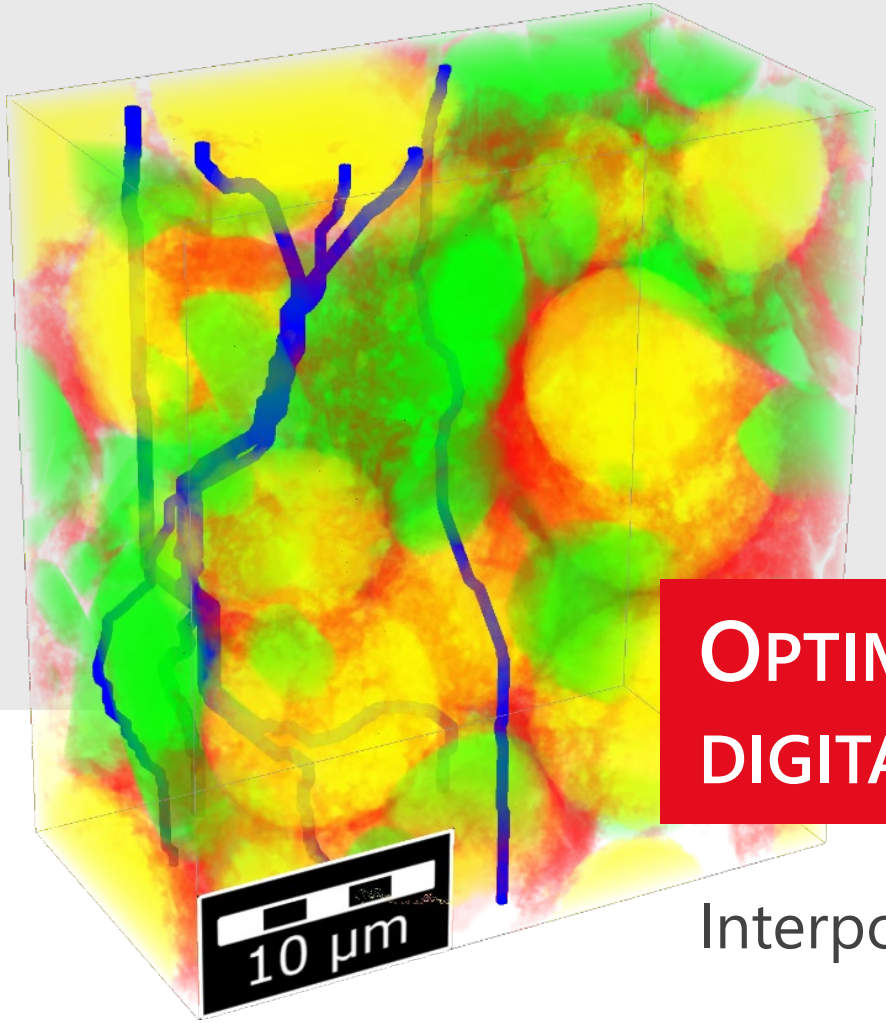

MATH
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Optimizing the performance of batteries using digital material engineering

