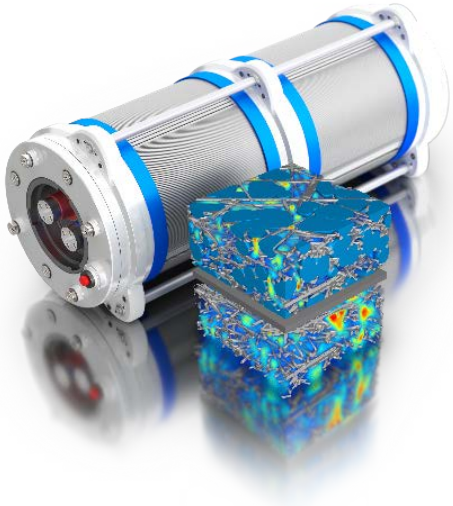
Simulation Based Design of Fuel Cell and Battery Materials

Math2Market GmbH



Who is Math2Market ?

- Math2Market GmbH was founded 2011 in Kaiserslautern.
- Spin-off of Fraunhofer Institute for Industrial Mathematics, ITWM.
- Today: 13 full-time, 6 part-time employees, turnover >2 Mio € / year

- Our product: GeoDict software
  - Sales
  - Development and Customization
  - Consulting

What is GeoDict?

GeoDict is a digital material laboratory

- Computer Aided Material Engineering and Design by providing Geometric models and preDictions of material properties.

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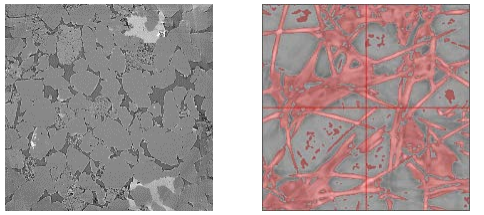

Import of CT Scans

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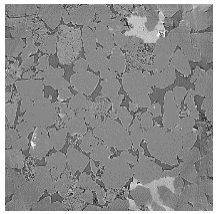

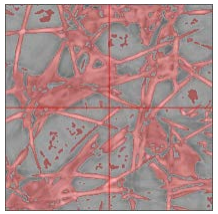

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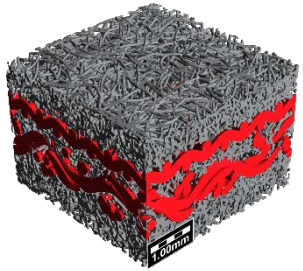

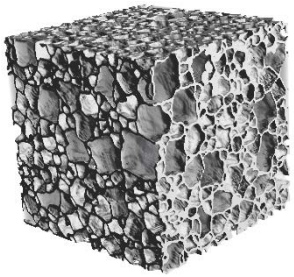

Create 3D Models of Micro-structures

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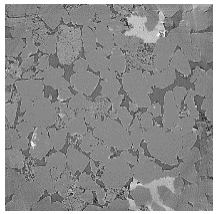

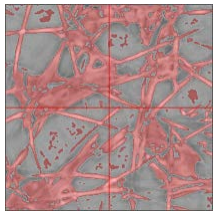

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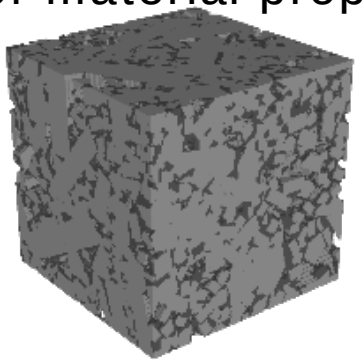
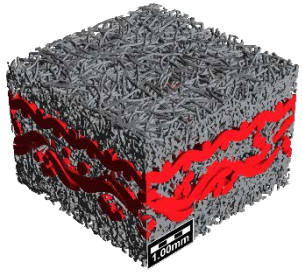
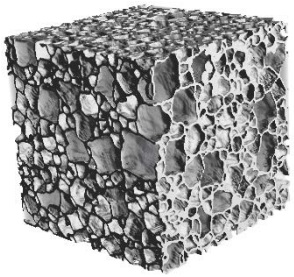


Geometric Analysis of 3D Structures





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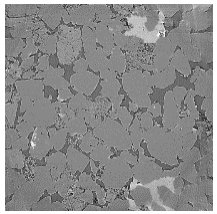

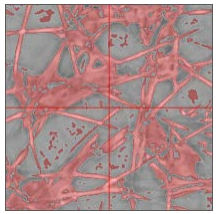

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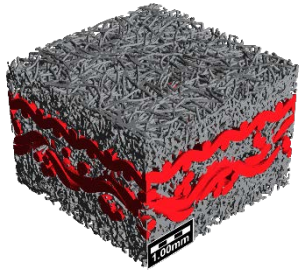

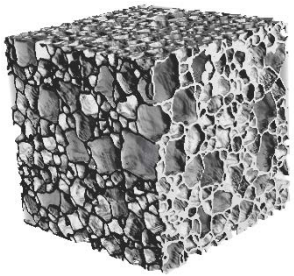

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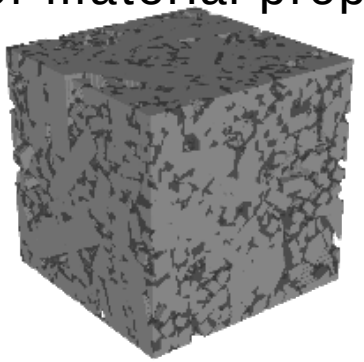

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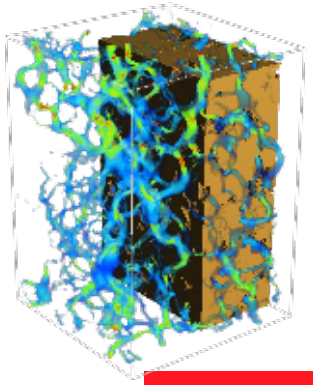
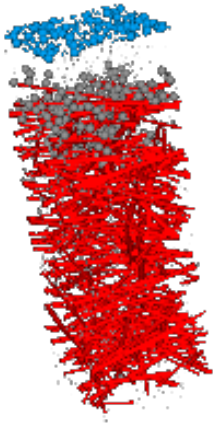
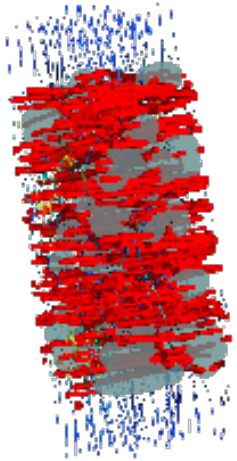




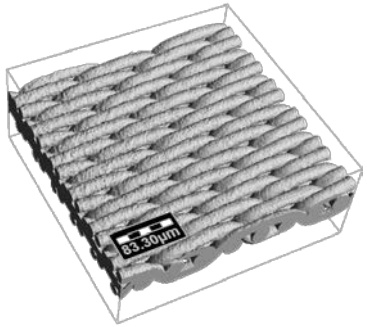


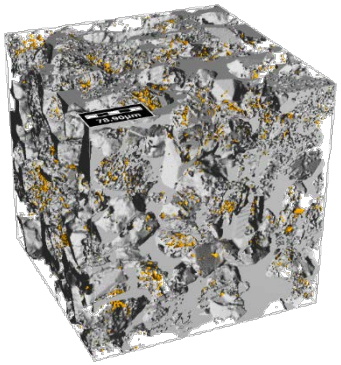
Simulate advection, diffusion particle transport, stiffness

Where GeoDict is used:

Electrochemistry	Fuel cell media & battery materials
Composites	Mostly automotive, lightweight materials
Filtration	Mostly automotive, filter media & filters
Weaves and Paper	Paper forming and dewatering, Metal Wire Mesh
Personal Care	Wipes, Feminine Care, Baby Care
Oil and Gas	Digital rock physics, digital sand control

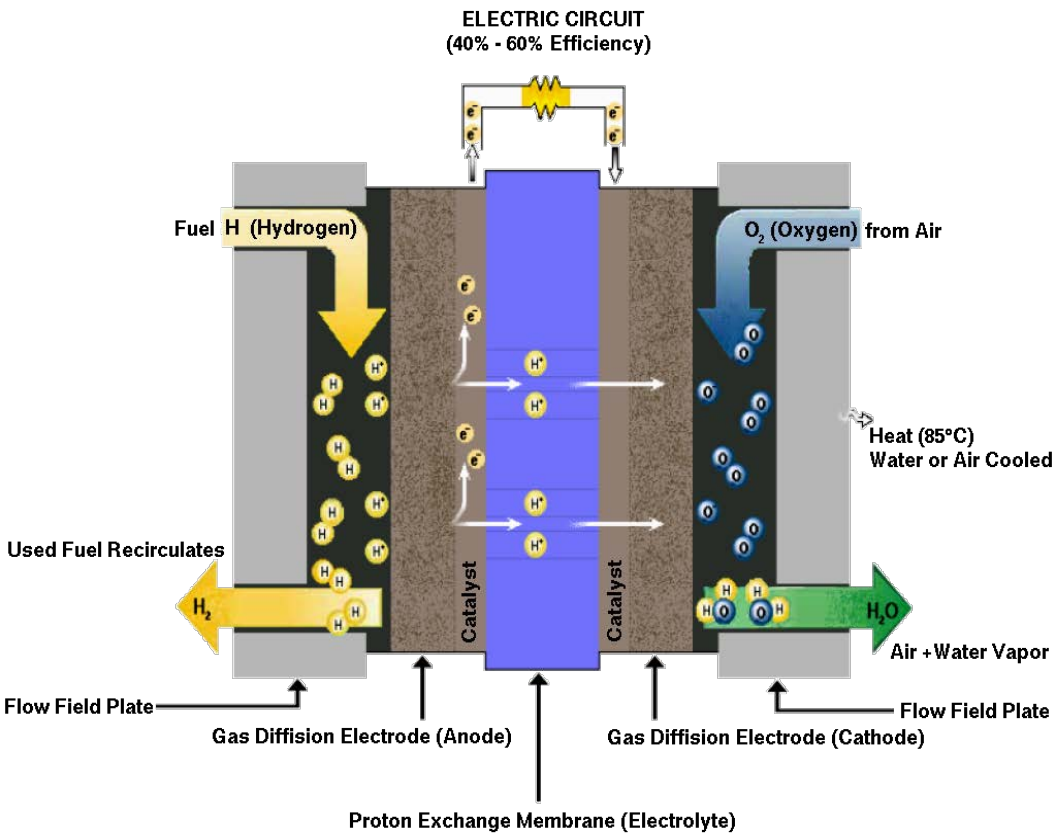
The basic idea:
Microstructures define macroscopic properties!





