coating

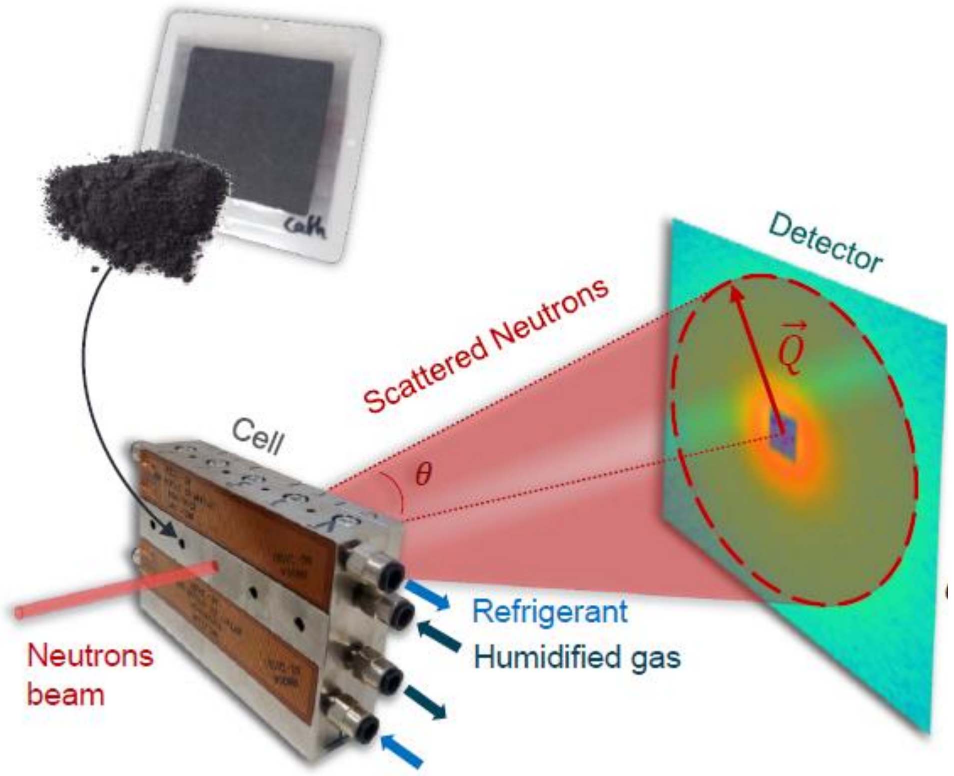
Molecular dynamic simulation (MD)

Pt surface	Graphite surface	Pt on Graphite surface
		
		

Self-assembly on different substrates in IPA

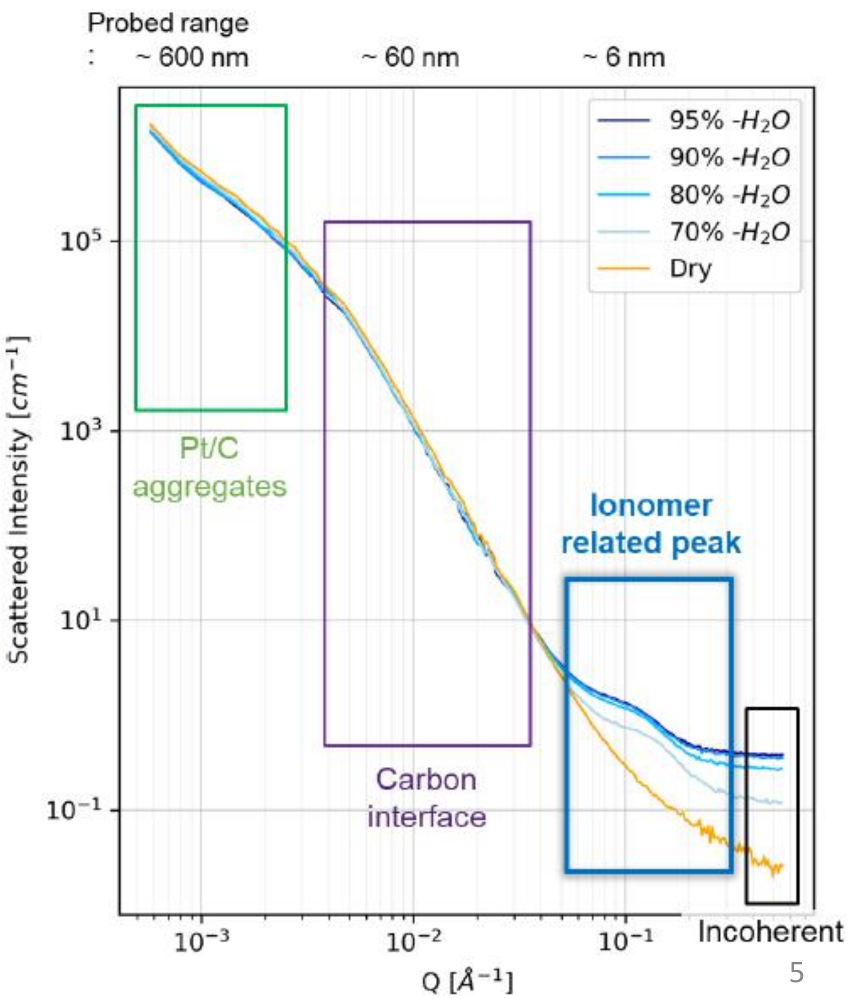
Sub-micrometer structure of CCL
Distribution/structure of ionomer and water

Small Angle Neutron Scattering (SANS)



Integration

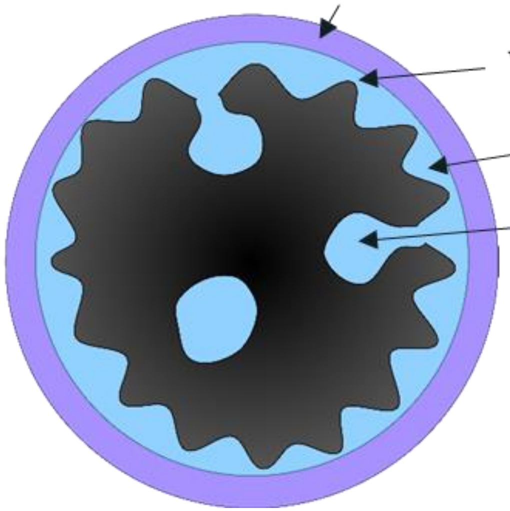
$$Q = \frac{4\pi}{\lambda}.\sin(\frac{\theta}{2})$$



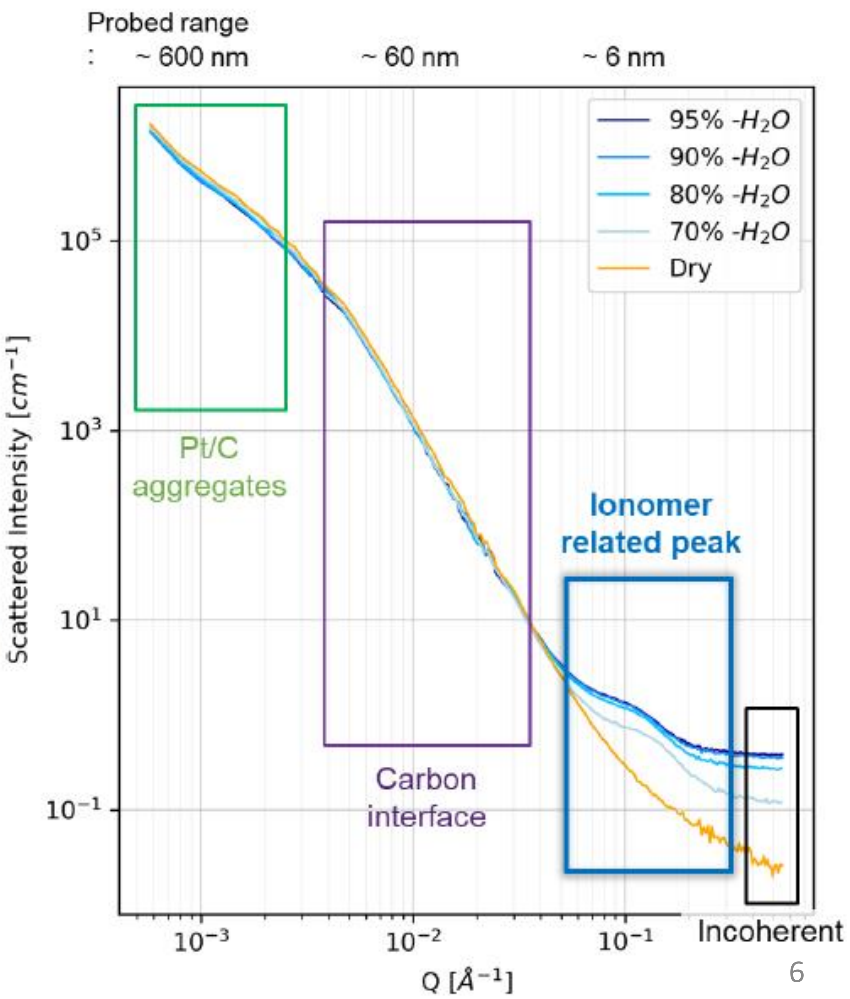
Sub-micrometer structure of CCL
Distribution/structure of ionomer and water

Small Angle Neutron Scattering (SANS)

50% HSA



@ 95%RH
- Ionomer film : 24 Å
- Water film : 8 Å
- Pores depth : 35 Å



Water volume fraction = **23%**
against 25% (water sorption)

Sub-micrometer structure of CCL
Ionomer coverage and thickness

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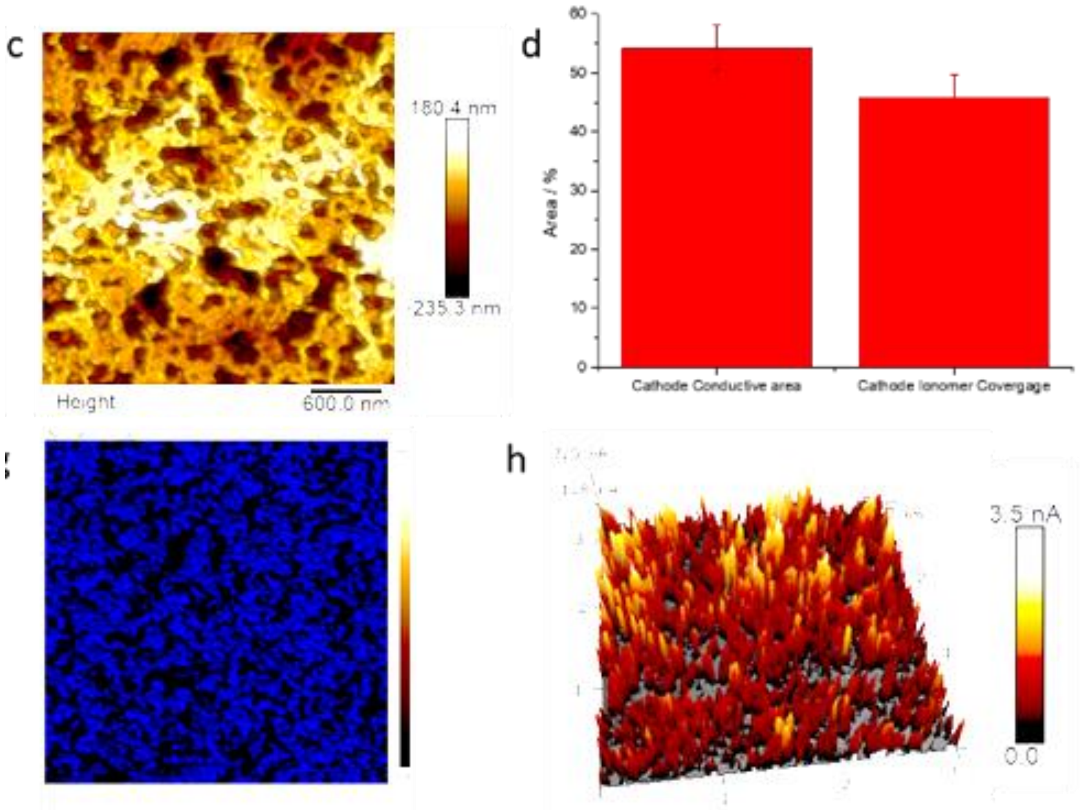
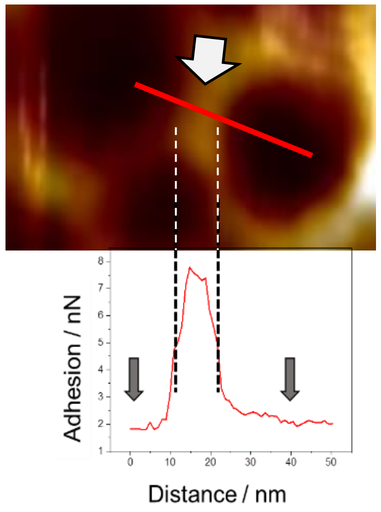
Atomic Force Microscopy (AFM)