Interpore, May 9, 2019

Erik Glatt, Fabian Biebl, Ilona Glatt, Christian Wagner, Andreas Wiegmann

OUTLINE

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1 Introduction

2 **ImportGeo**: import of cathode FIB-SEM image

3 **GrainFind**: segmentation of the two active materials

4 **BatteryDict**: battery charging simulations

5 Outlook

Who we are

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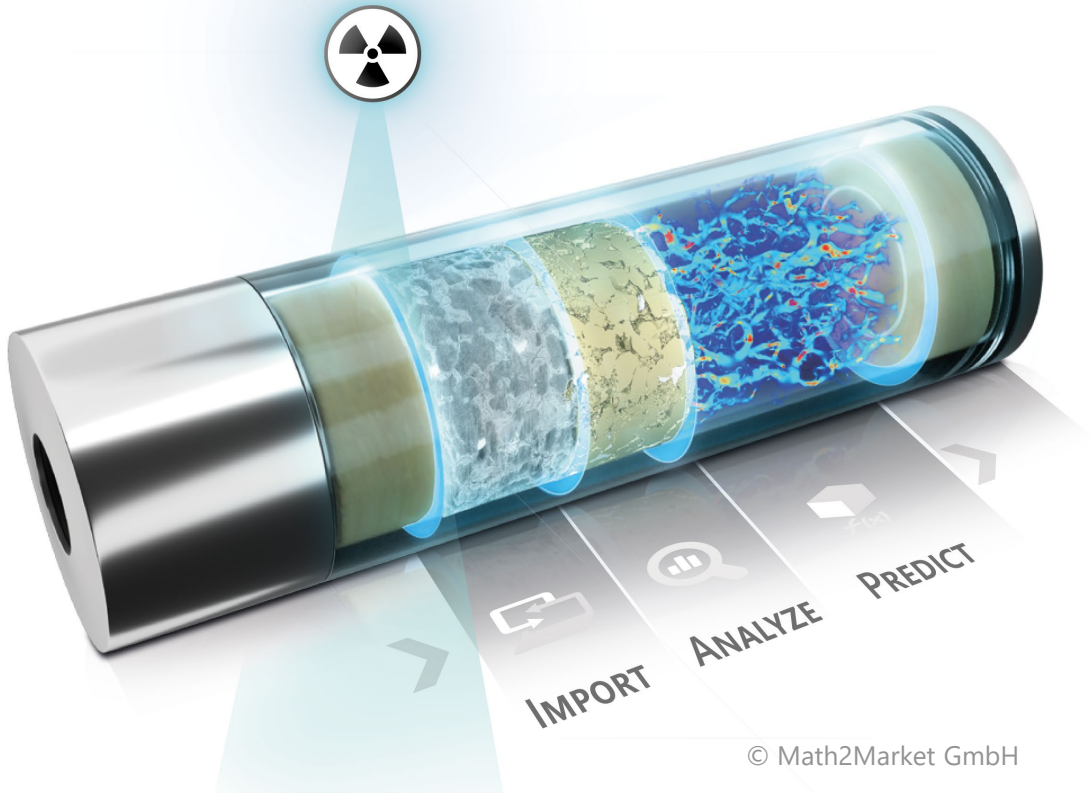
Math2Market GmbH

- creates and markets the scientific software GeoDict®.
- was spun off in 2011 from Fraunhofer ITWM in Kaiserslautern.
- is a privately owned company based in Kaiserslautern, Germany.

GeoDict® - The Digital Material Laboratory

- is a software tool to analyze and design the microstructure of porous media and composites.
- works on
  - µCT and FIB-SEM 3D images or
  - random geometric material models.

GeoDict
The Digital Material Laboratory



Digital material engineering with GeoDict®

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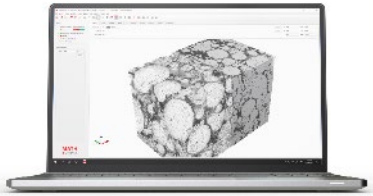
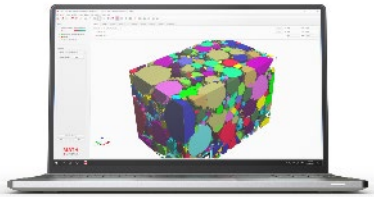
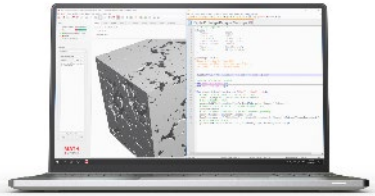
1. Import	2. Analyze	3. Model	4. Design
			
Import of 3d images captured by µCT or FIB/SEM techniques	In-depth digital analysis and evaluation of material properties	Digital material design based on the statistical material properties	Design by varying the statistics of the geometry that govern the material properties
Digital Material	**Quantification of** geometrical, structural, and physical **material properties**	**Digital Twin**	**Digital Prototypes**