Li-Ion Cathode	Gas Diffusion Layer	Fiber Reinforced Polymer	Metal Wire Mesh	Sandstone
Diffusion and electrochemistry in the micro-structure define the behavior of a battery.	Two-phase flow properties of the GDL influence the behavior of a PEM fuel cell	Fiber orientation and fiber solid volume fraction define the strength / failure behavior of a FRP component	Through pore and permeability define the filtration properties and the pressure loss	Pore space and permeability define the oil/gas reservoir behavior

Porous Transport Layers in a PEM Fuel Cells



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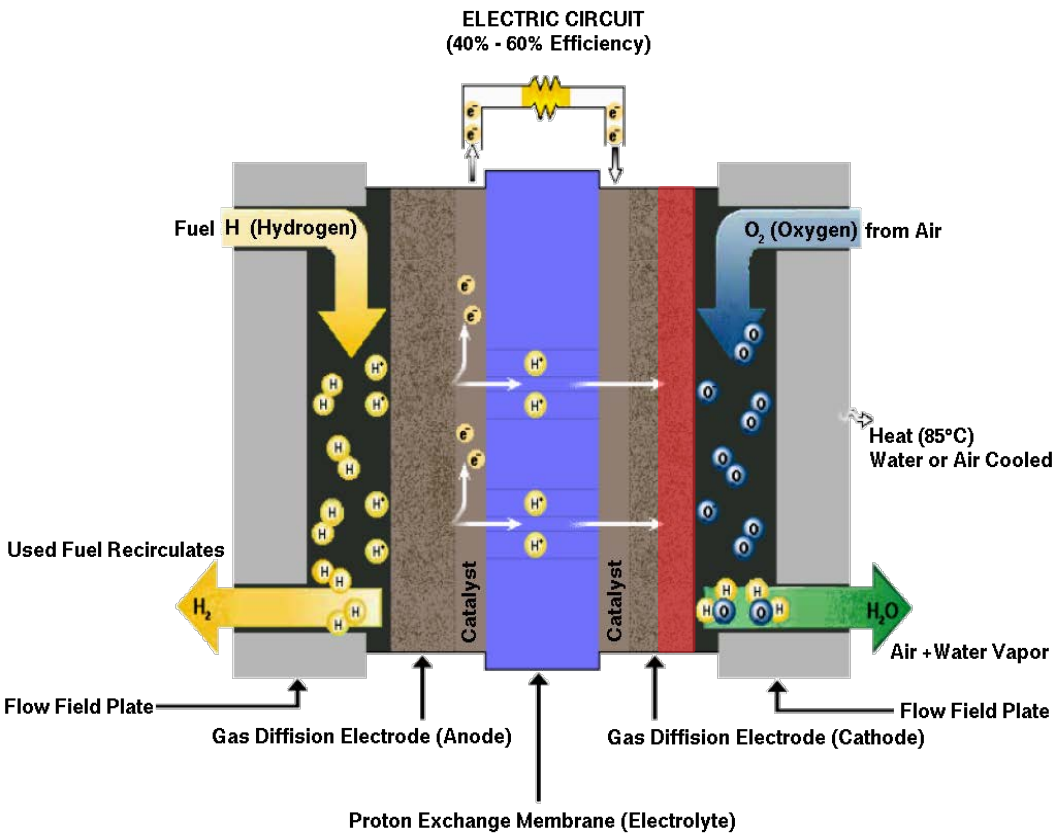
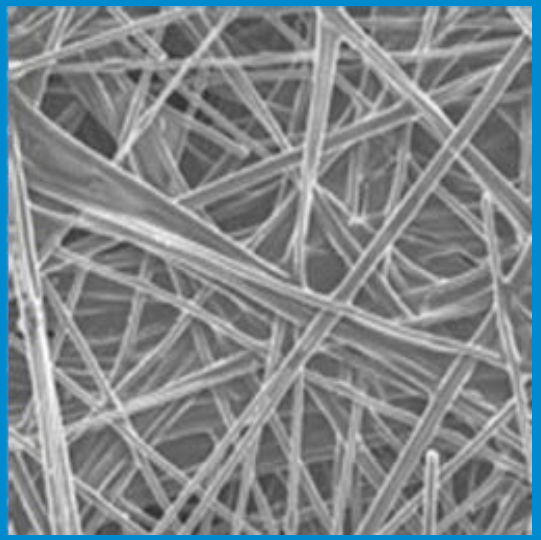


Gas Diffusion Layer (GDL)



- Fibers (~ 7 µm diam.)
- Pore Sizes ~ 30 µm
- Thickness 200-400 µm

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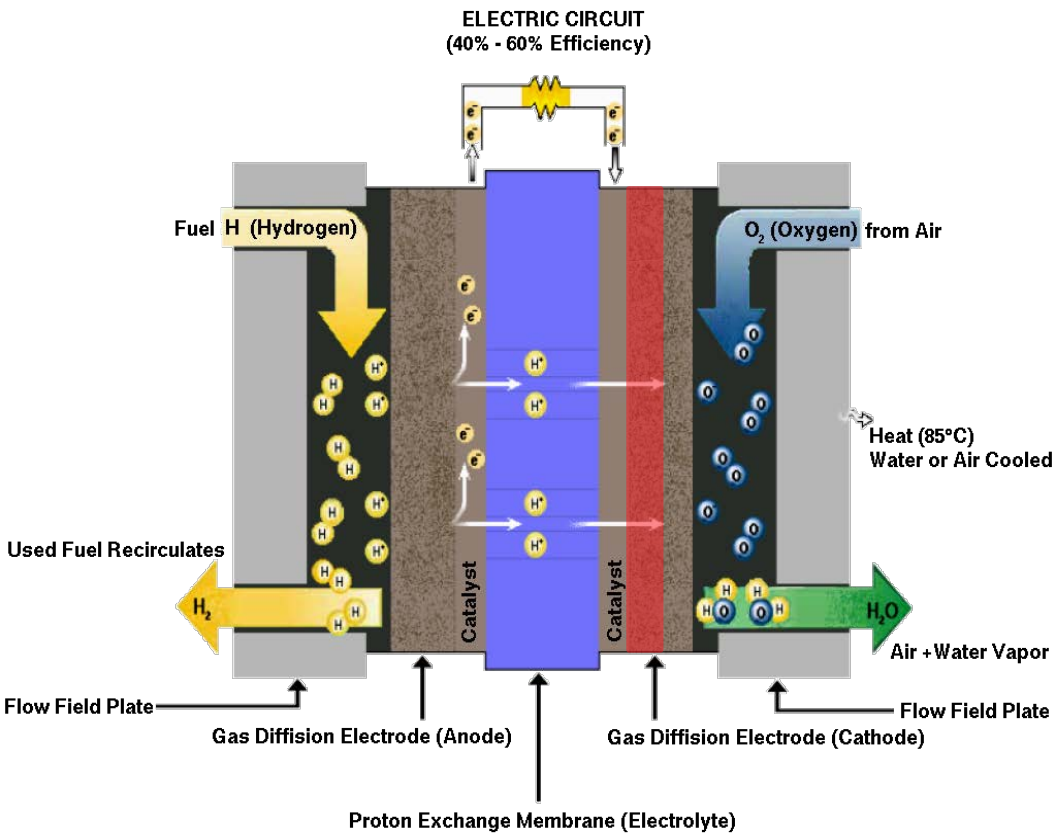
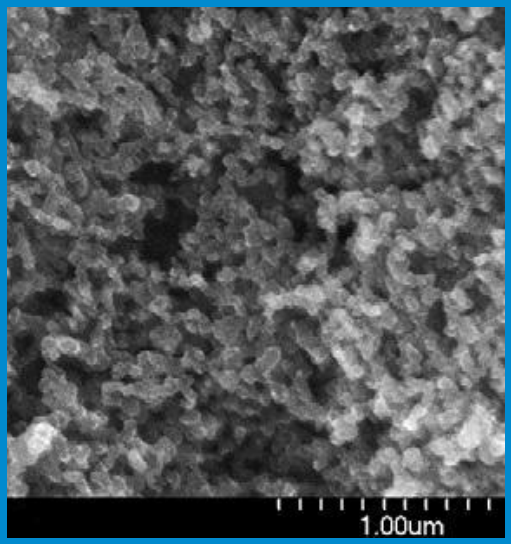
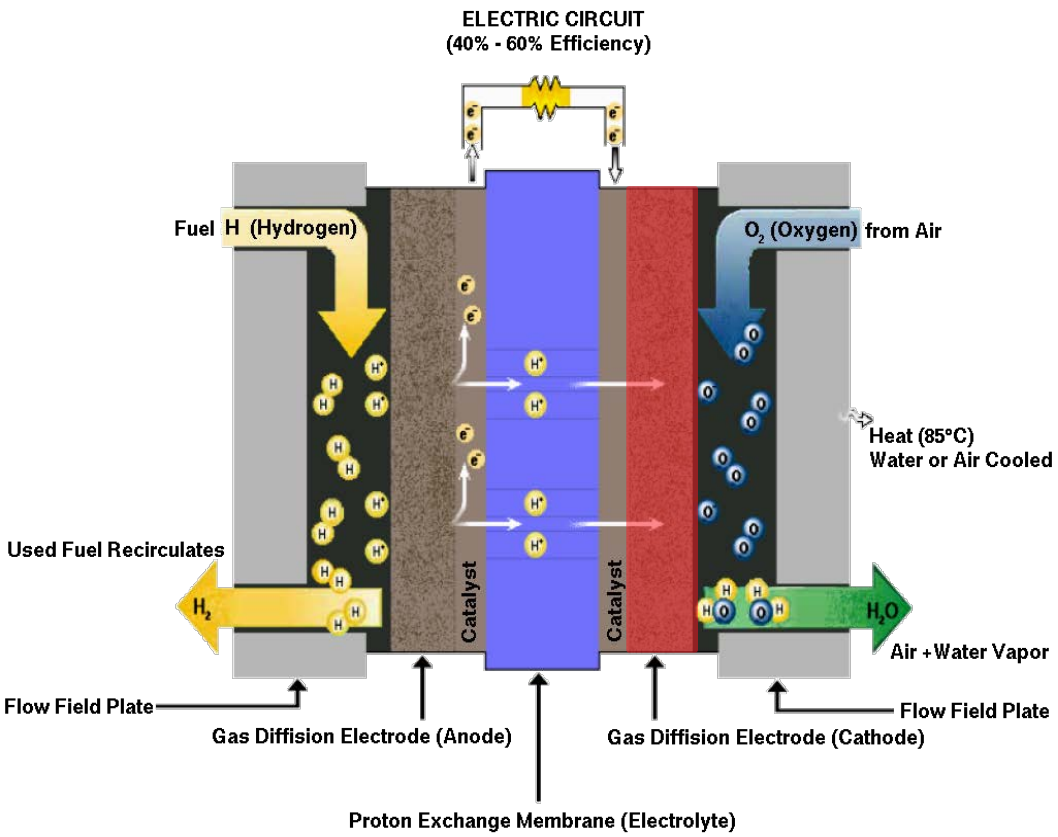