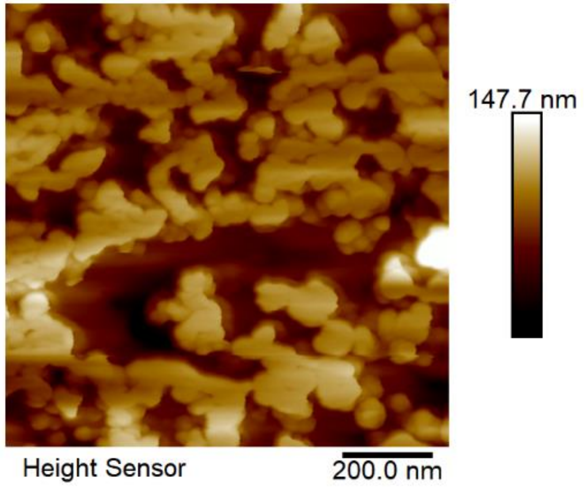
Coverage

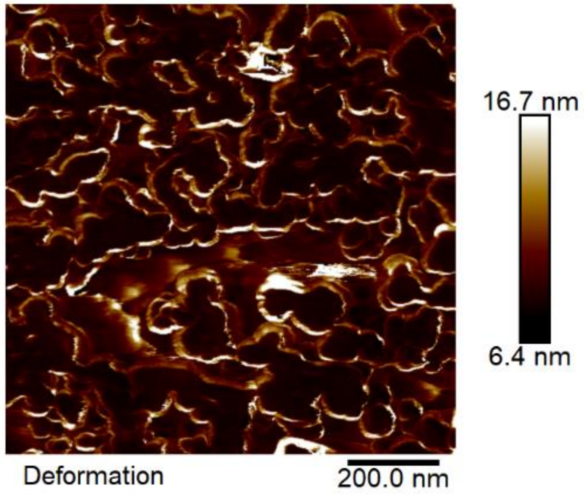


MATLAB Evaluation



Thickness

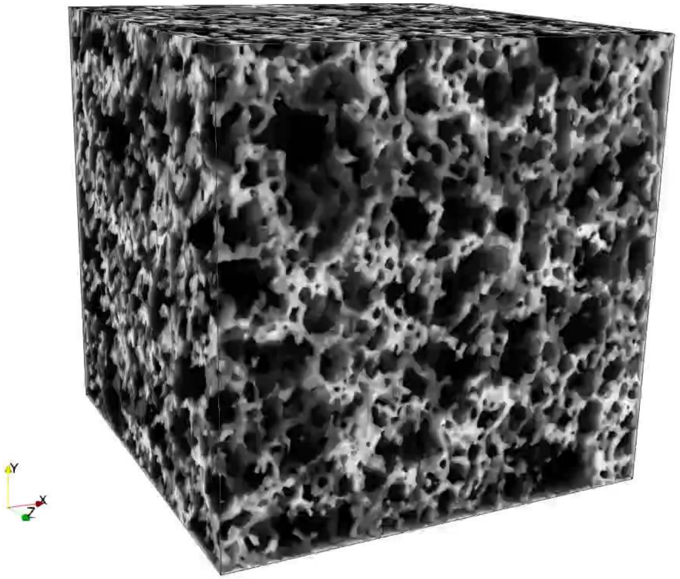


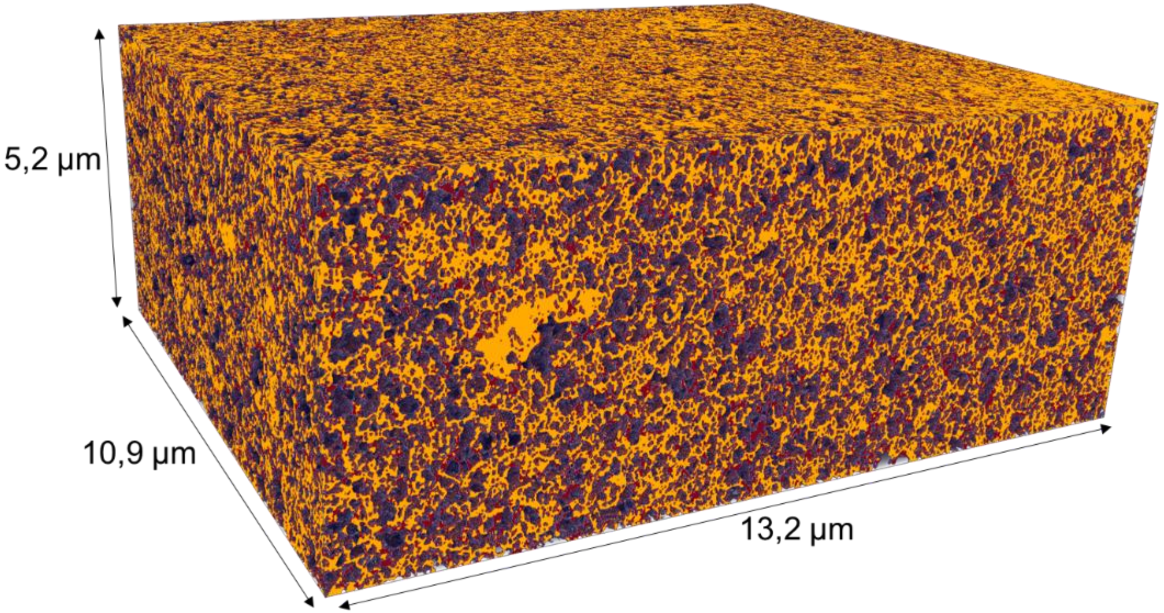


Structure of CCL
3D porous structure

3D FIB-SEM

Voxel size: 5x5x5 nm^3

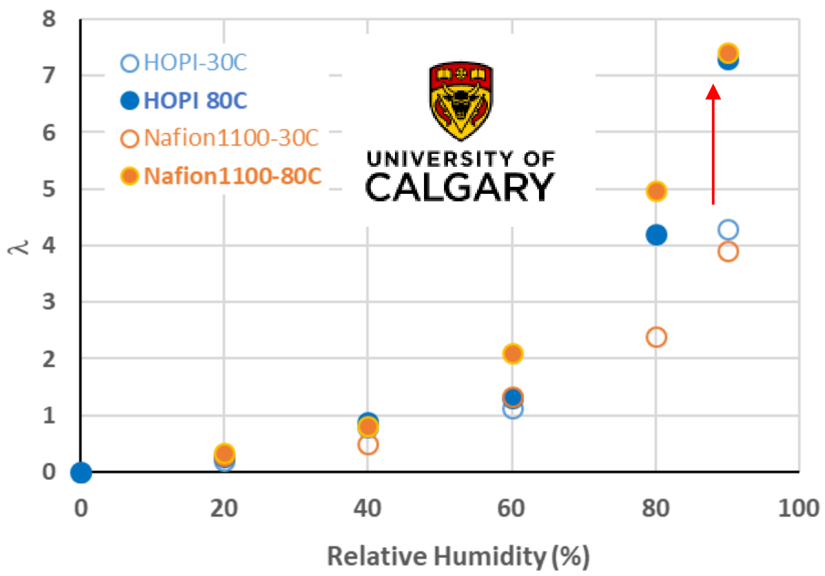




Measurement of thin ionomer films properties
Structure and mechanic

Swelling

Ellipsometry



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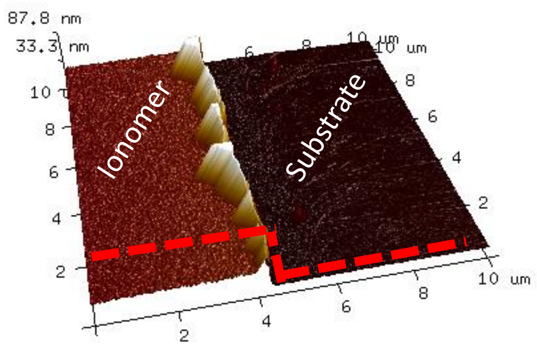
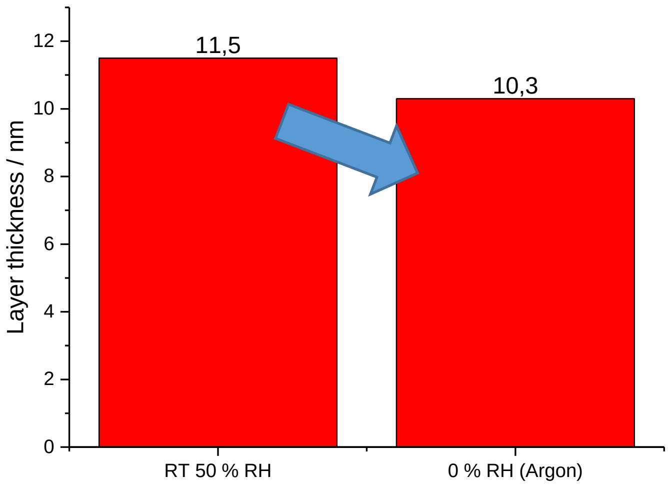
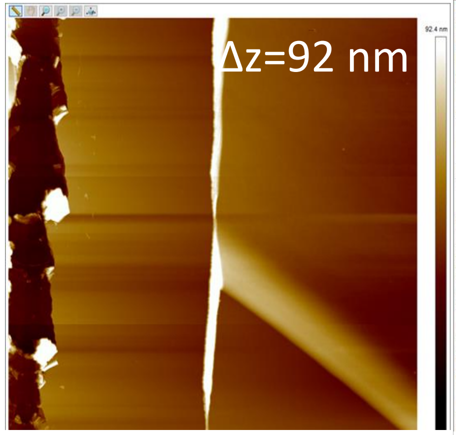
AFM



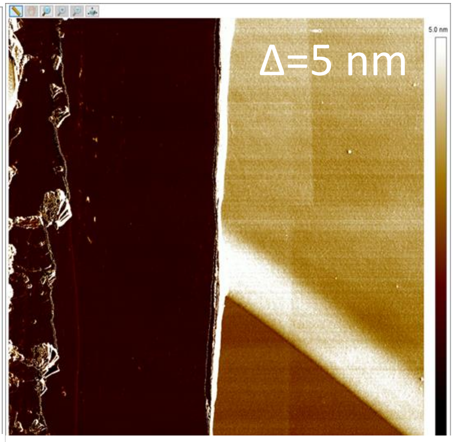


AFM

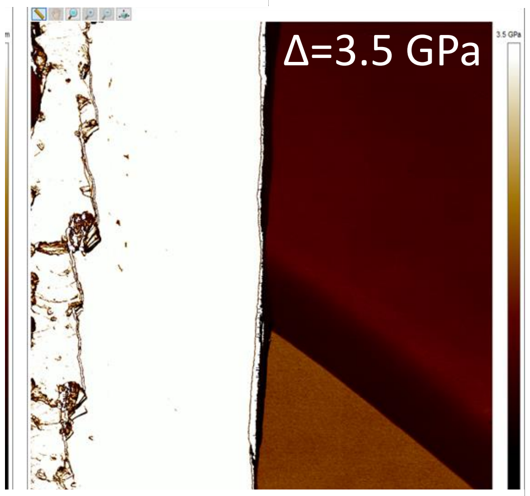
Nanomechanical Properties



Height (20 µm)