Schematic of a Li-ion battery

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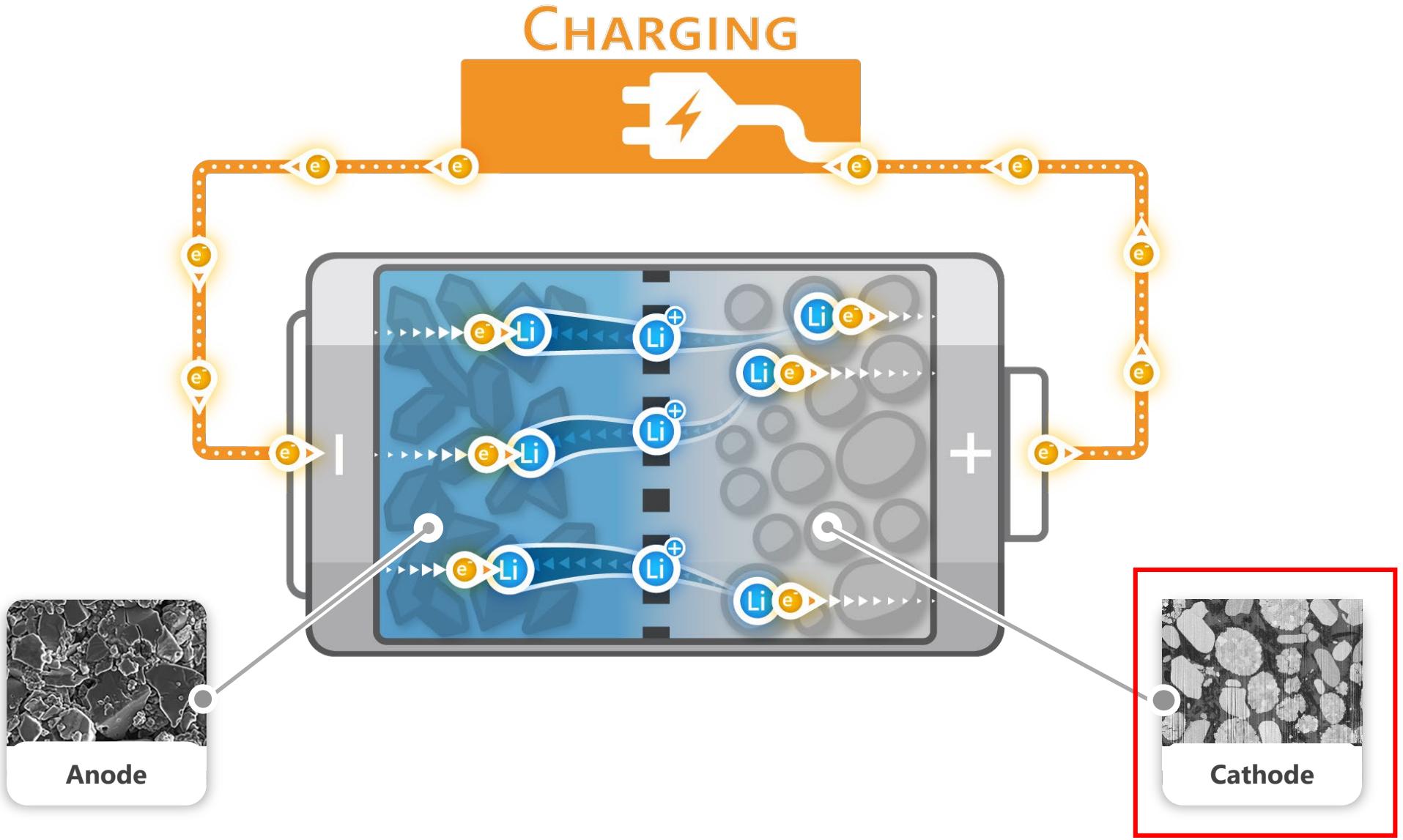