Microporous Layer (MPL)

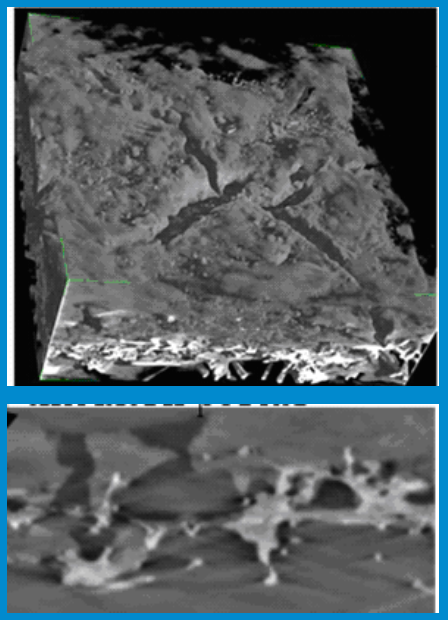


- Carbon Agglomerates
- Pore Sizes ~ 100 nm

Porous Transport Layers in a PEM Fuel Cells

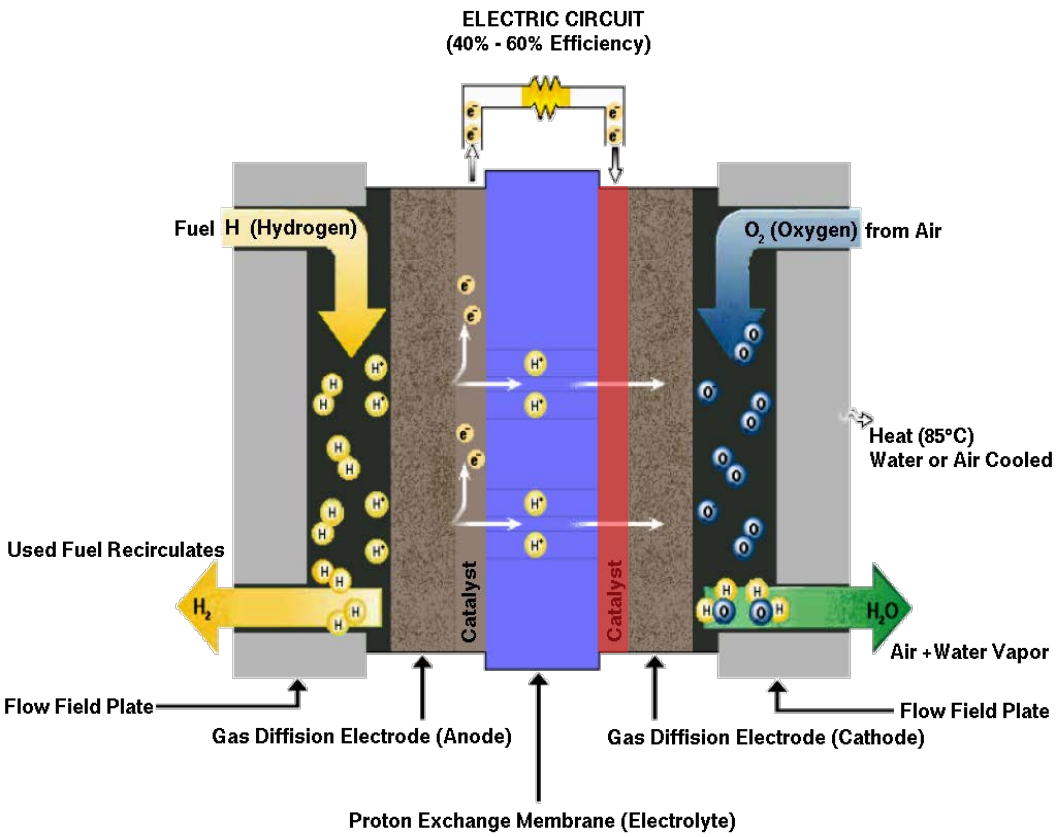


GDL and MPL

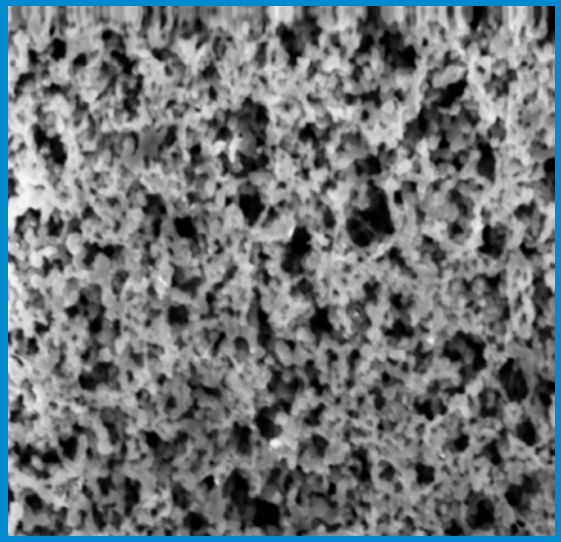


- MPL Penetration
- Cracks

Porous Transport Layers in a PEM Fuel Cells

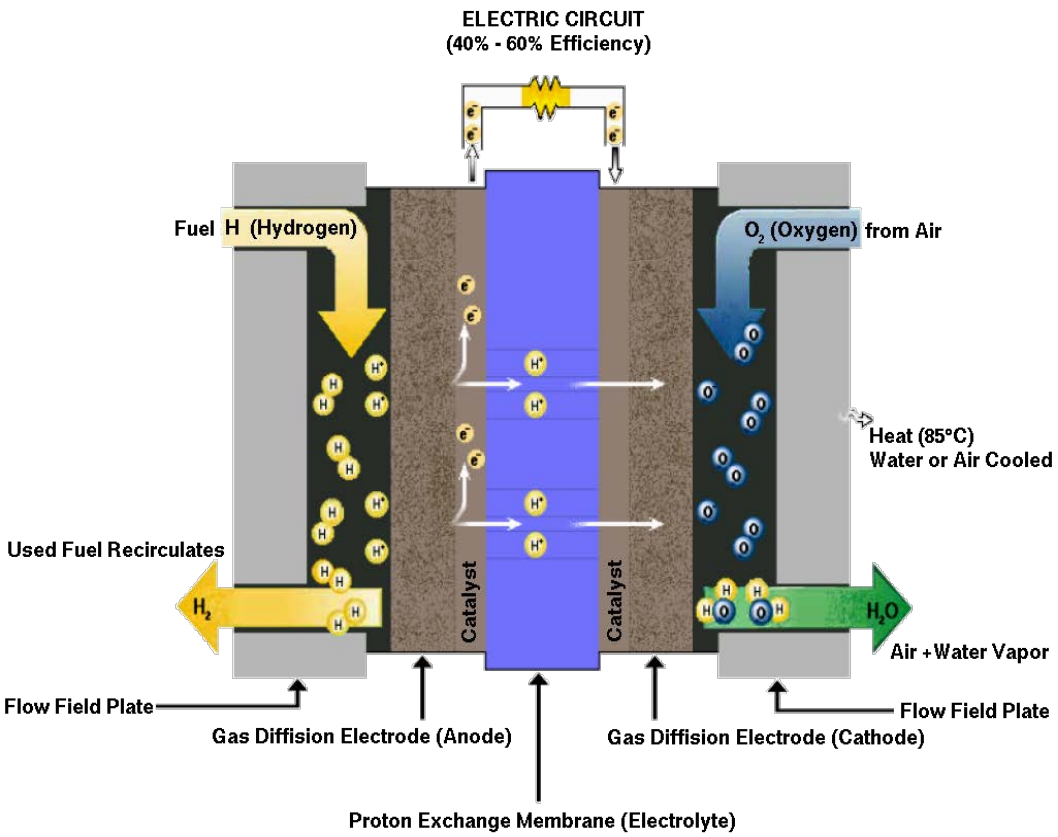


Catalyst Layer (CL)



- Carbon Agglomerates
- Ionomer
- Platinum Particles
- Pore Sizes ~ 100 nm

Porous Transport Layers in a PEM Fuel Cells



Functions of pores:

- Oxygen transport
- Water removal

Functions of solids:

- Electric conductivity
- Heat distribution
- Mechanical stability

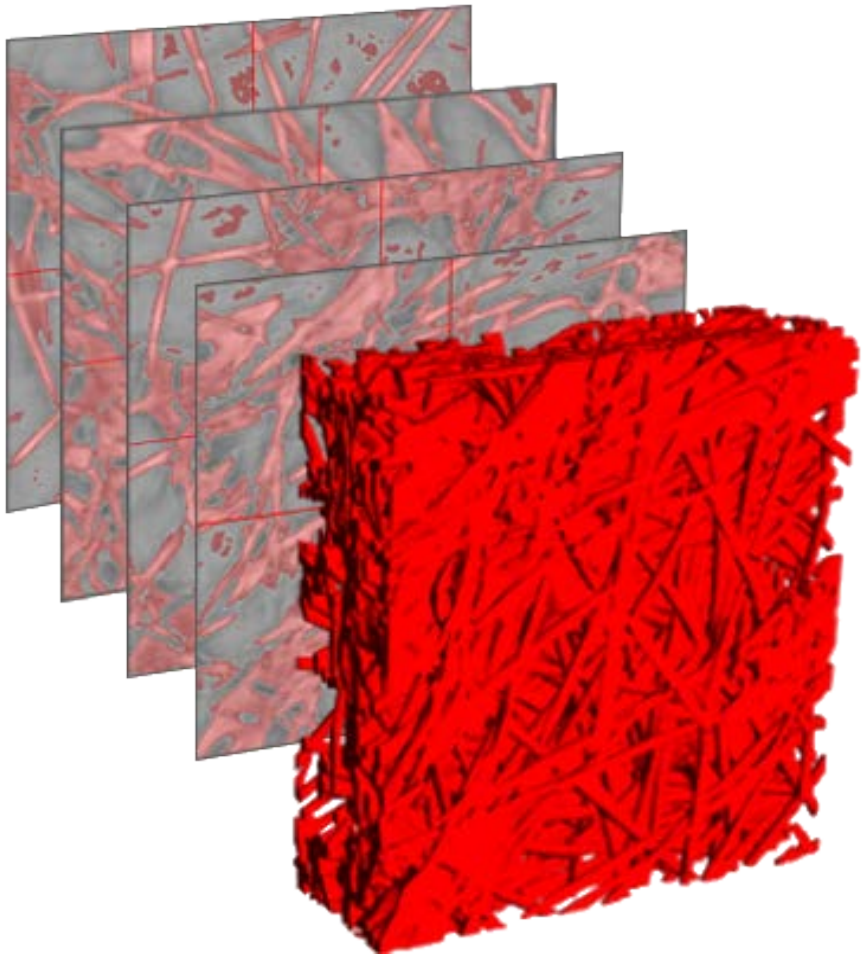
Computer Aided Material Engineering

Step 1: Get your material into the computer

CT-Scan

- Allows resolutions down to 0.5 µm / voxel
- Result is an 3D image with up to 2000^3 voxels