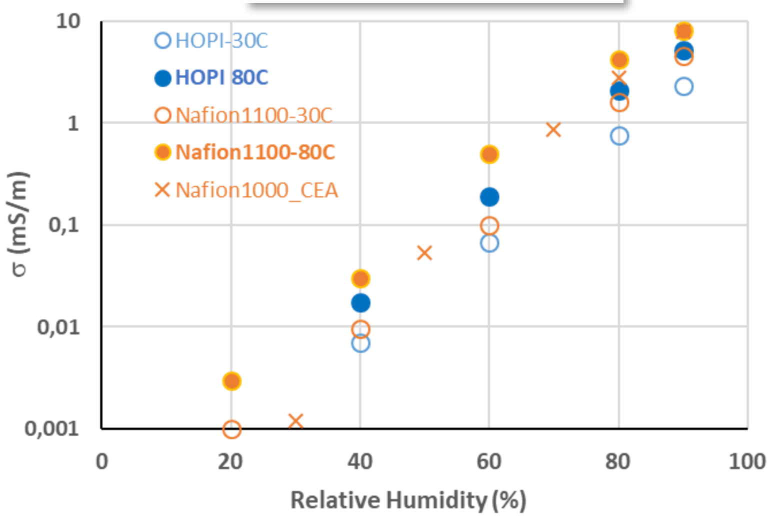
Deformation (20 µm)

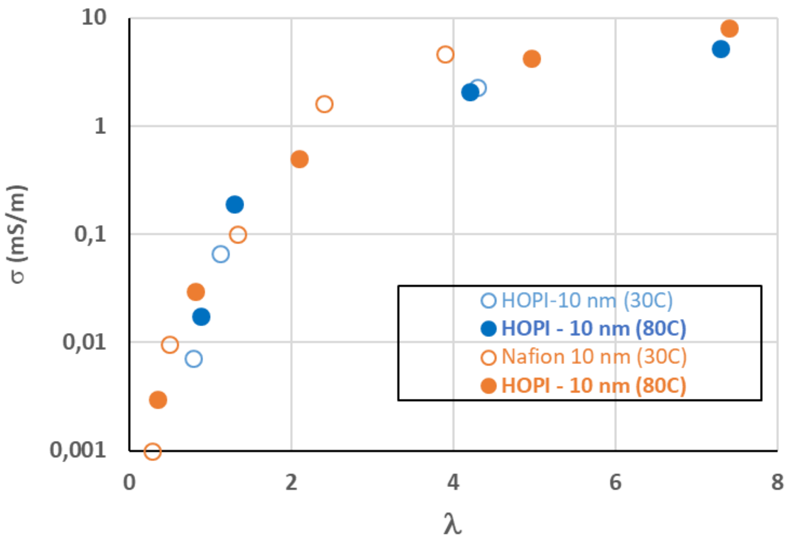


Stiffness (20 µm)

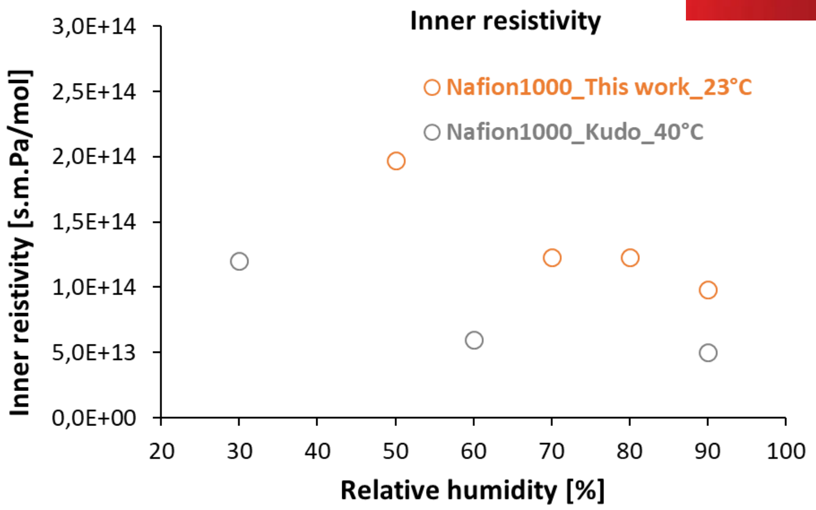
Measurement of thin ionomer films properties
Transport

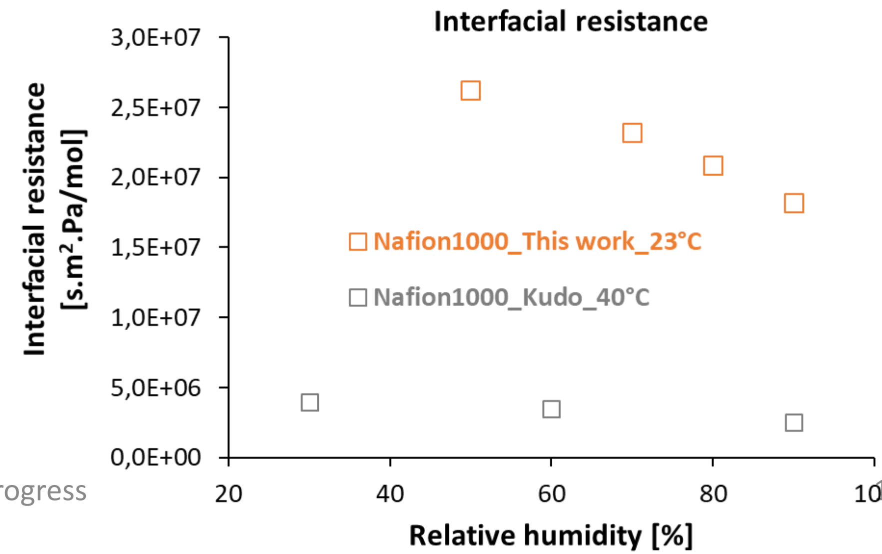
H^+ conductivity





O_2 effective resistance





Measurement of CCL properties
Hydrophilicity/Hydrophobicity

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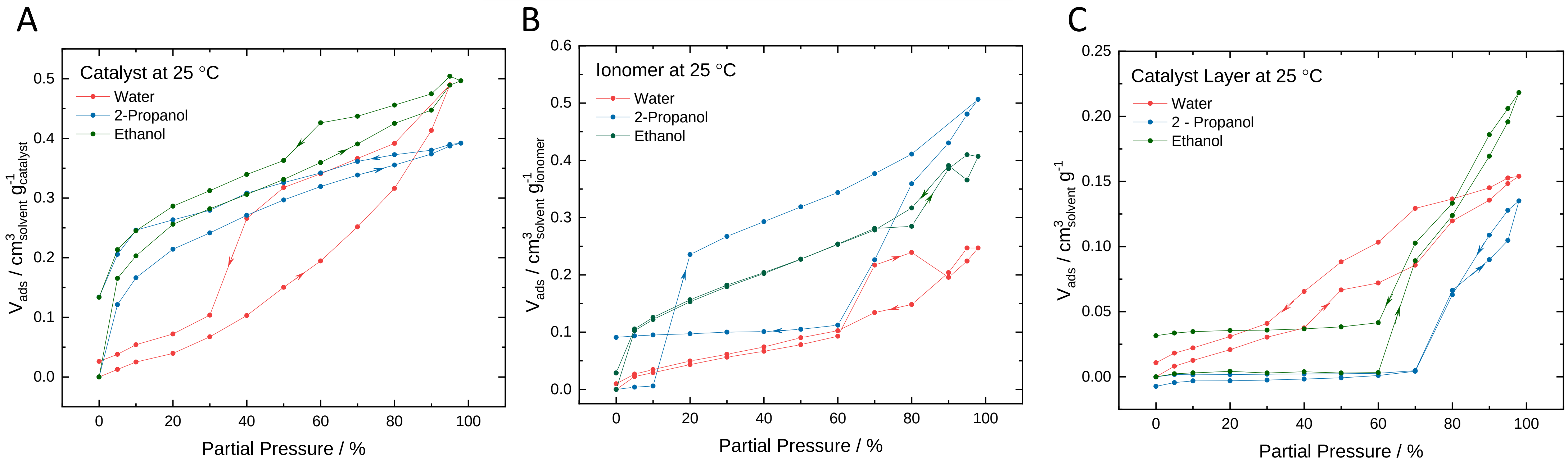
Solvent sorption measurements



Calculated parameters	Catalyst Powder	Catalyst Layer
γ_s / mJ m^{-2}	117 ± 3	105 ± 1
γ_s^d / mJ m^{-2}	19.4 ± 6.3	2.5 ± 0.3
γ_s^p / mJ m^{-2}	97.8 ± 9.4	103 ± 1
π_e / mJ m^{-2}	29.2 ± 8.7	6.1 ± 7.0
W_{s-l} / mJ m^{-2}	105 ± 67	85 ± 64

$$\pi_e = \frac{RT}{MS}\int_P^{P'} \frac{Q}{P}\, dP$$

$$W_{s-l} = 2\gamma_L + \pi_e = 2\sqrt{\gamma_L^d \times \gamma_s^d} + 2\sqrt{\gamma_L^p \times \gamma_s^p}$$

$$\gamma_s = \gamma_s^p + \gamma_s^d$$

P = Partial pressure
$\boldsymbol{\gamma_s}$ = surface tension of the catalyst
comγ_s^d = dispersive component of catalyst surface tension
γ_s^p = polar ponent of catalyst surface tension
$\boldsymbol{\gamma_L}$ = surface tension of the liquid
π_e = spreading pressure (θ=0º)
W_{s-l} = Work of adhesion
M = molar mass of liquid, S = specific surface area, T = temperature and R = gas constant and Q = total amount adsorbed.

Catalyst layer wetting properties does not seem to be a simple combination of the individual components