Cathode with two active materials

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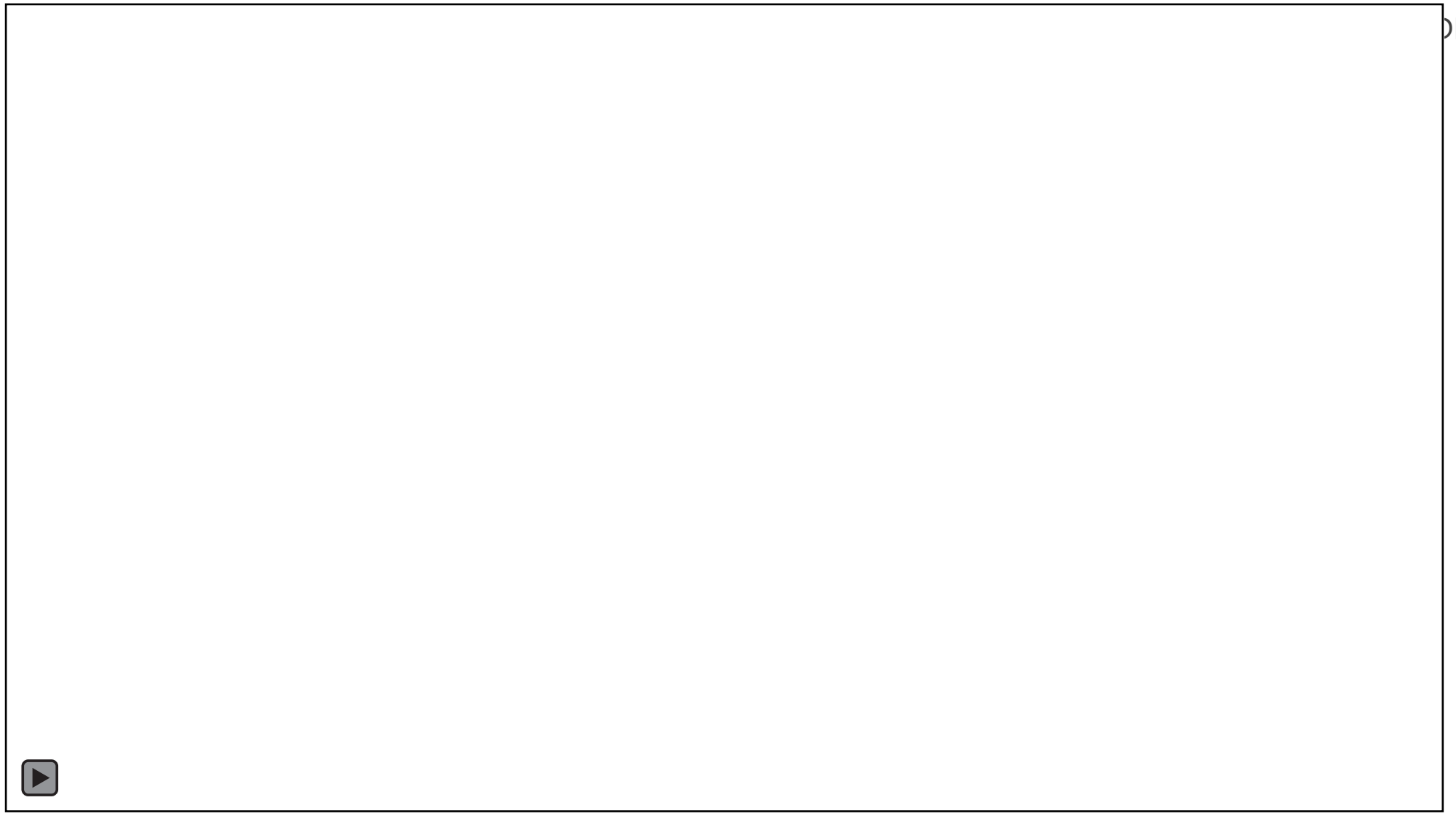

de ($LiNiCoAlO_2$)