(voxel = volume pixel)



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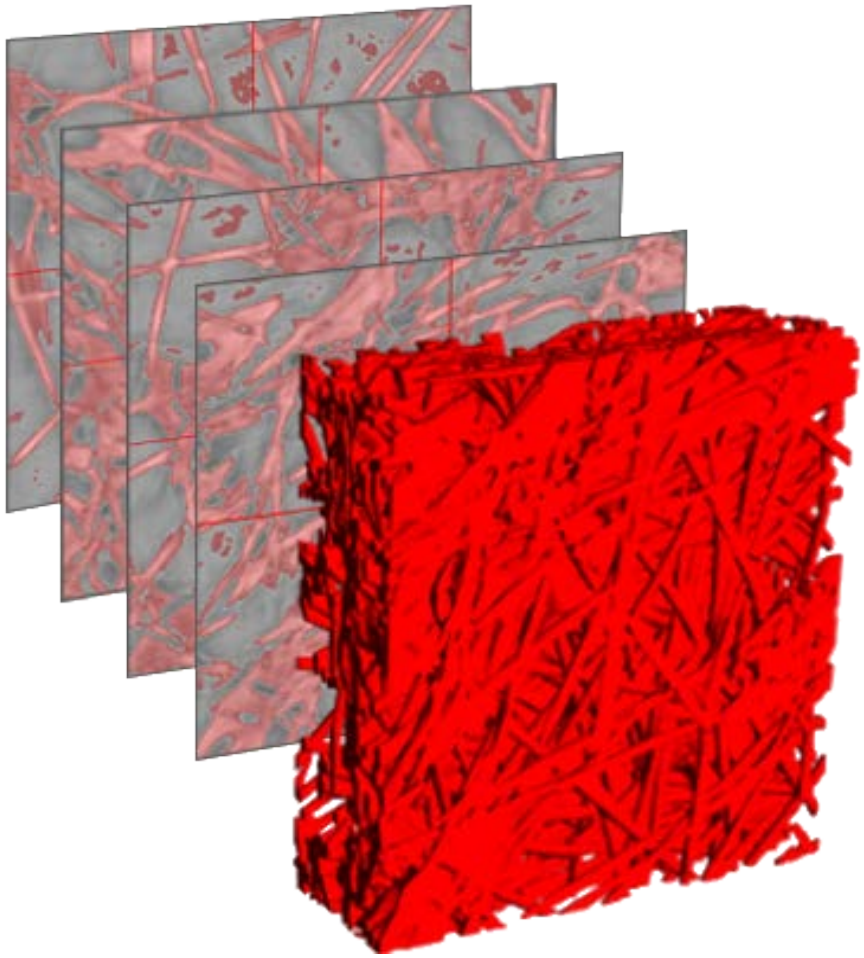
Large number of grid cells requires specialized solutions.



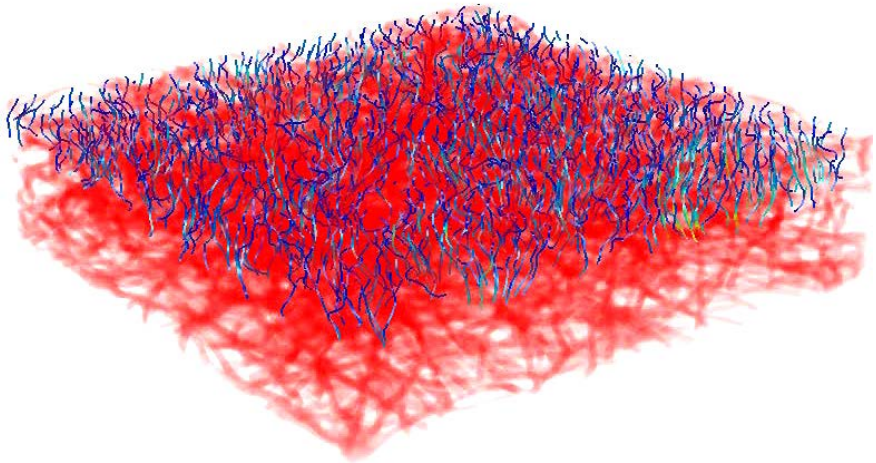
Step 2: Analyze your material

Compute geometrical properties:

- Pore size distribution
- Percolation paths
- Fiber diameters

Compute physical properties:

- Effective diffusivity
- Thermal conductivity
- Permeability

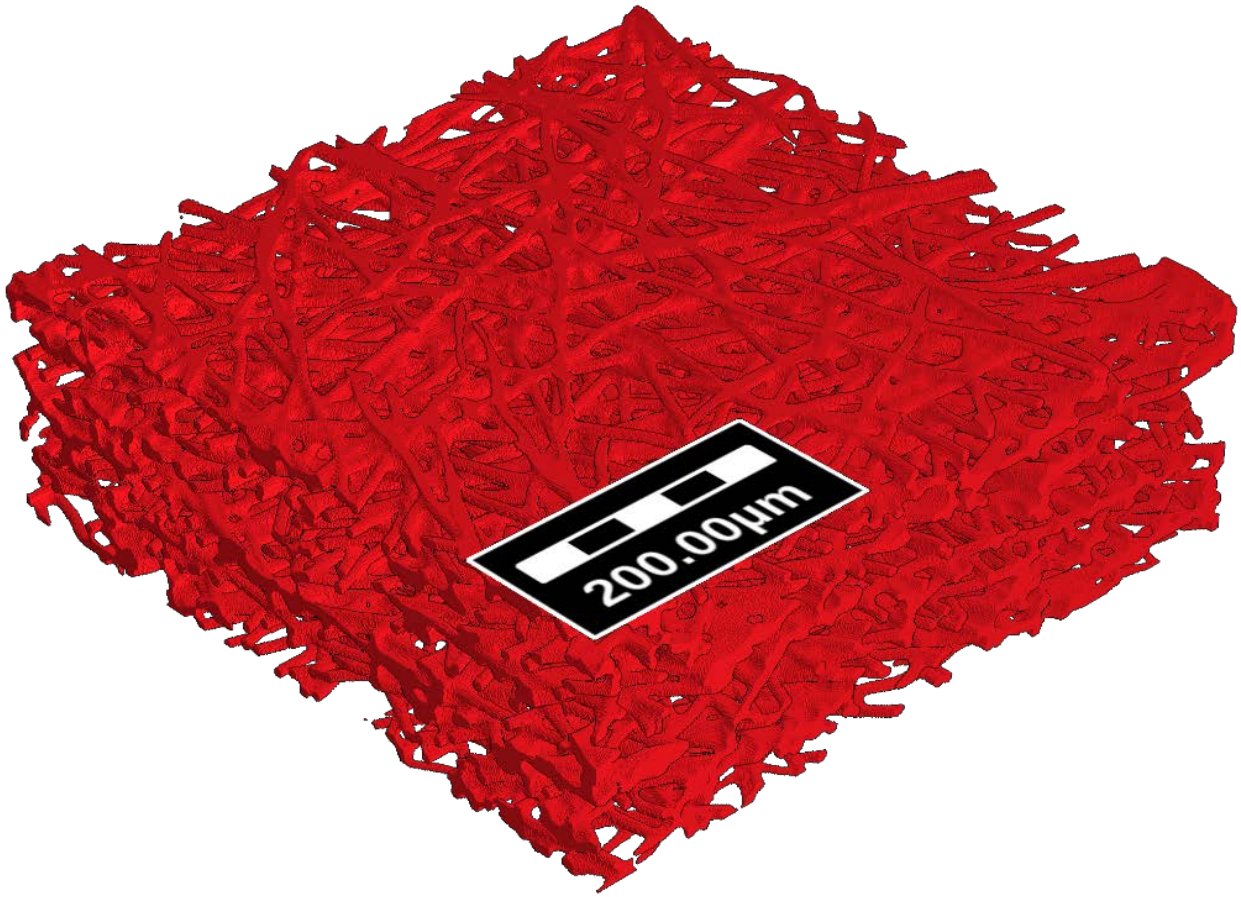


Step 3: Create new materials virtually

Choose e.g.

- Porosity
- Fiber diameter
- Fiber length
- Anisotropy

...and let FiberGeo generate a nonwoven model



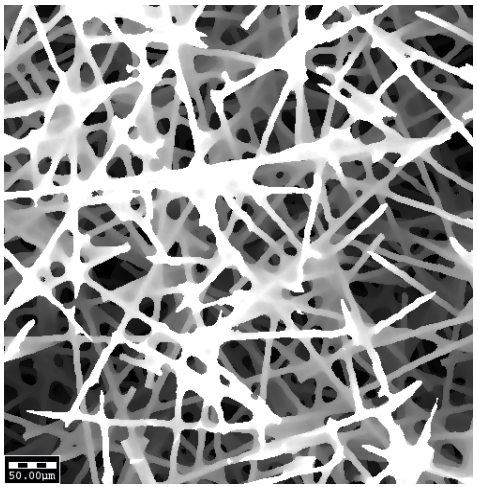
Step 4: Analyze and Optimize

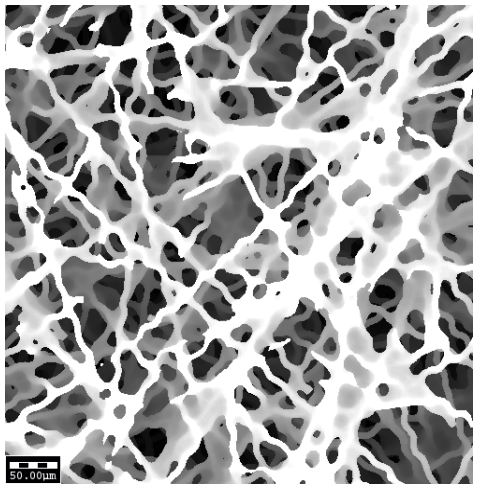
Vary geometrical input:

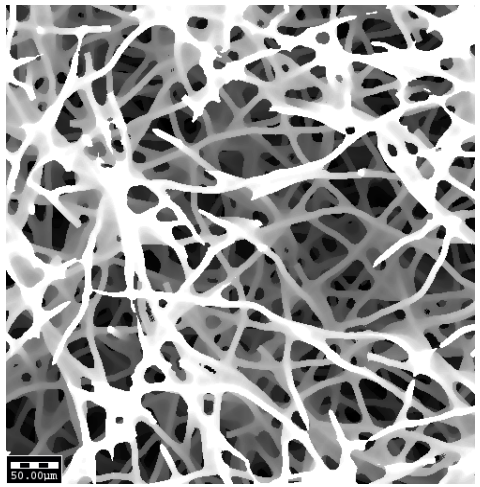
- Binder content
- Porosity
- Fiber shape