Measurement of CCL properties
Transport: local distribution in properties

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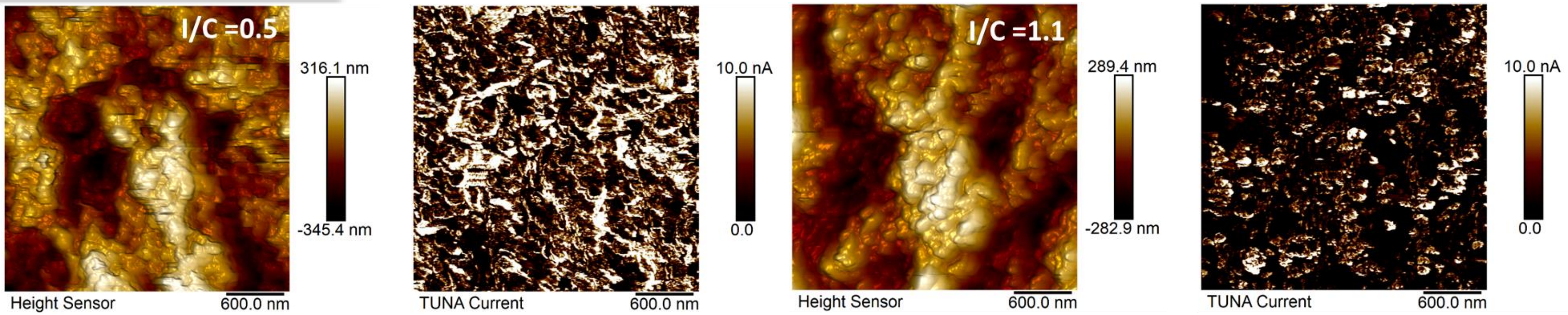
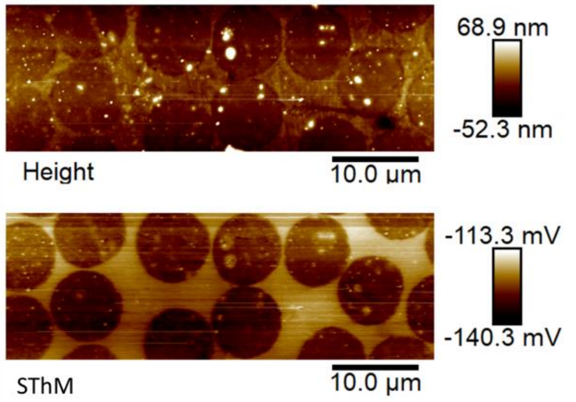
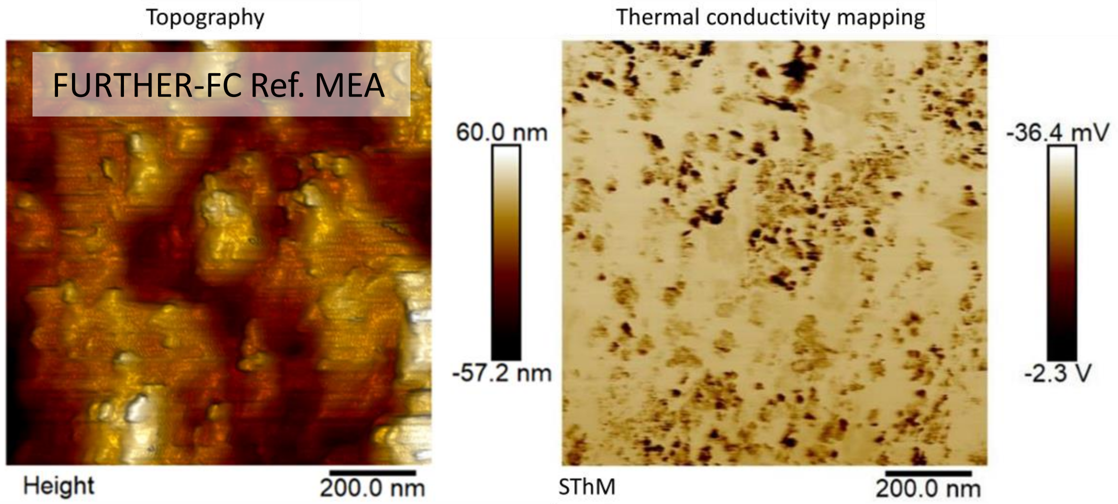
Electronic conductivity



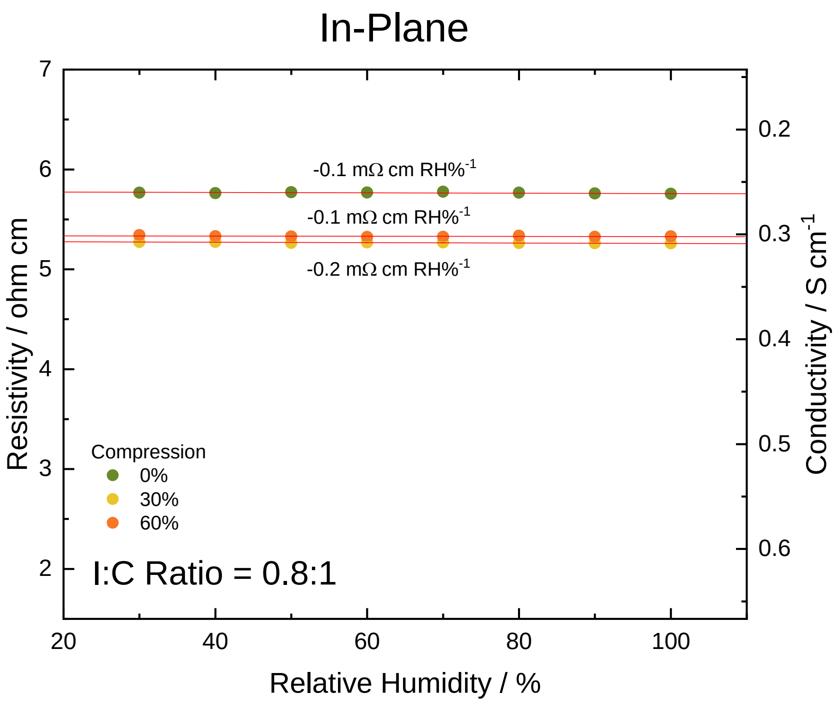
Thermal conductivity

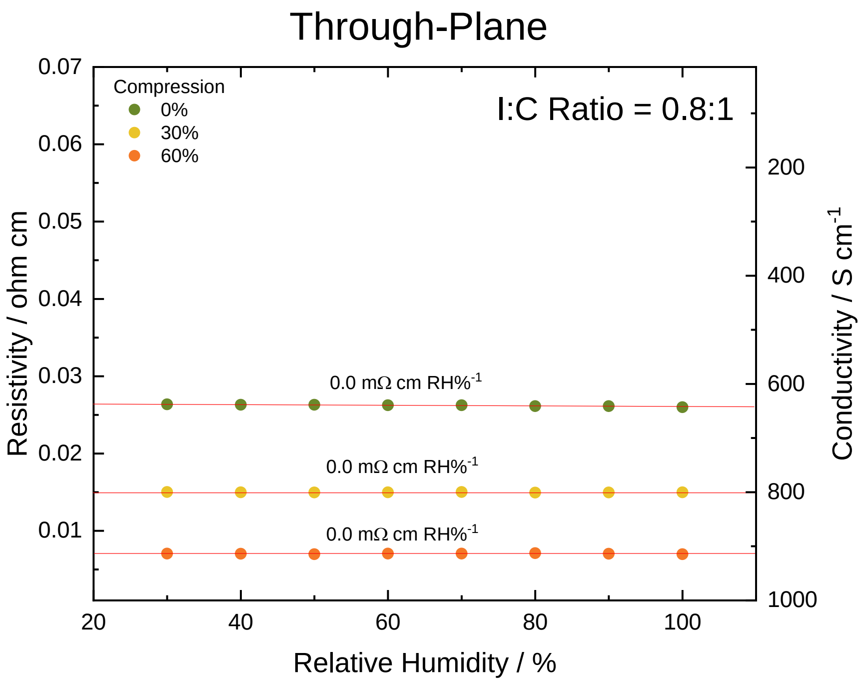
Reference sample: Carbon fibers in resin





Measurement of CCL properties
Transport: effective electronic conductivity

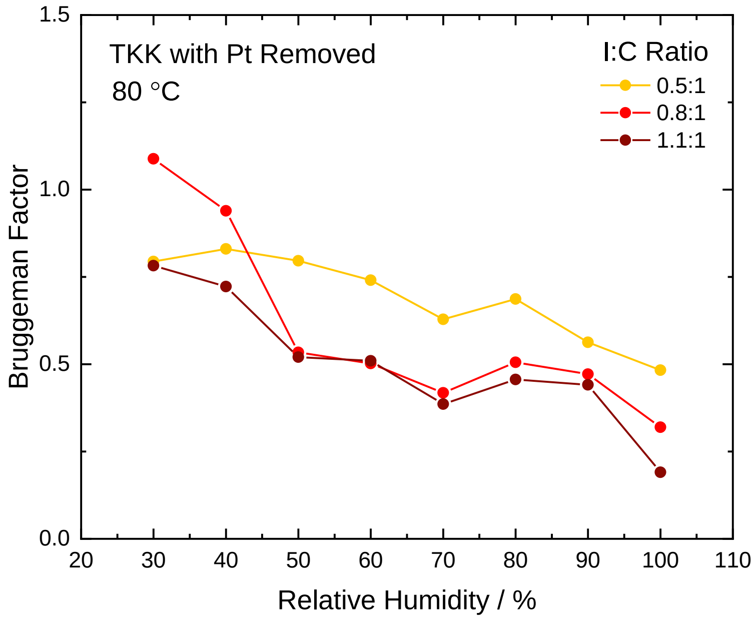


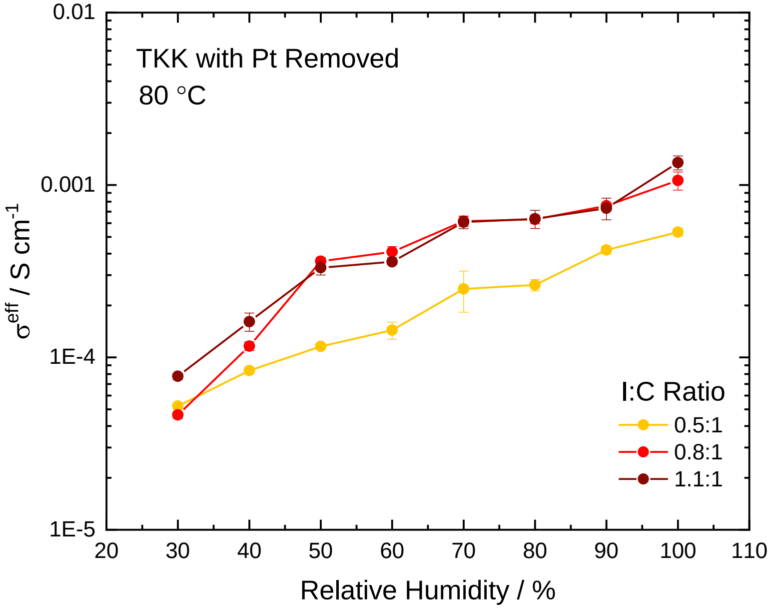


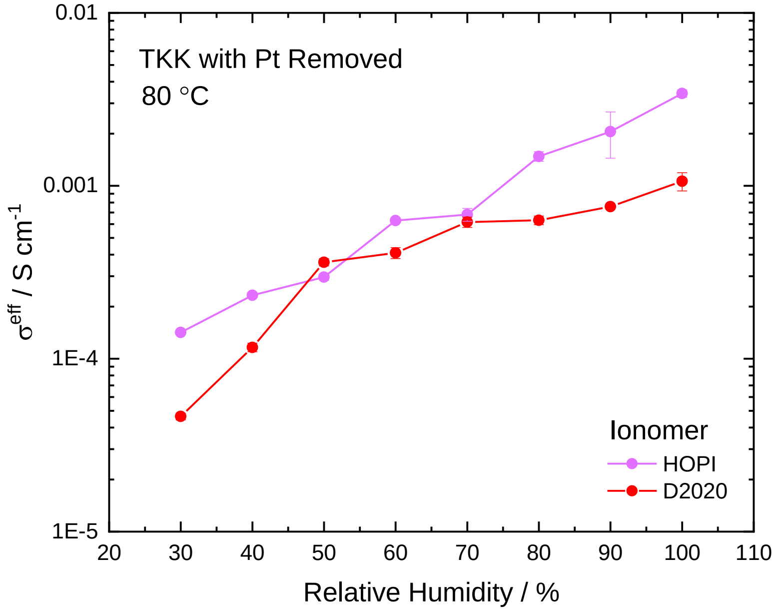
- Increase in electronic conductivity as compression is increased
- Little change in conductivity as relative humidity is increased
- Two orders of magnitude lower conductivity in catalyst layer only for in-plane conductivity
- Increase in conductivity as I:C ratio is decreased
- Two orders of magnitude higher conductivity in through-plane vs in-plane

RH has little effect on electronic conductivity
➔ swelling of ionomer does not affect particle-particle contact

Measurement of CCL properties
Transport: effective through-plane proton conductivity