Well organized transport is key

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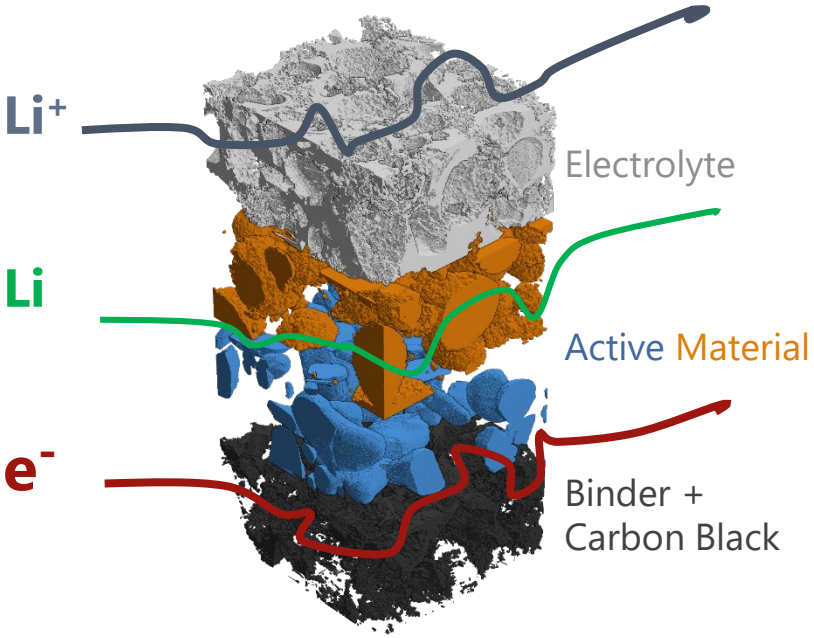

Infrastructure in Ludwigshafen
Source: https://www.stuttgarter-zeitung.de

Like in a city, certain transportation pathways are reserved for certain species

Dissolved Li^+ moves through the electrolyte	Ships sail on rivers
Lithium moves through the active material	Pedestrians walk on the sidewalk
e^- move through the carbon black + binder	Cars drive on streets

DIGITAL BATTERY DEVELOPMENT

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The development of new electrode microstructures is a **costly and time-consuming** process.

The workflow using the **GeoDict®** software significantly **reduces the development process**:

- Where are the bottlenecks of ionic transport?
- How do I improve the life-time of my battery?
- Smaller or larger grains? More or less binder?

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FIB-SEM SCANS OF CATHODE

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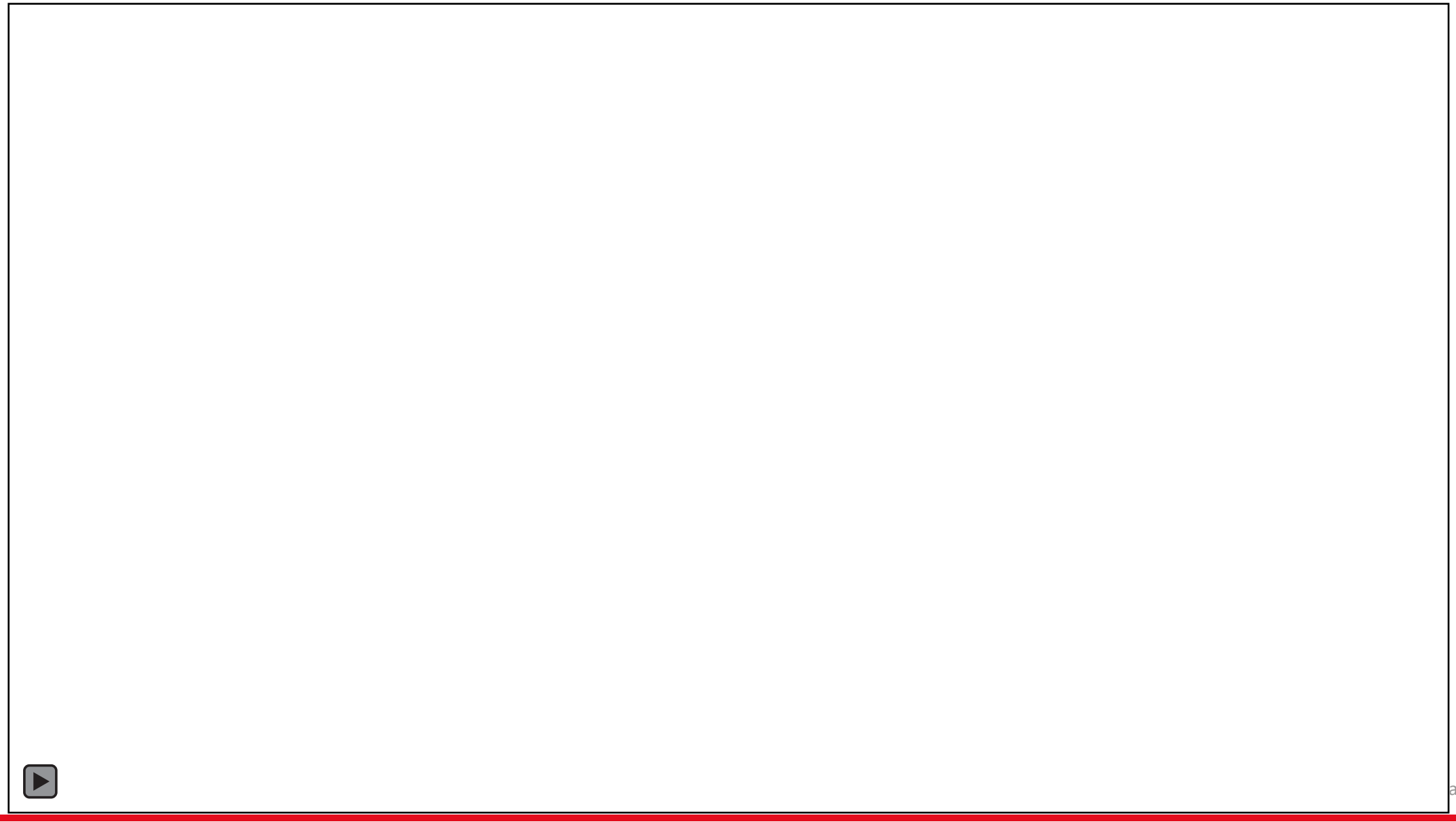