Optimize for:

- Ohmic resistance
- Oxygen and Water Transport
- Mechanical stability







Project Examples

Project Example:
Compression of a Gas Diffusion Layer (GDL)

Fibers: linear elastic, transverse isotropic

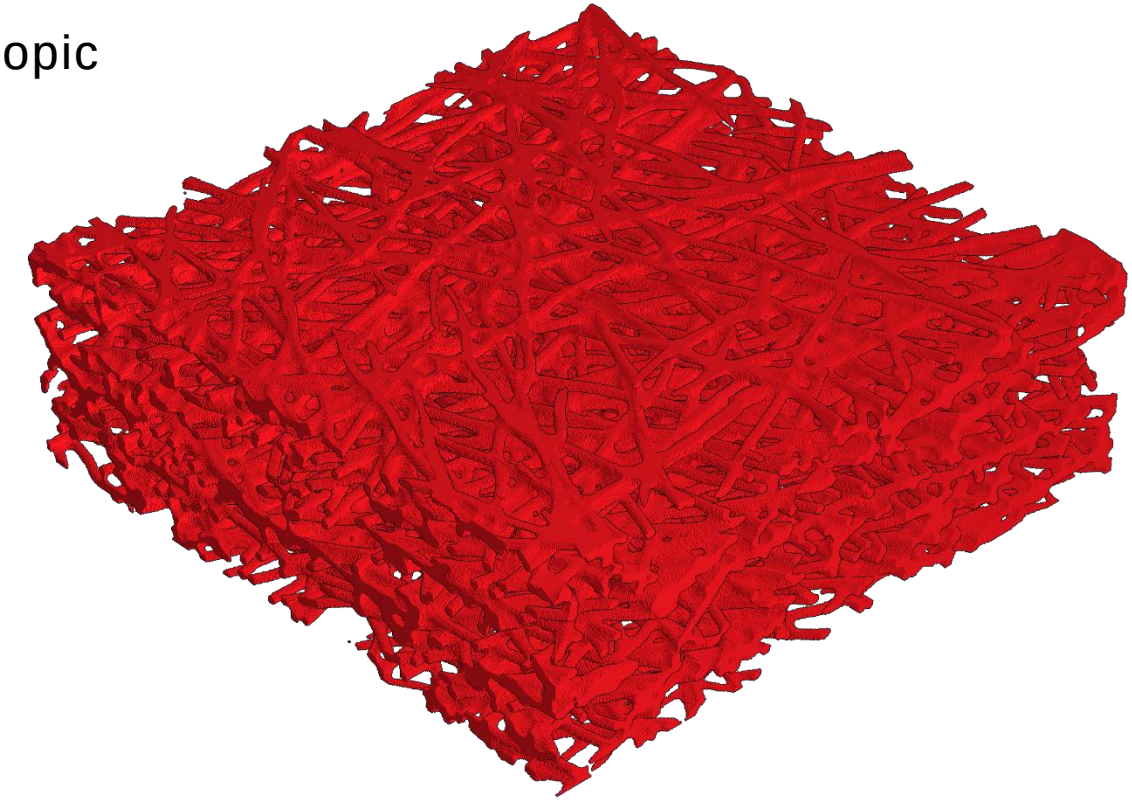
Binder: linear elastic, isotropic

Solver:

FeelMath

Fraunhofer ITWM

Runtime: 1h 17 min (8x)



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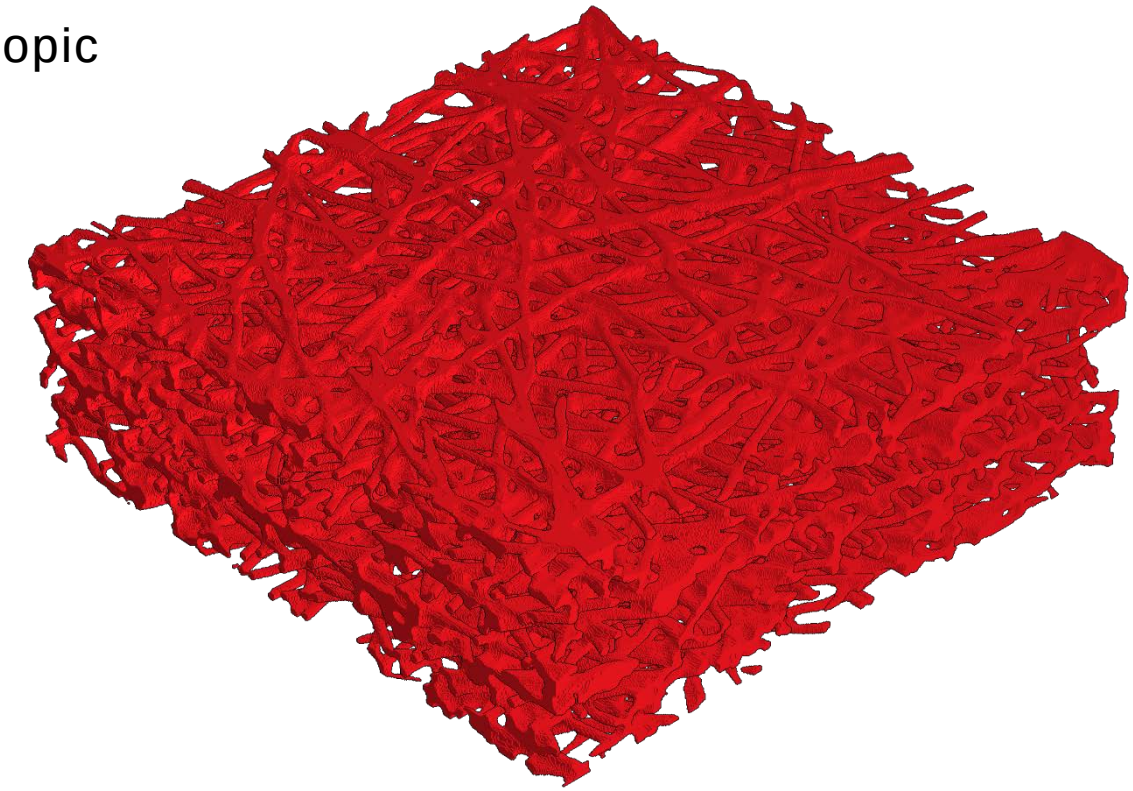

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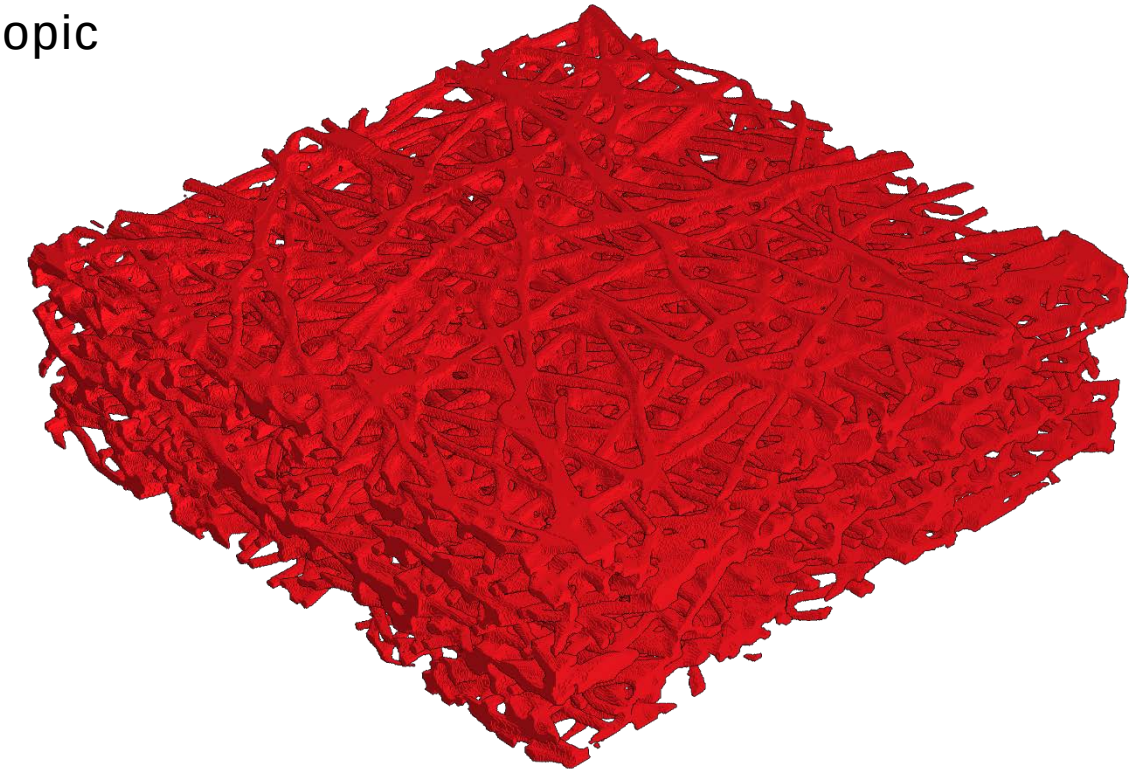

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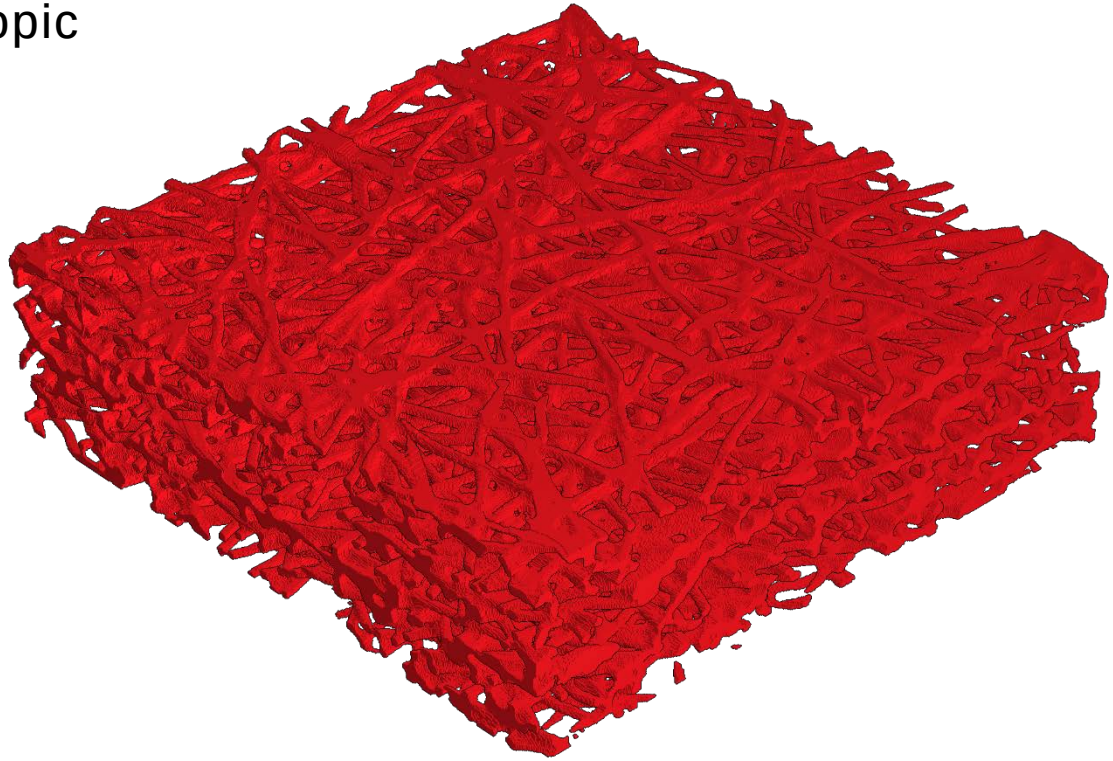