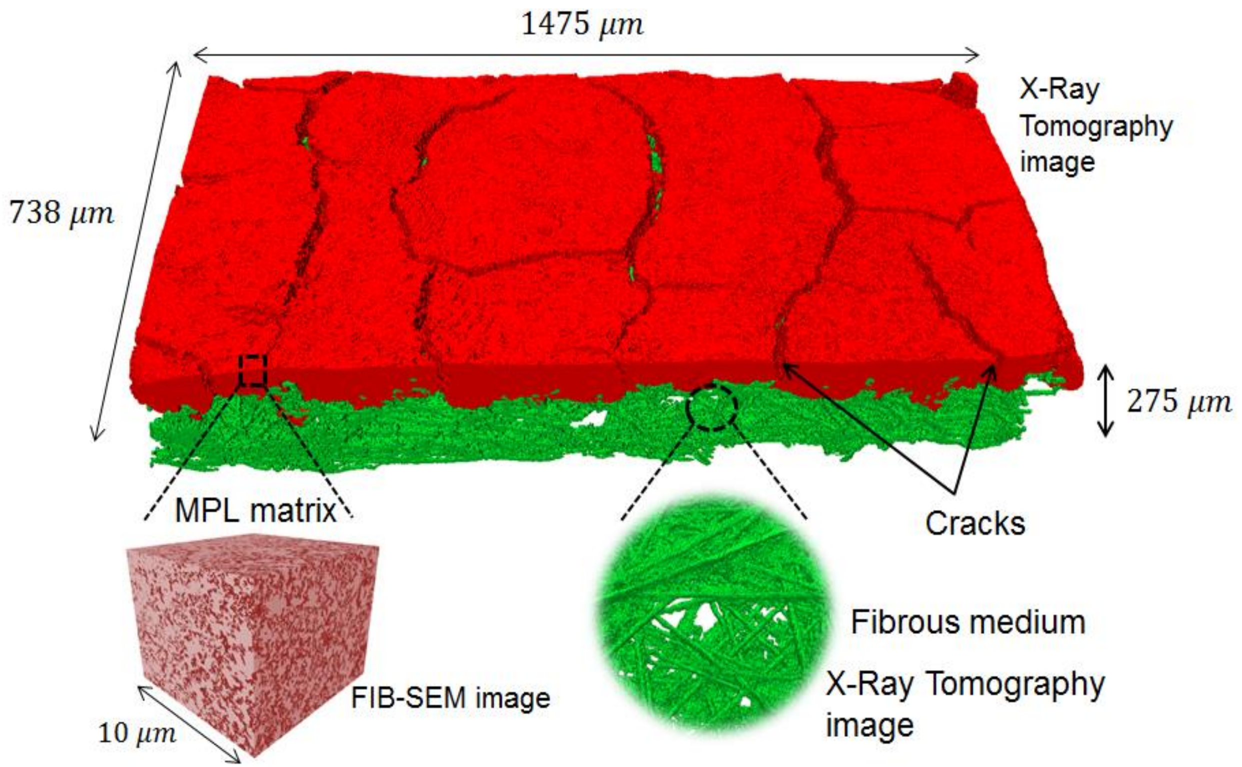




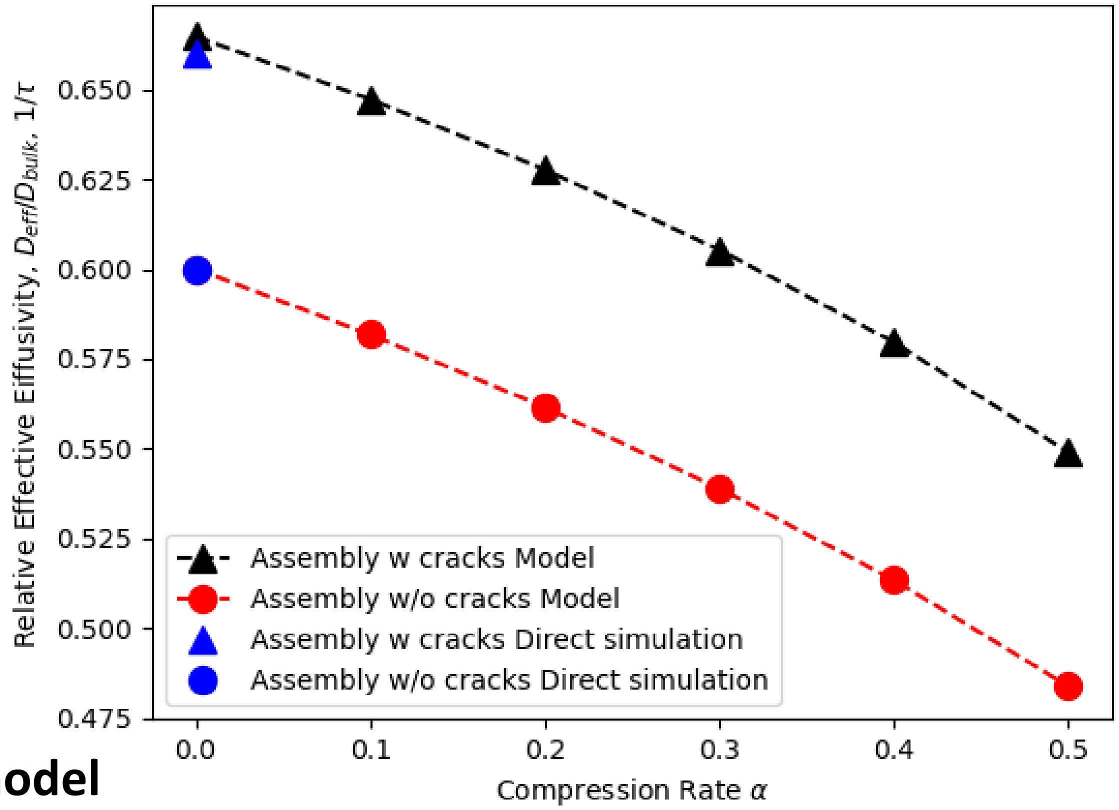
- Increase in proton conductivity as RH increases
- Increase in proton conductivity as I:C ratio increases
- Increase in proton conductivity when using HOPI ionomer
- Decrease in Bruggeman Factor as RH increases
- Little change in Bruggeman Factor with different I:C ratios

Proton conductivity in catalyst layer is liable to be a limiting factor in performance

Computation of properties from 3D structure
Transport: (ex. MPL)



Relative effective diffusivity



MPL computation from FIB-SEM
GDL/MPL assembly computation from X-ray Tom.
GD/MPL compression effect computation via resistance model

Simulation of sub-micrometer CL operation
Lattice-Boltzmann Modeling

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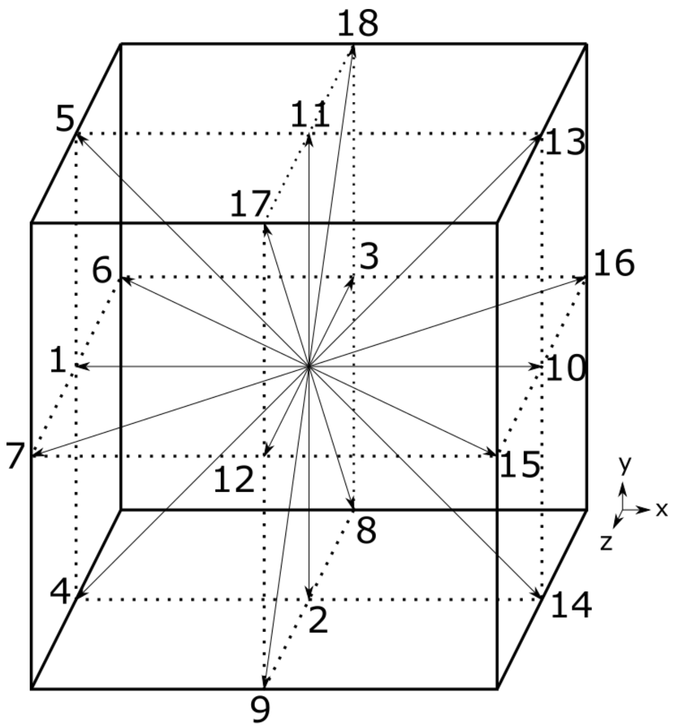
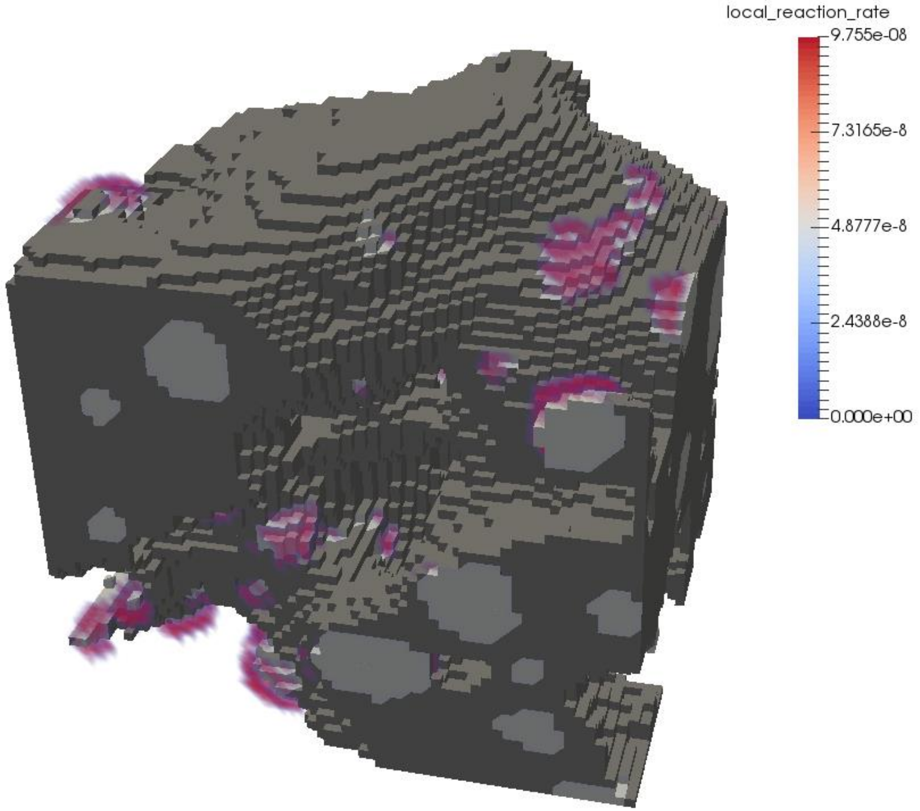