FIB-SEM IMAGE ALIGNMENT

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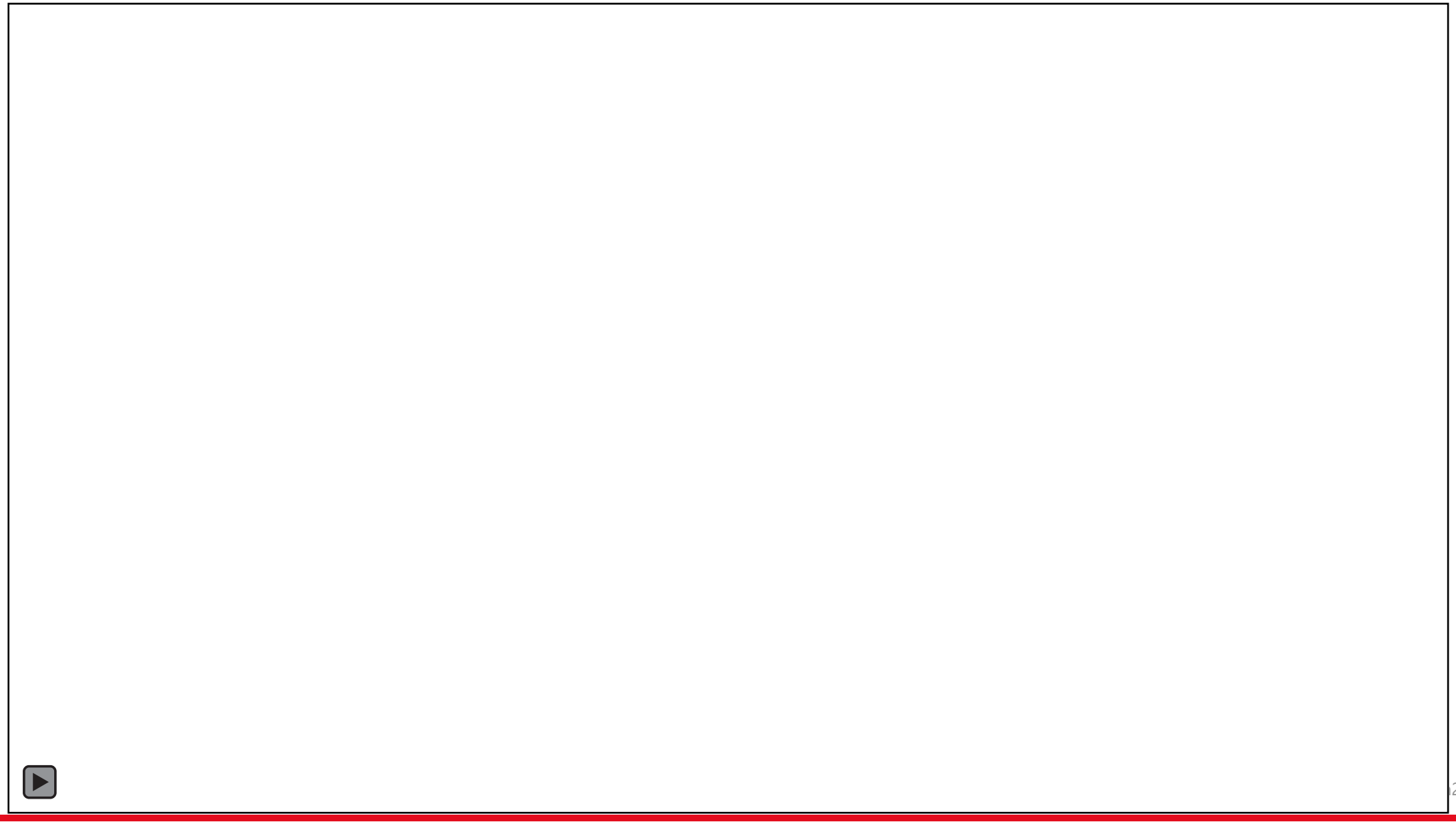