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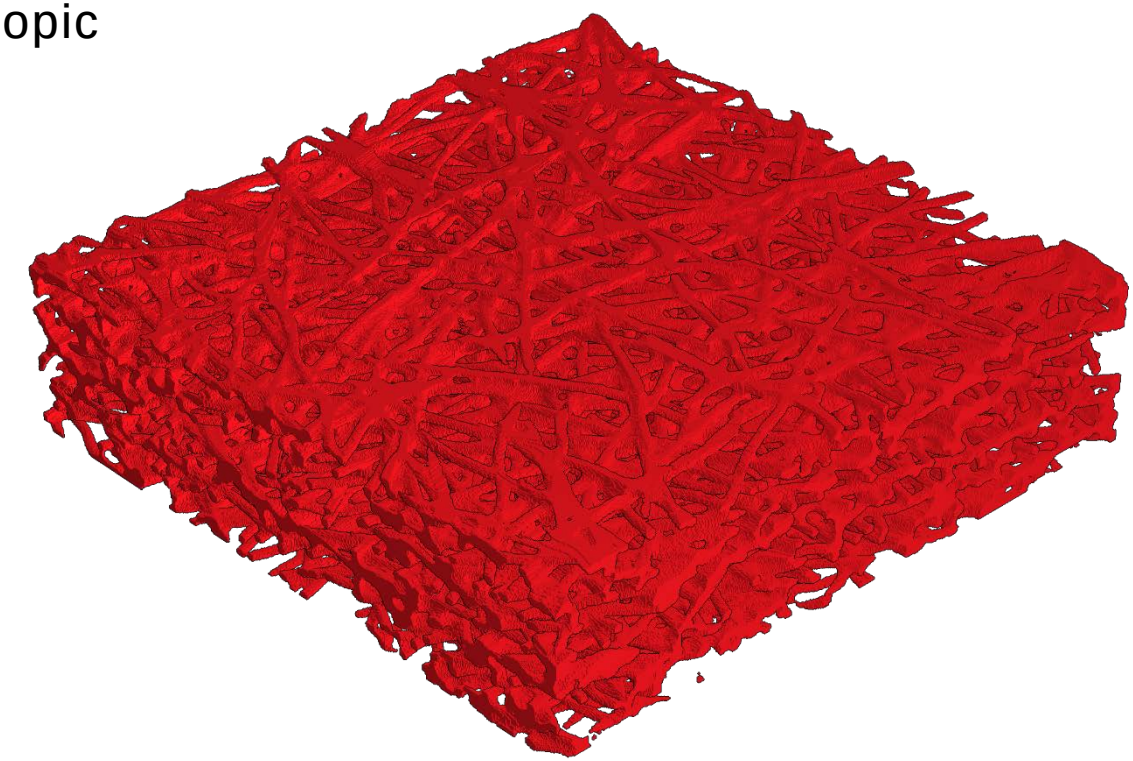

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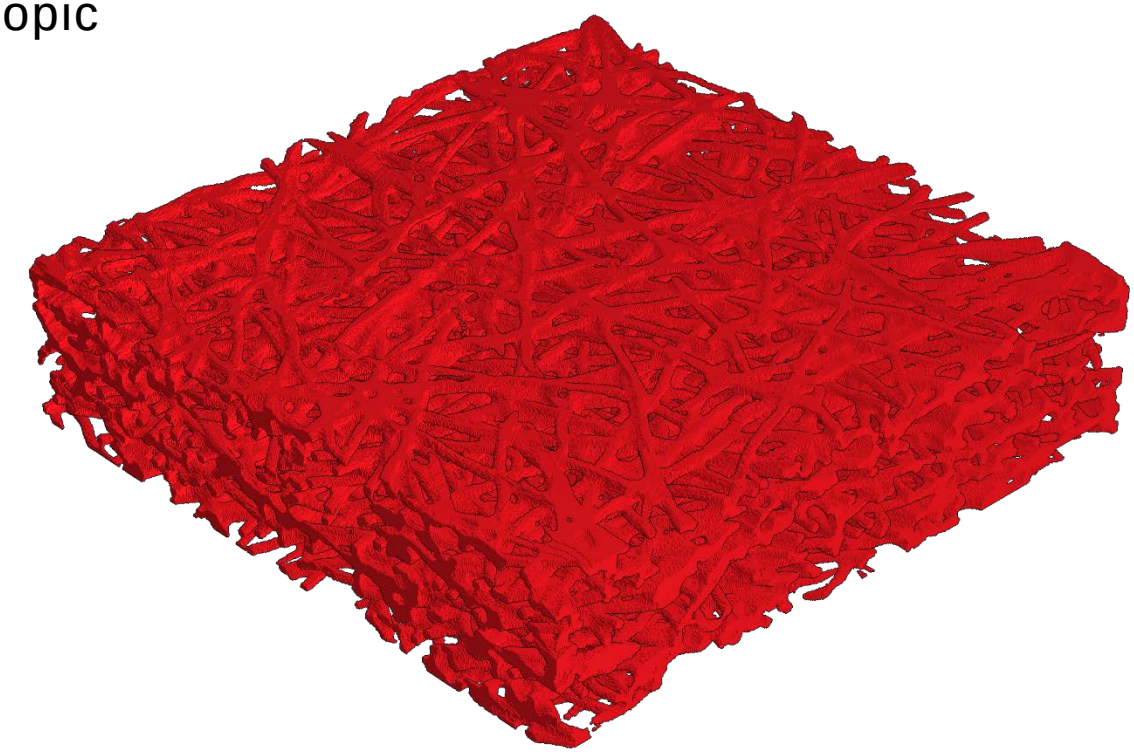

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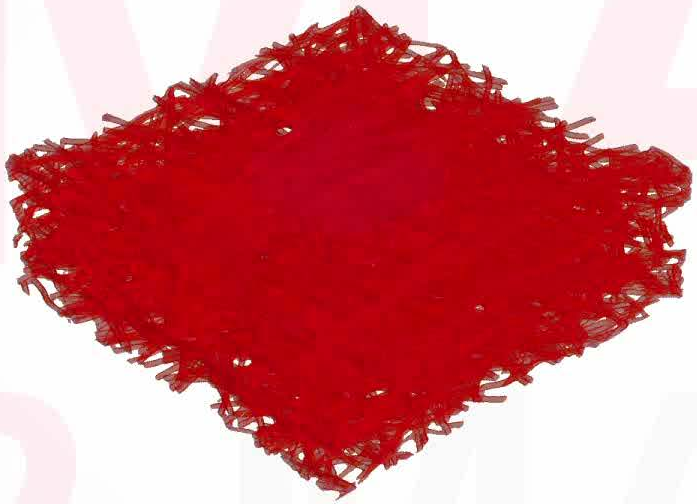
Project Example:
Water Entering into the GDL

GEO DICT



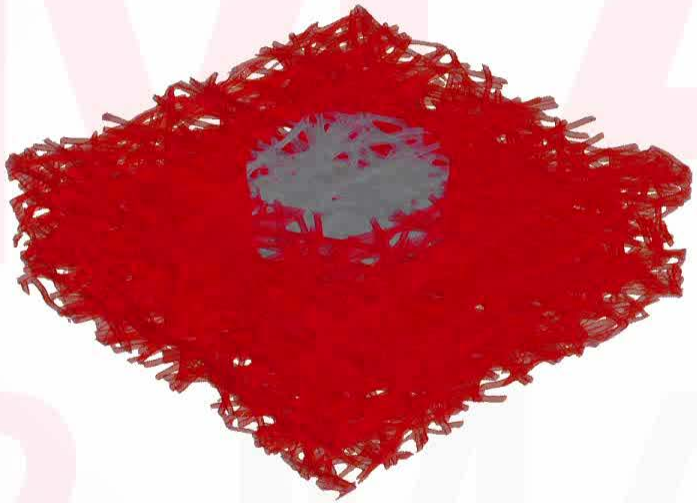
Top View

Bottom View

SatuDict Simulation with constant contact angle; uncompressed

Project Example:
Water Entering into the GDL – Patterned Wettability

GEO DICT



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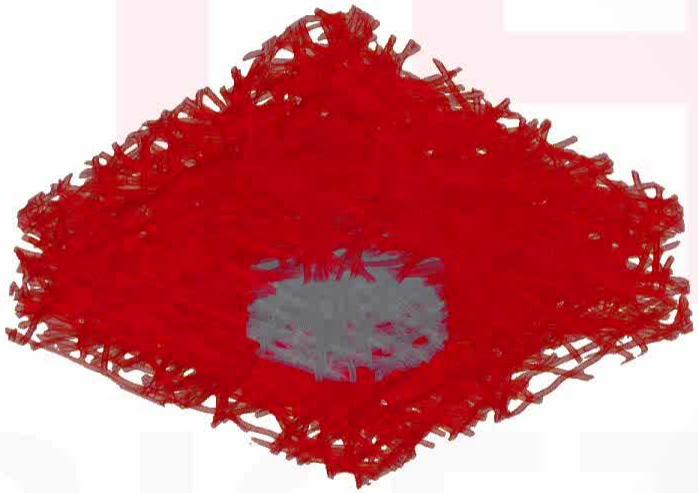