D3Q19

Local reaction rates within real CCL microstructures



Effect of CL structure on the local ORR rate and transport

Simulation of sub-micrometer CL operation
Direct numérical simulation

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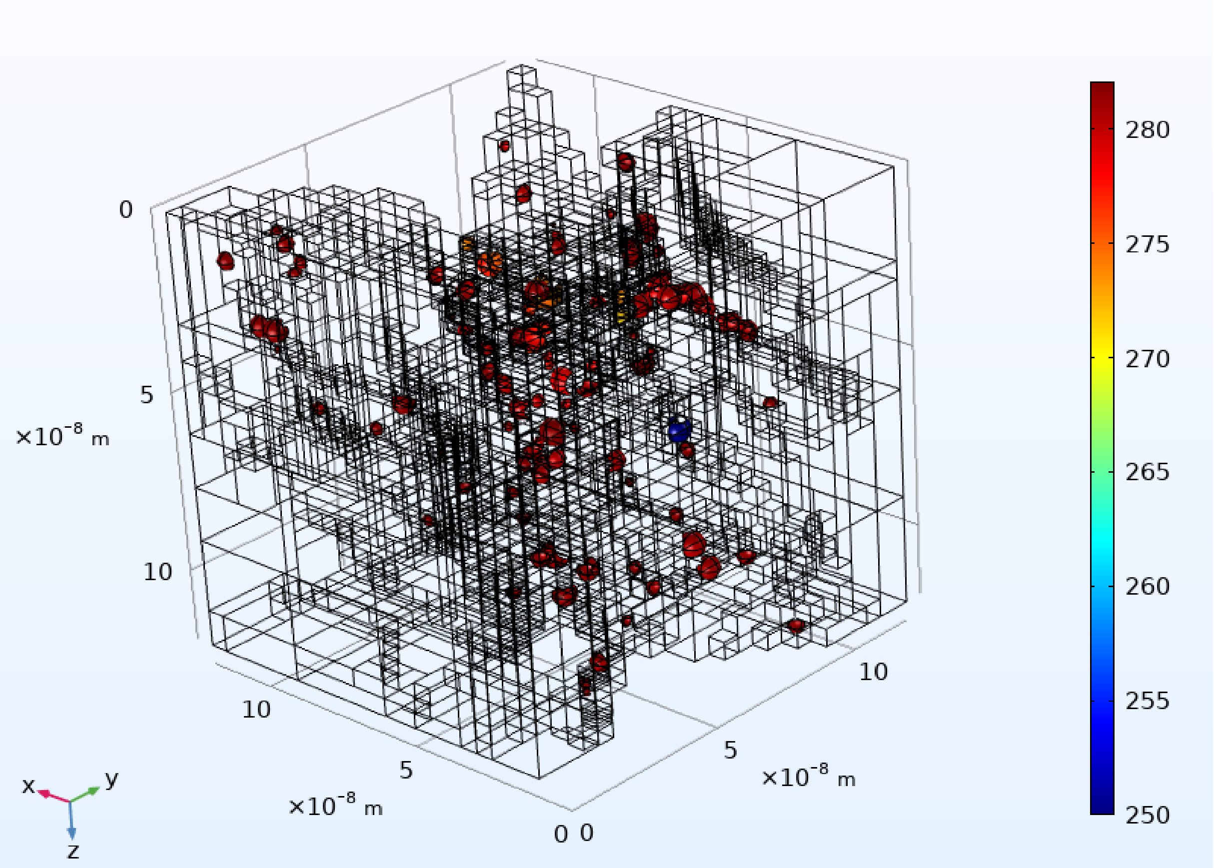
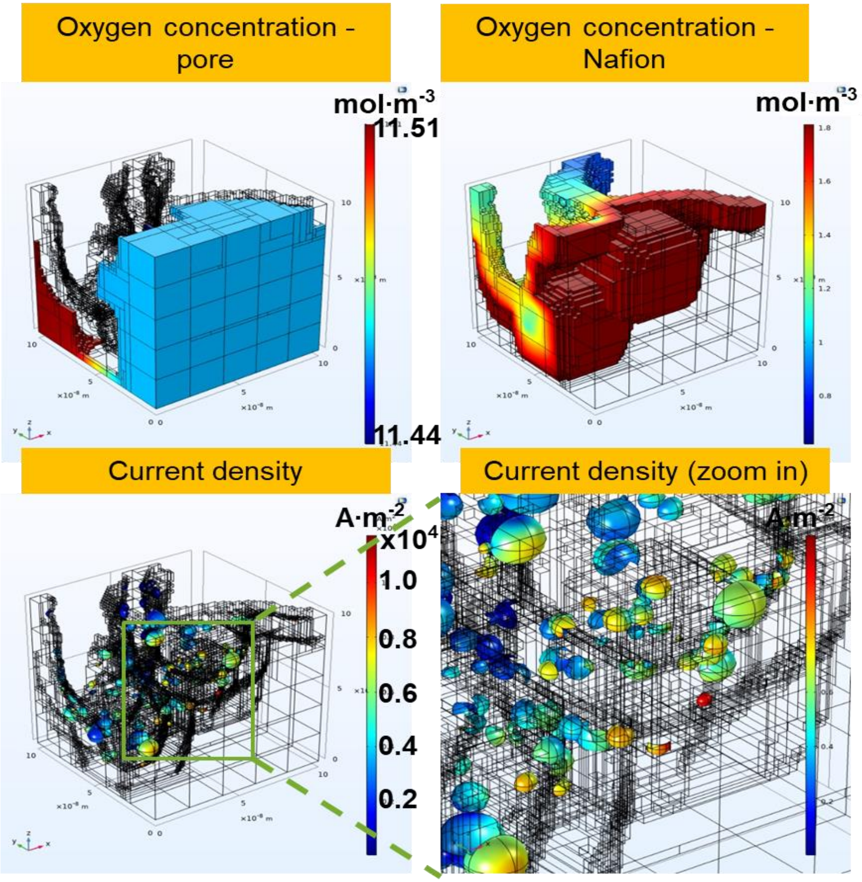
Local O_2 concentration and current density within real CCL microstructures





Fuel cell characterisations
Reproducibility between partners

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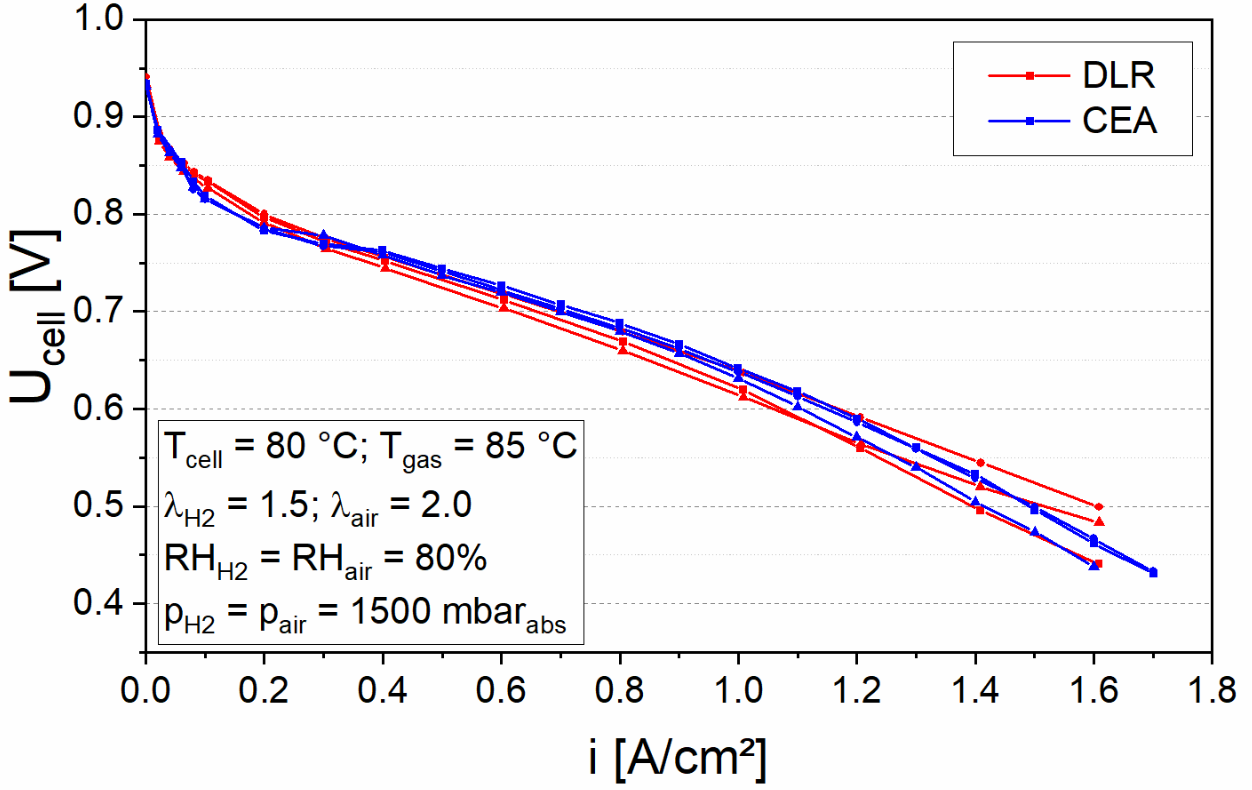
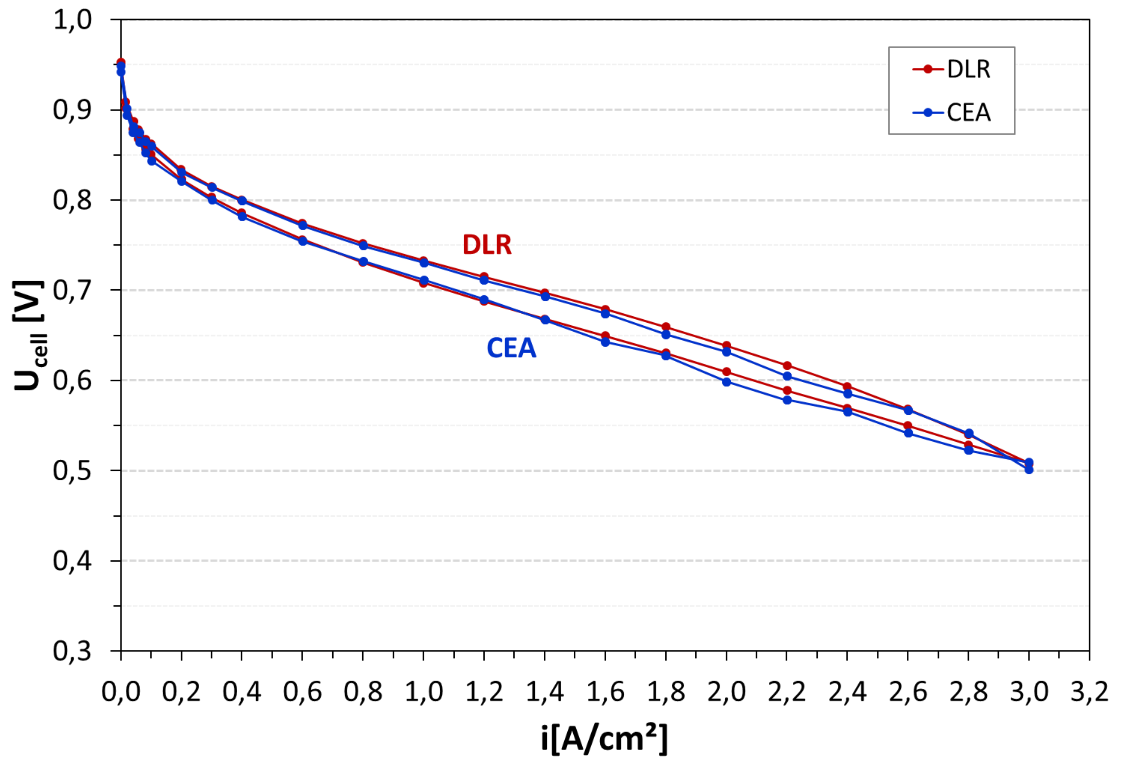
German Aerospace Center

Technical cell

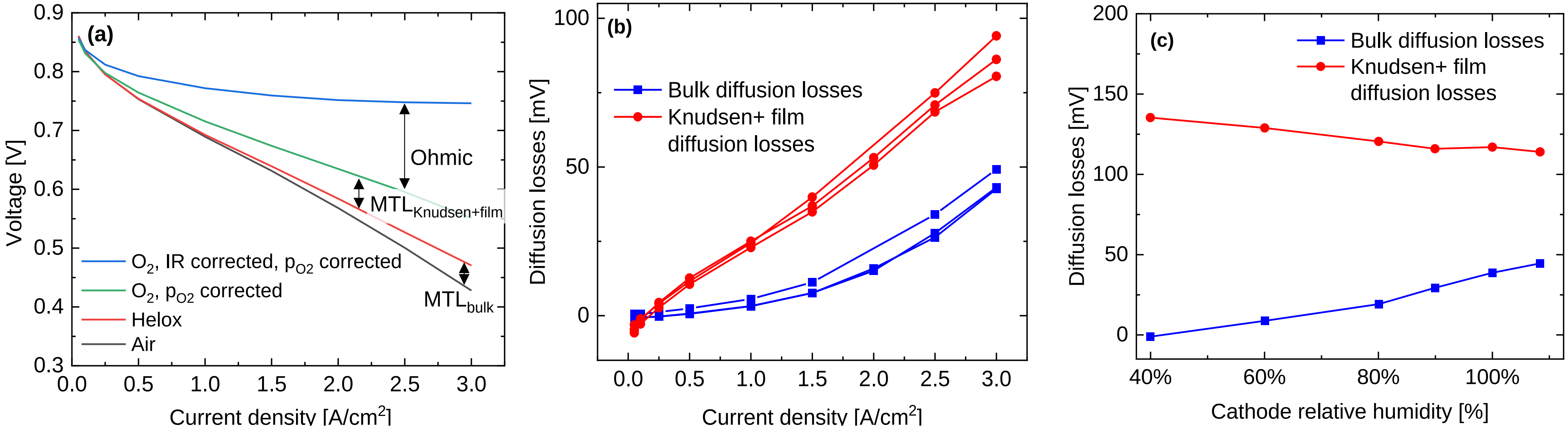


Differential cell



Fuel cell characterisations
O2 transport limitations

Pulse Gas Analysis (PGA)

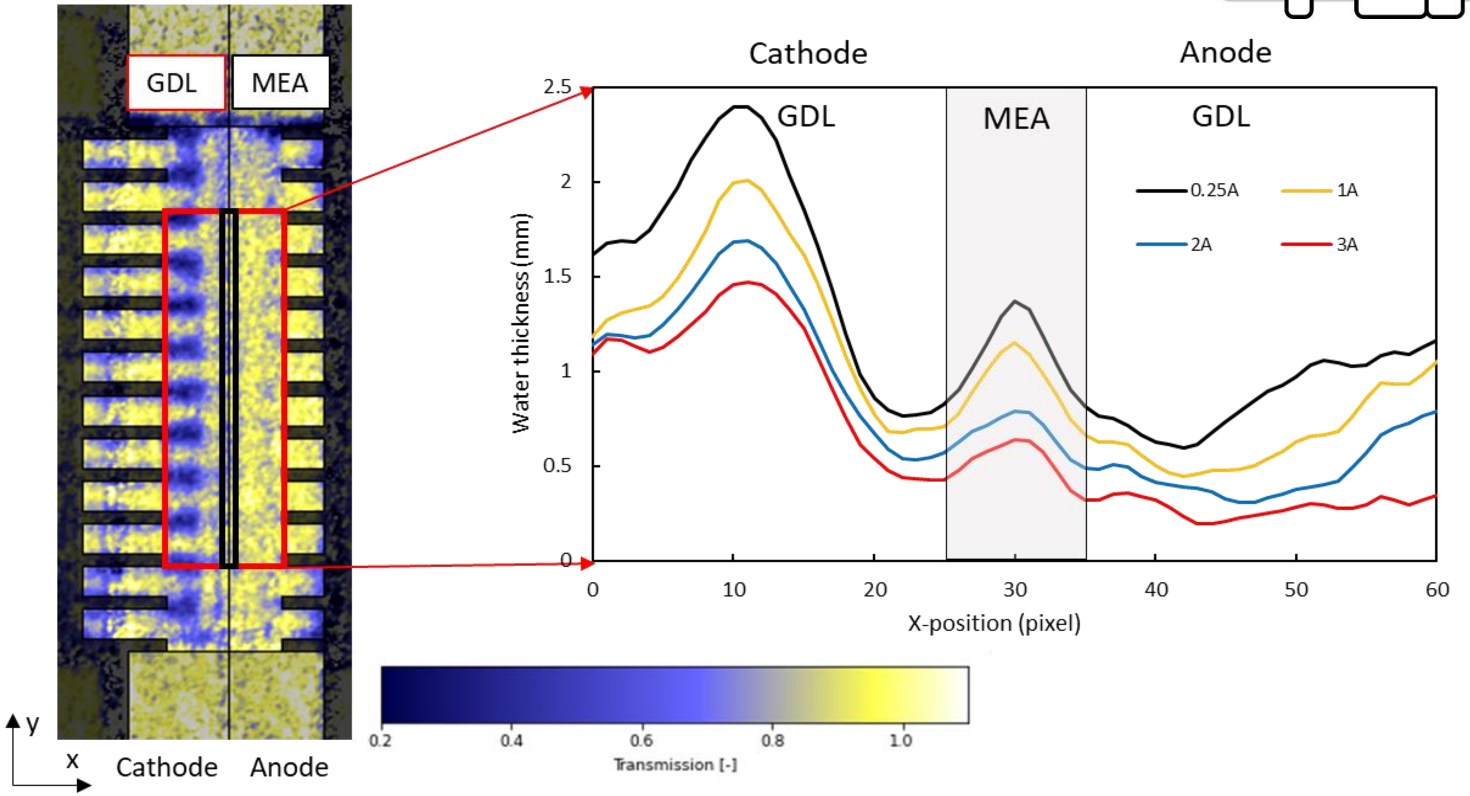


Bulk diffusion losses only observed at high cathode humidity

« Knudsen+film » diffusion losses dominate, in particular at low humidity

Local operating conditions
Water content in MPL/GDL

Neutron Radiography

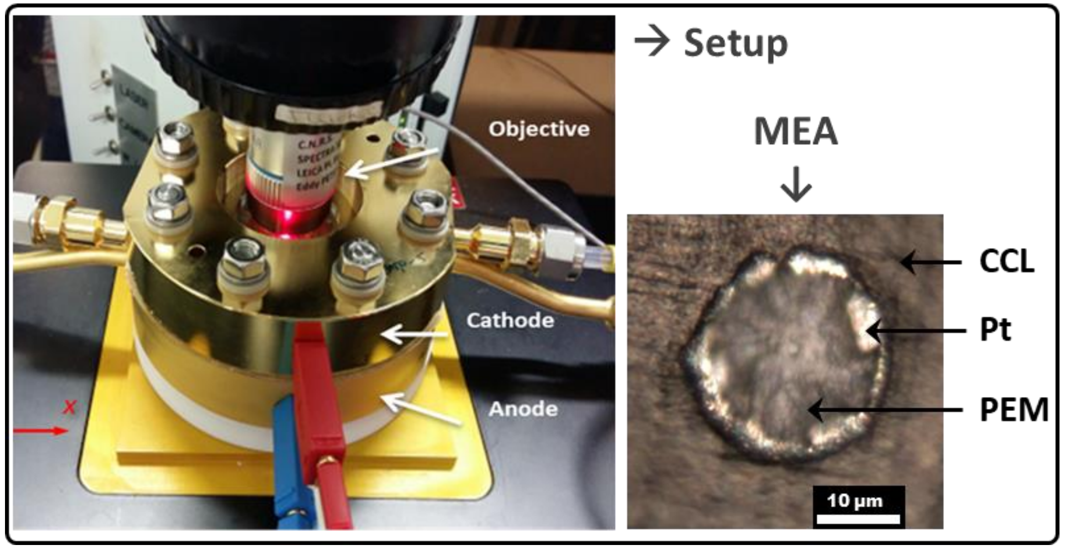


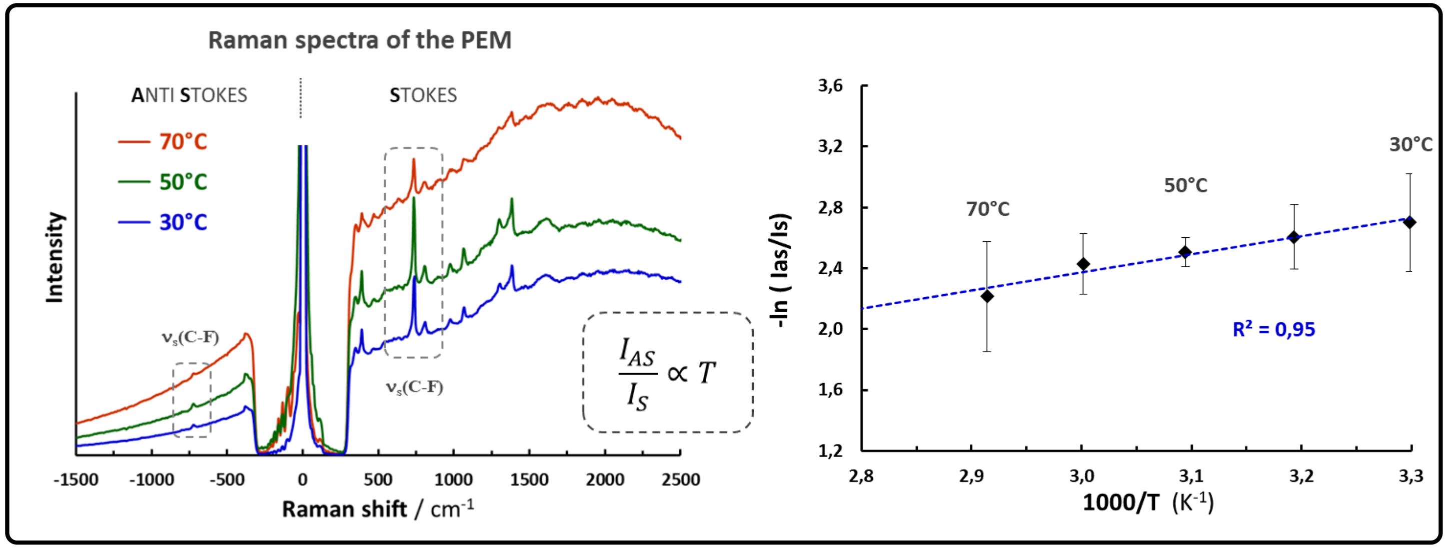
Even with these narrow land flow fields, land/channel differences are observed