Bottom View

SatuDict Simulation with two different contact angles; uncompressed

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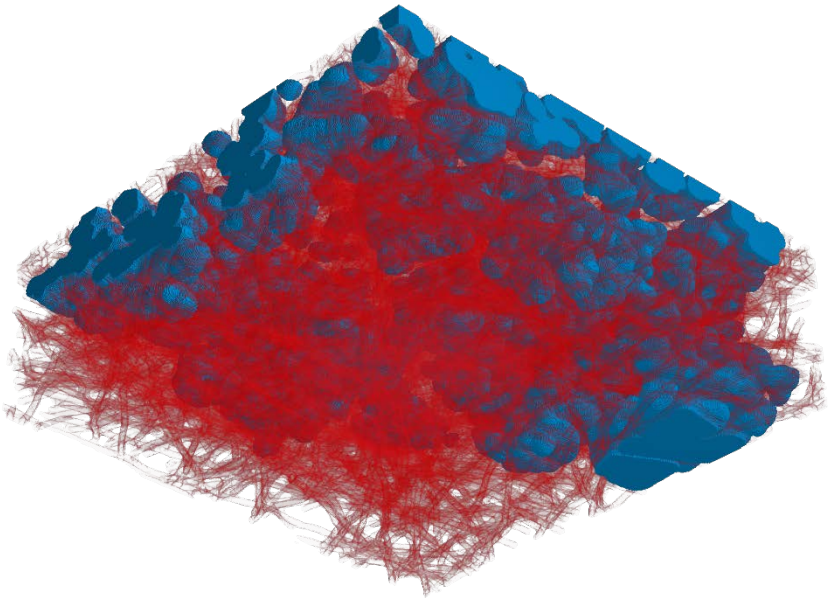
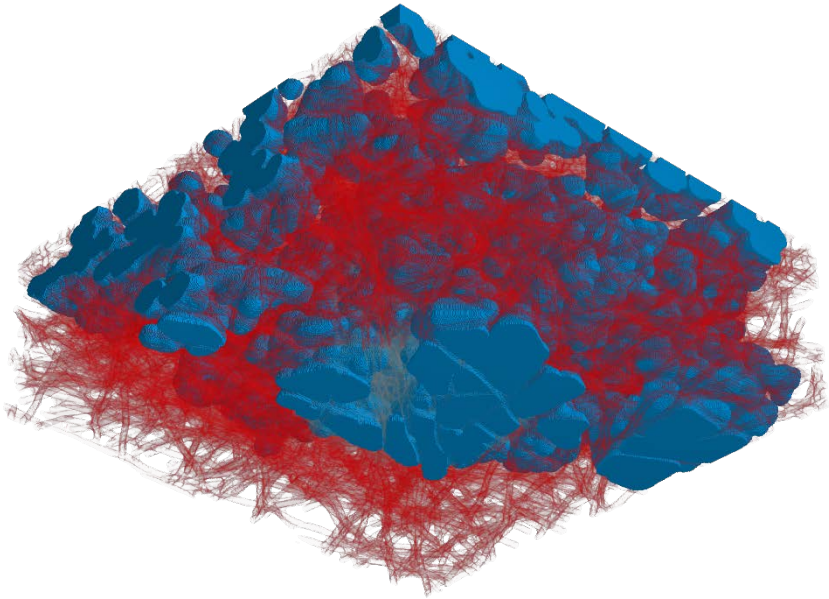
Water Entering into the GDL -

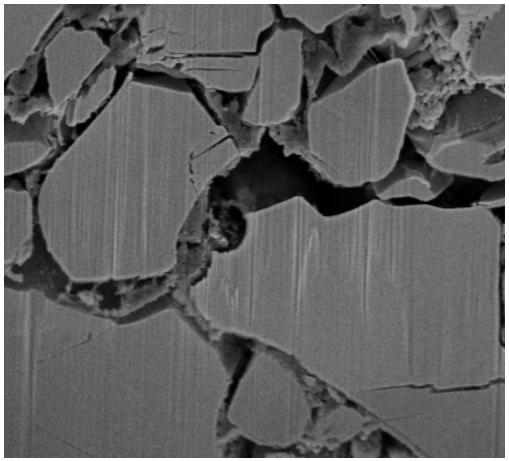


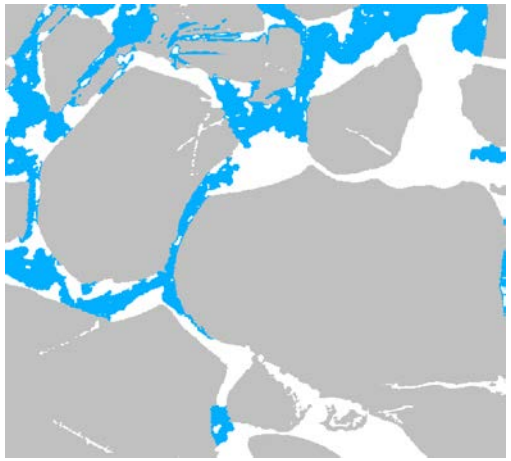


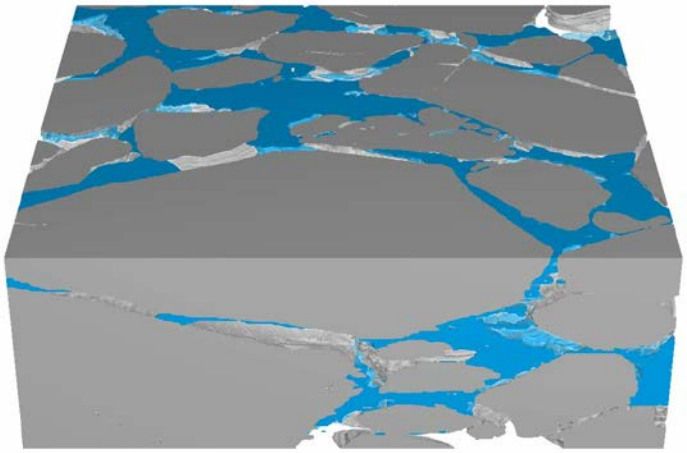
Constant Hydrophobicity

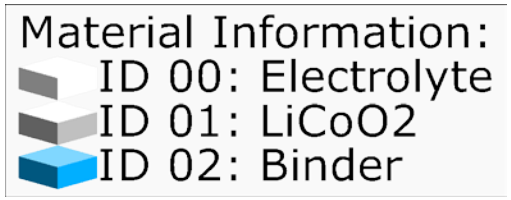
Patterned Wettability

Project Example:
Li-Ion Battery Cathode from FIB-SEM





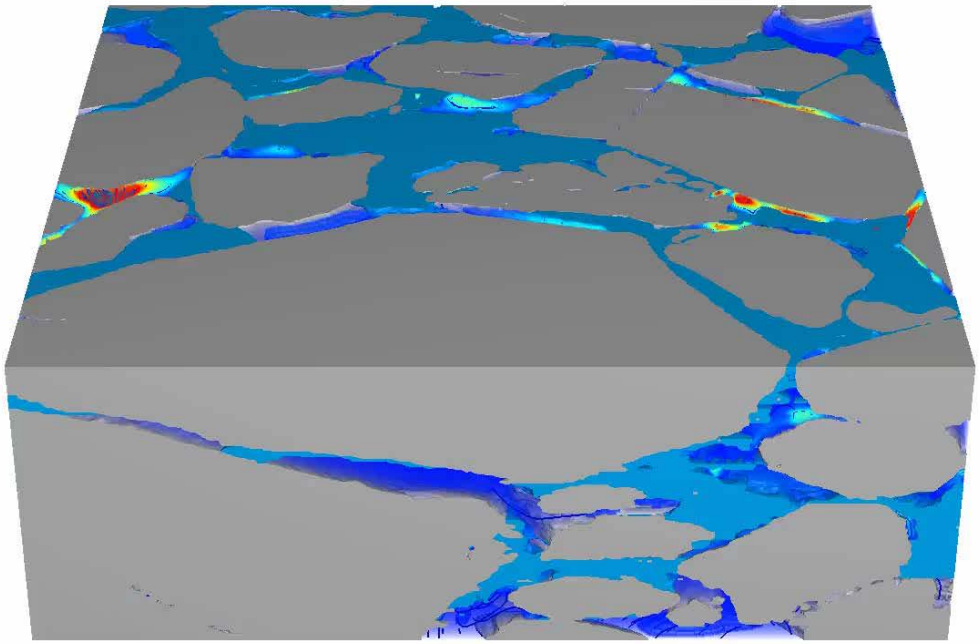




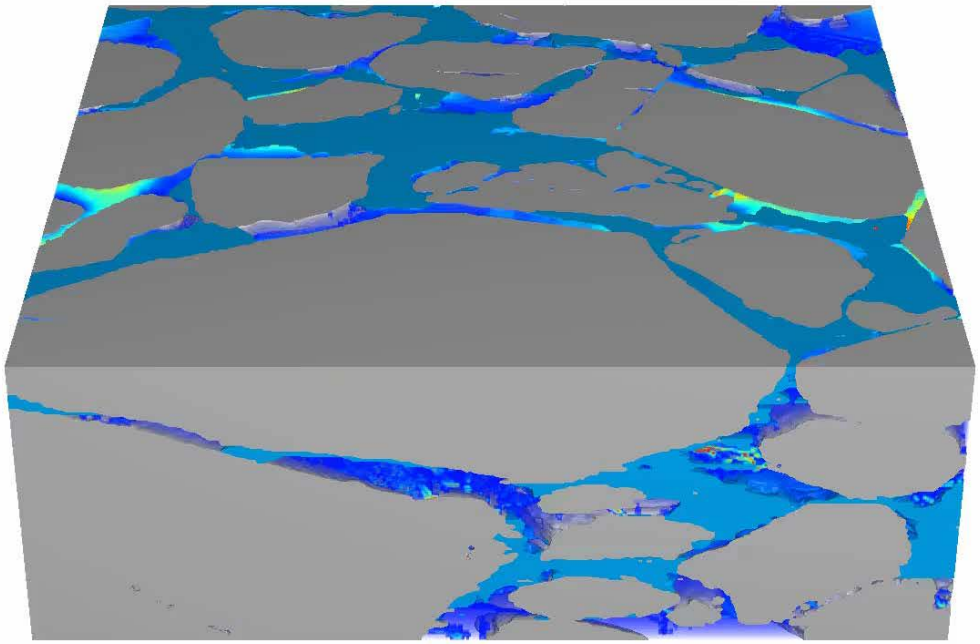
Three-dimensional reconstruction of a LiCoO2 Li-Ion battery cathode
Tobias Hutzenlaub, Simon Thiele, Roland Zengerle, and Christoph Ziegler