At full humidity, water saturation is reduced when increasing current density

Local operating conditions
Local temperature

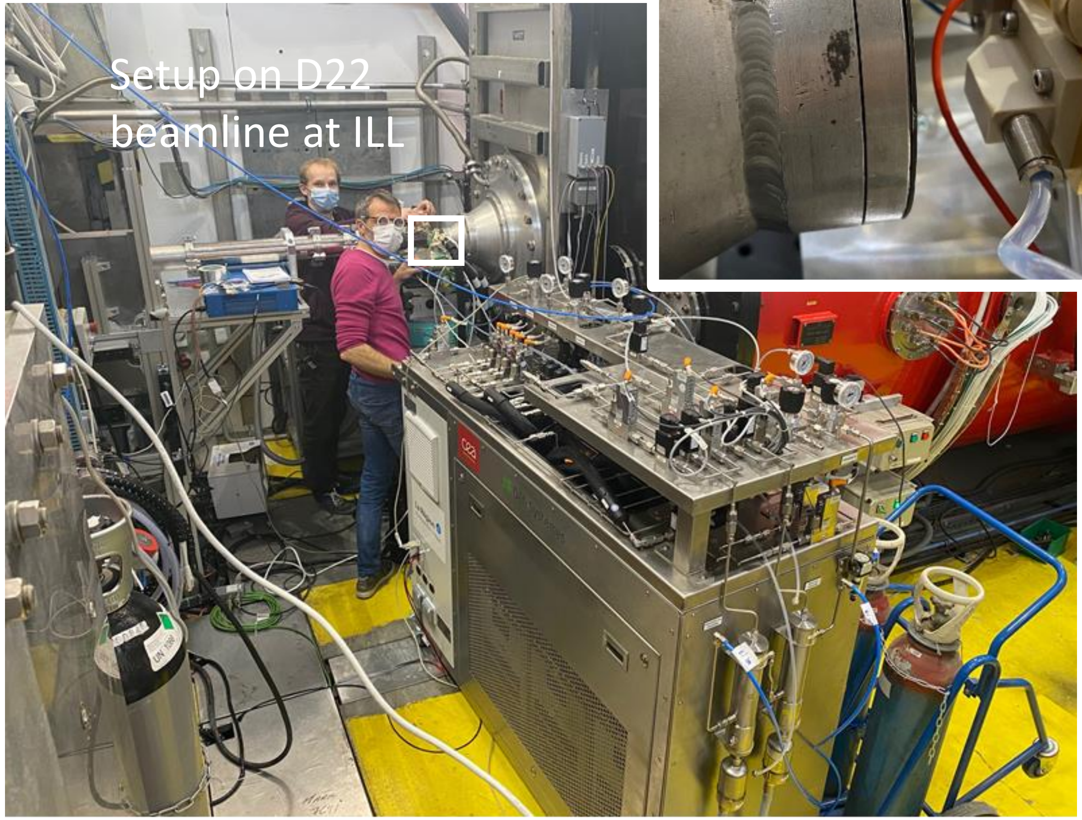
Raman microspectroscopy thermography



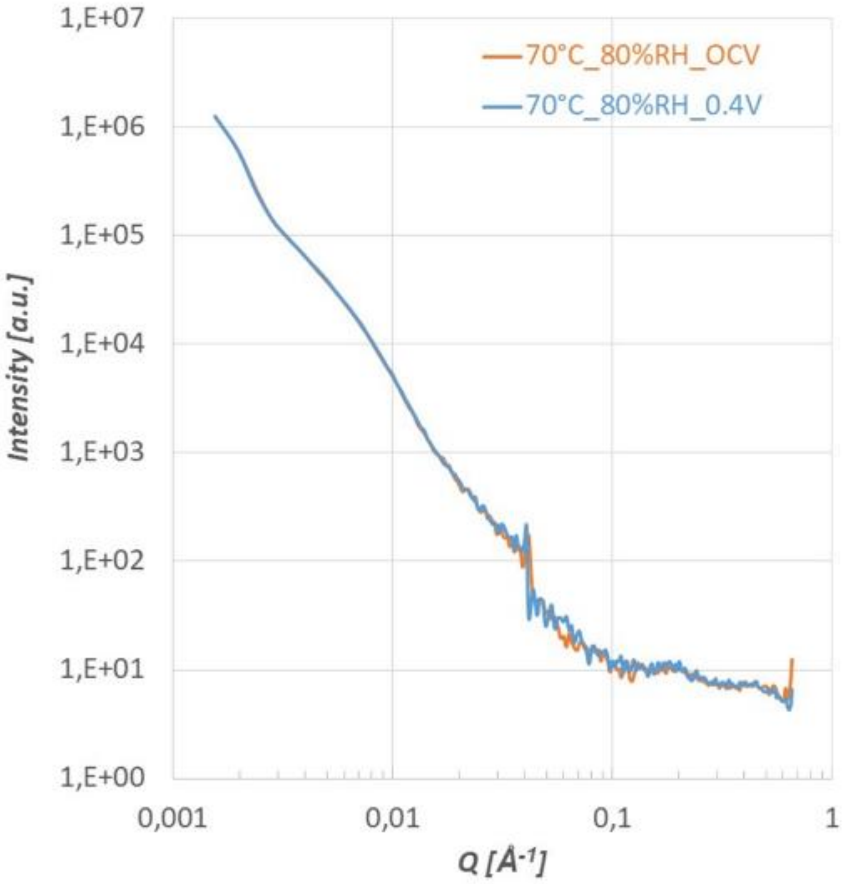


Local operating conditions
Water content in CL

Small Angle Neutron Scattering



1D SANS profiles during operation



Simulation of fuel cell operation

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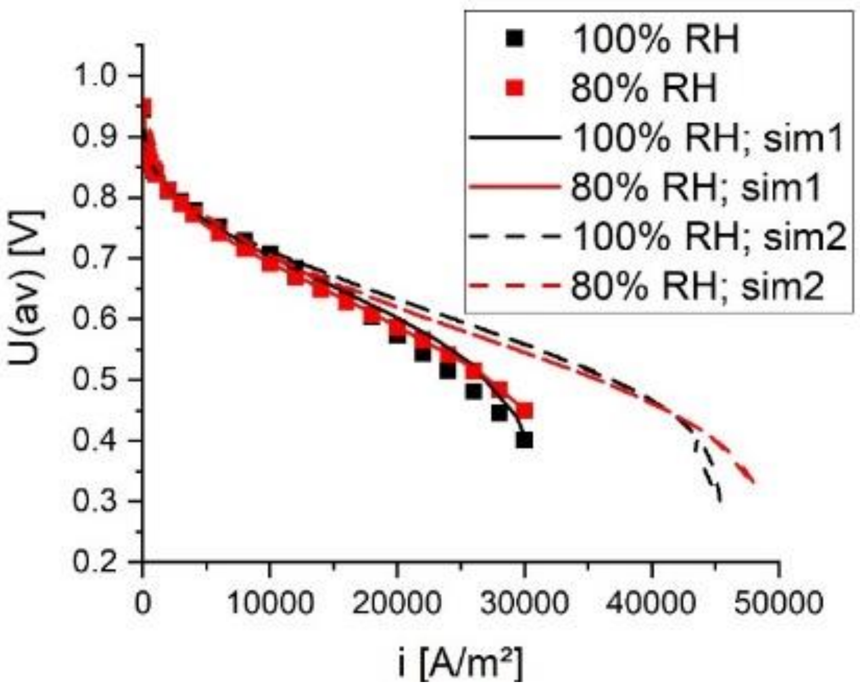
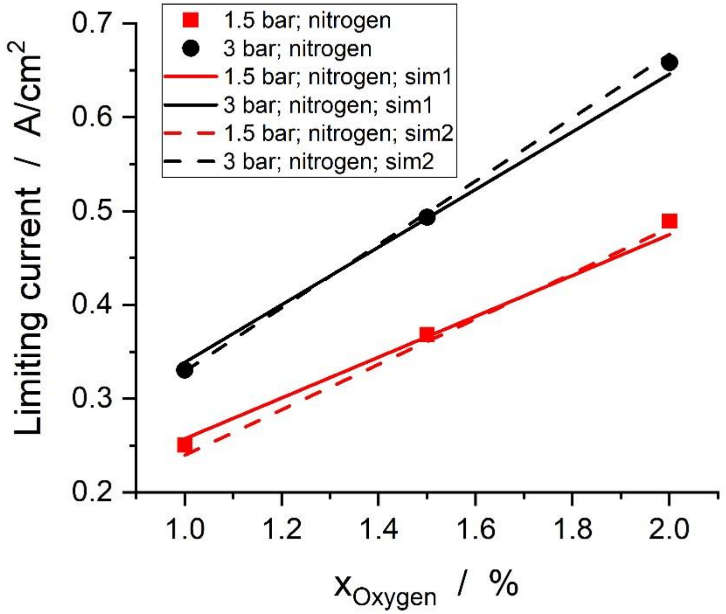
Development and validation of single cell model

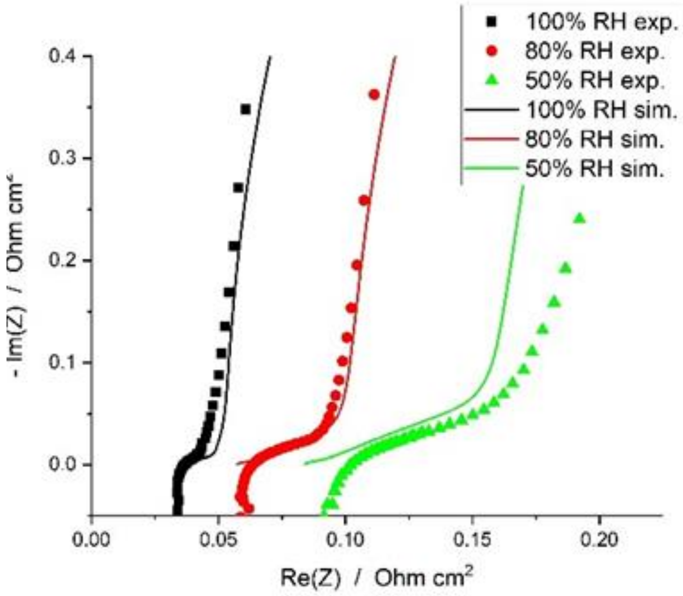
Polarisation curves



LCA

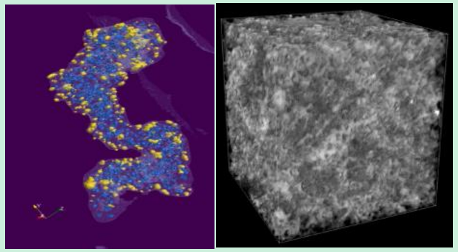


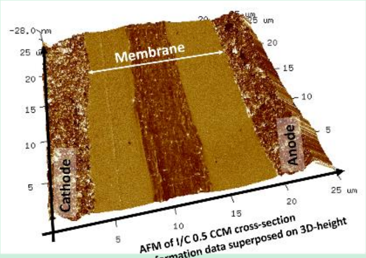
EIS



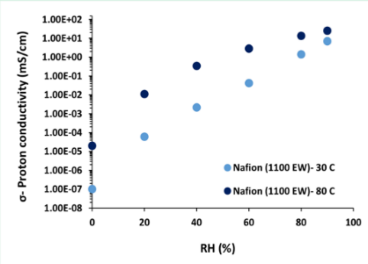
Thank you for your attention.
Your questions are welcome!

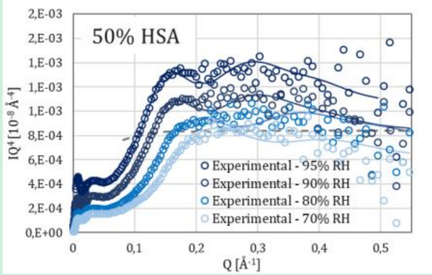
Multiscale characterization



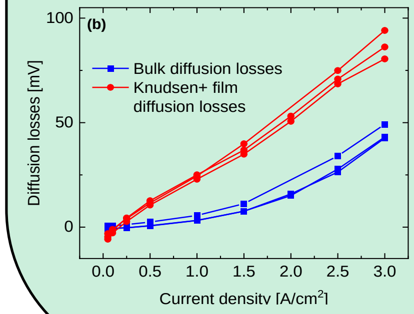


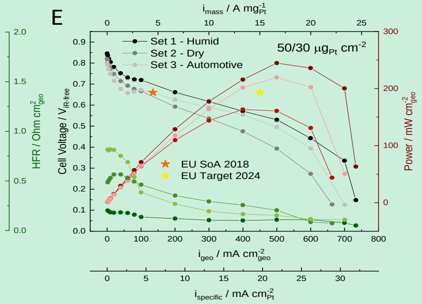
3D TEM and FIB/SEM *AFM*



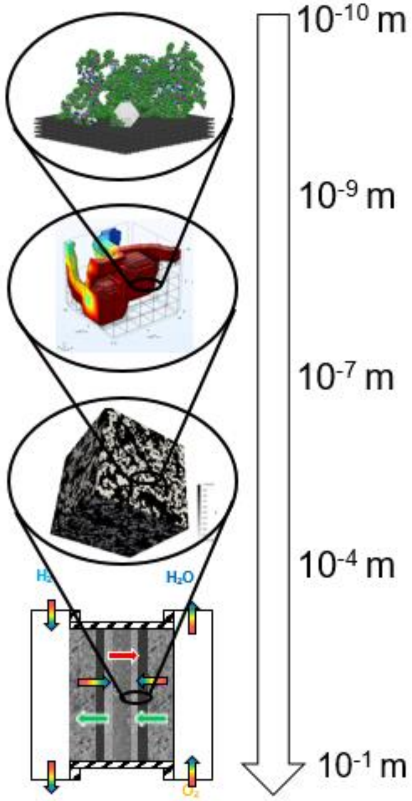


Ionomer transport properties *Small Angle Scattering*



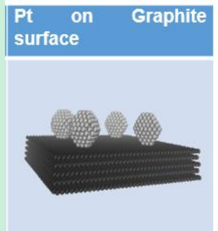


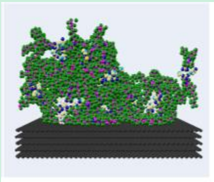
Mass transport losses *Ultra-thin electrode*

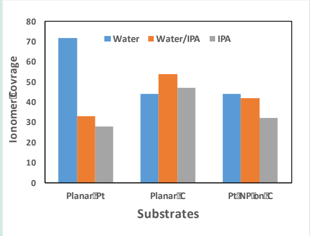


Multiscale modeling

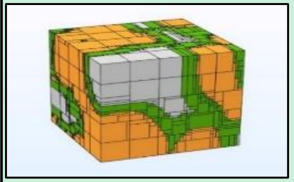
Ionomer film scale



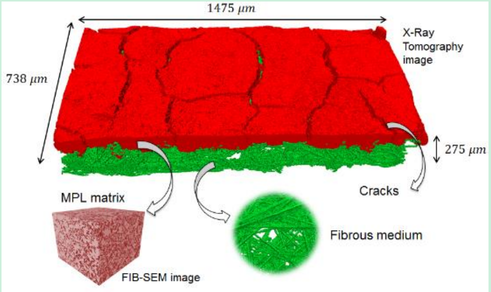




Sub µm scale



CCL scale



Cell scale