Raw Image Stack | Segmented Images | 3D-Material

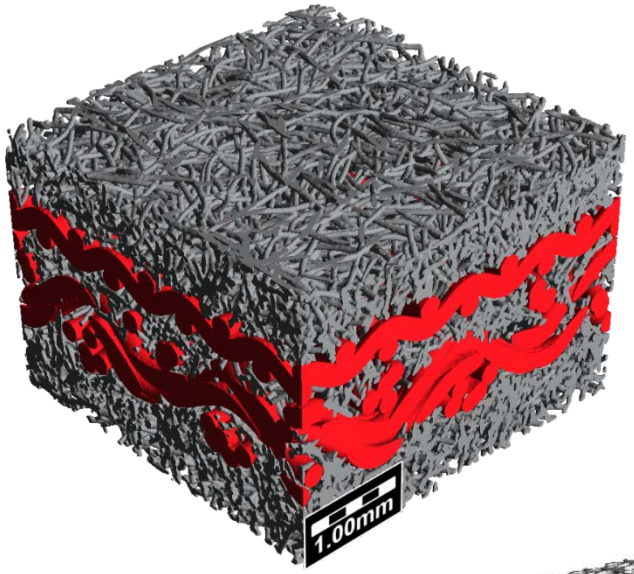
Project Example:
Pressure Driven Flow



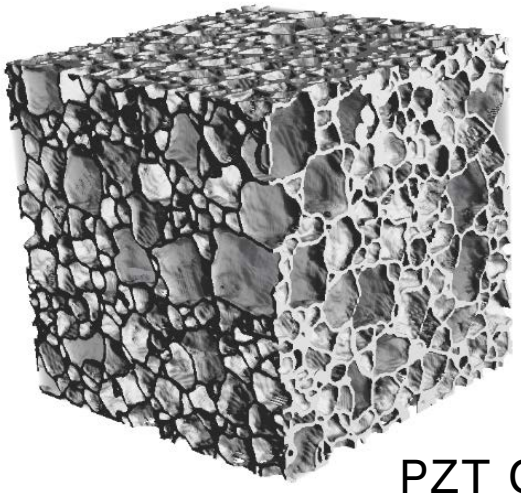
Project Example:
Diffusive Flux



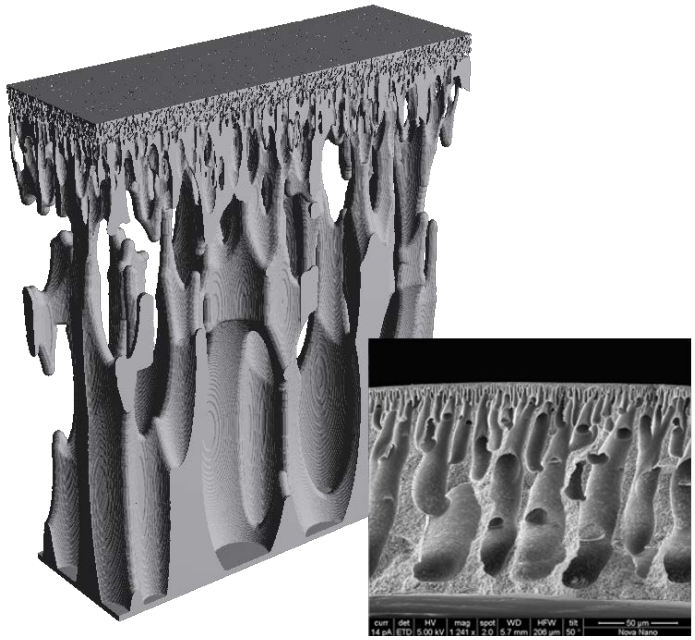
Beyond Fuel Cells & Batteries: Create Structure Models



Paper dewatering felt



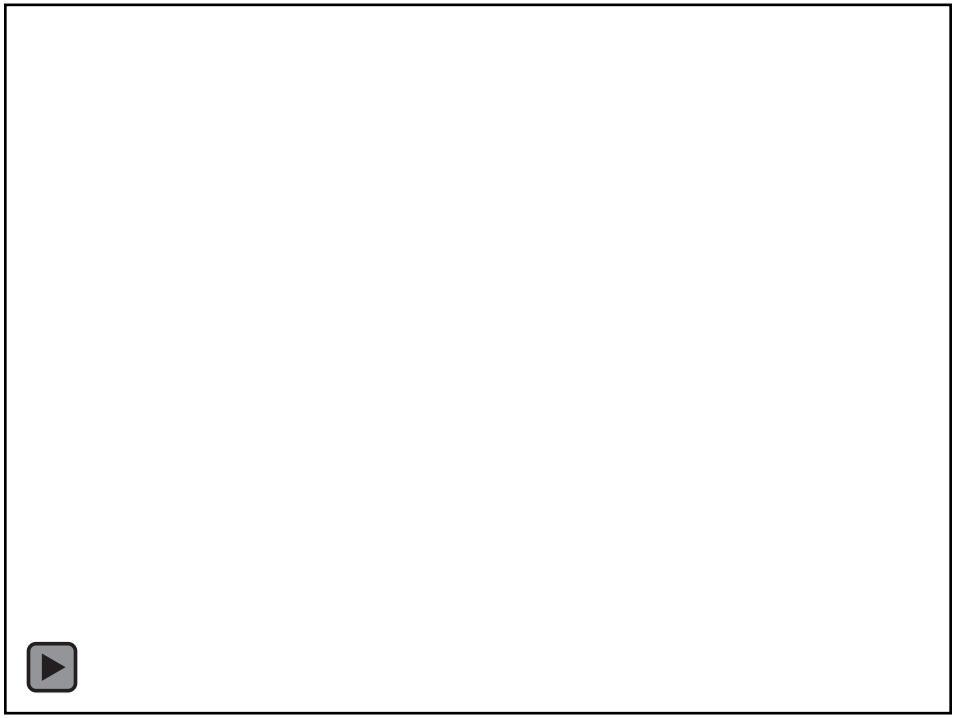
PZT Ceramics

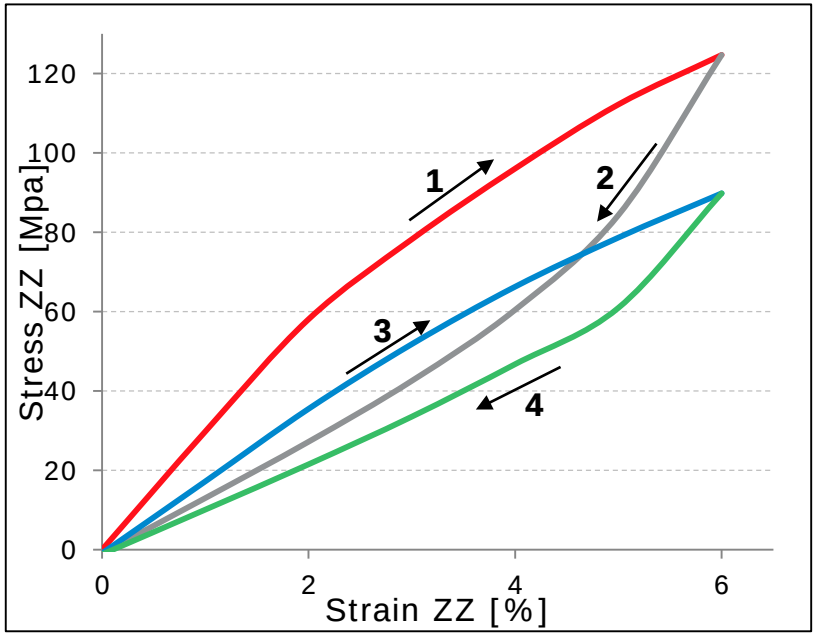


Desalination membrane

Beyond Fuel Cells & Batteries:
Simulate Damage Tests of Composite Materials

- Compute stress-strain curve under cyclic loading
- Use nonlinear material laws (UMAT)
- Use damage model (UMAT)

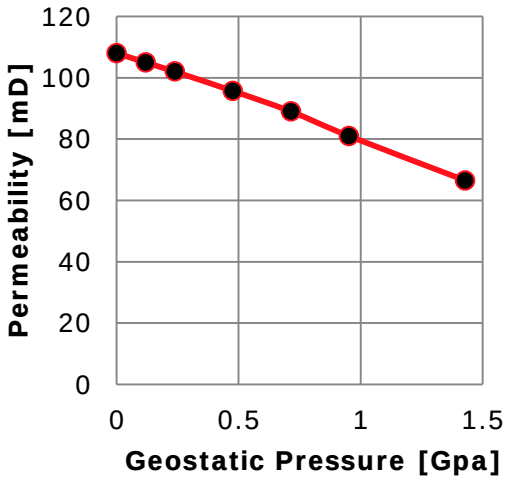


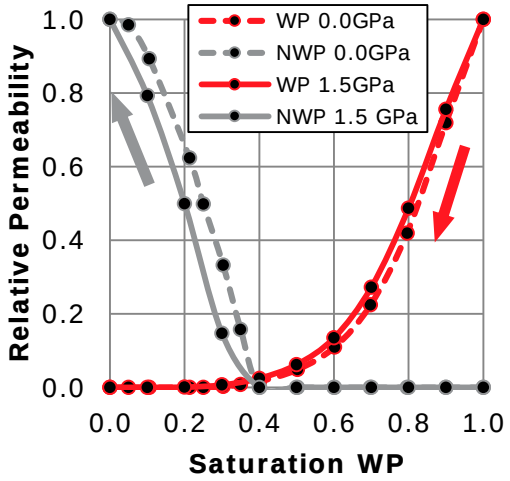


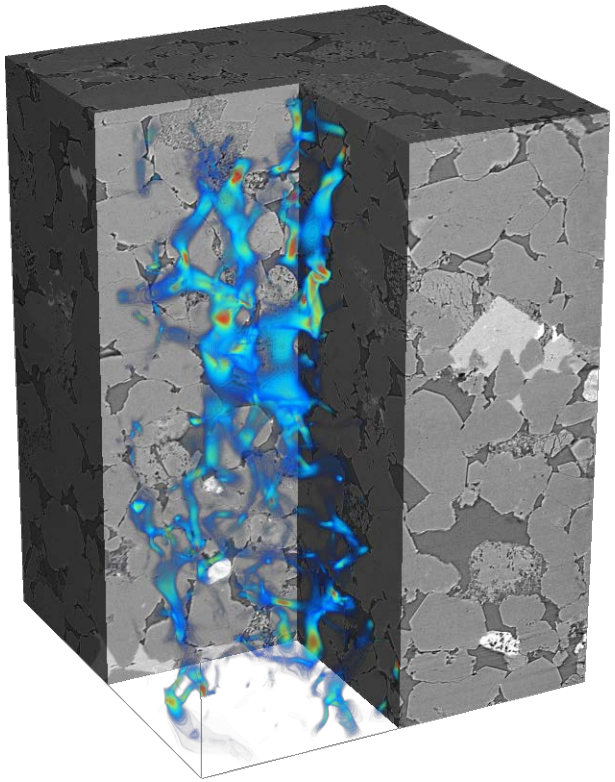
Beyond Fuel Cells & Batteries: Simulate Flow Through Rock Pores

- Permeability: 108 mD (ex-situ)
- Permeability: 66 mD (in-situ @ 1.4 GPa geostatic pressure)

- Relative permeability at different saturations







Velocity field

Summary

The digital material laboratory GeoDict allows to

1. Import CT scans
2. Create 3D micro-structure models
3. Analyze 3D structures geometrically
4. Predict physical properties that depend on the micro-structure

Thank You!

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