Image filtering: streak removal & NLM filter

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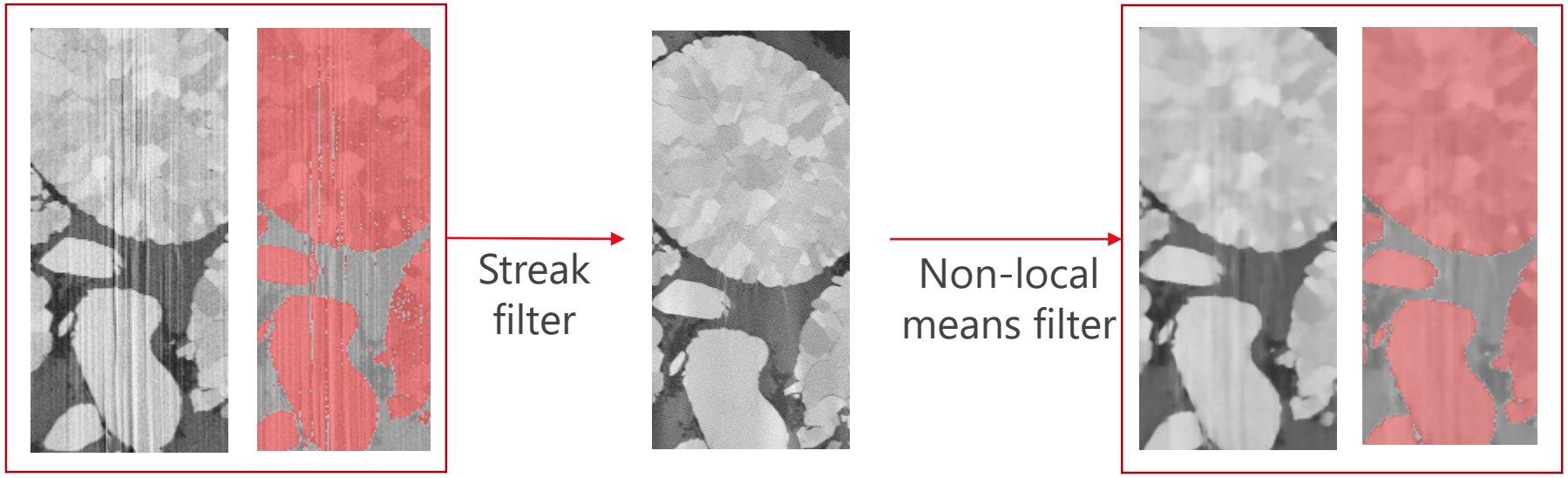
- Streak Removal in GeoDict 2019
  - Fills in strong streaks but leaves some shadows
  - Still experimental
  - In combination with good filtering (non-local means) possibly better segmentations



Segmented image first step

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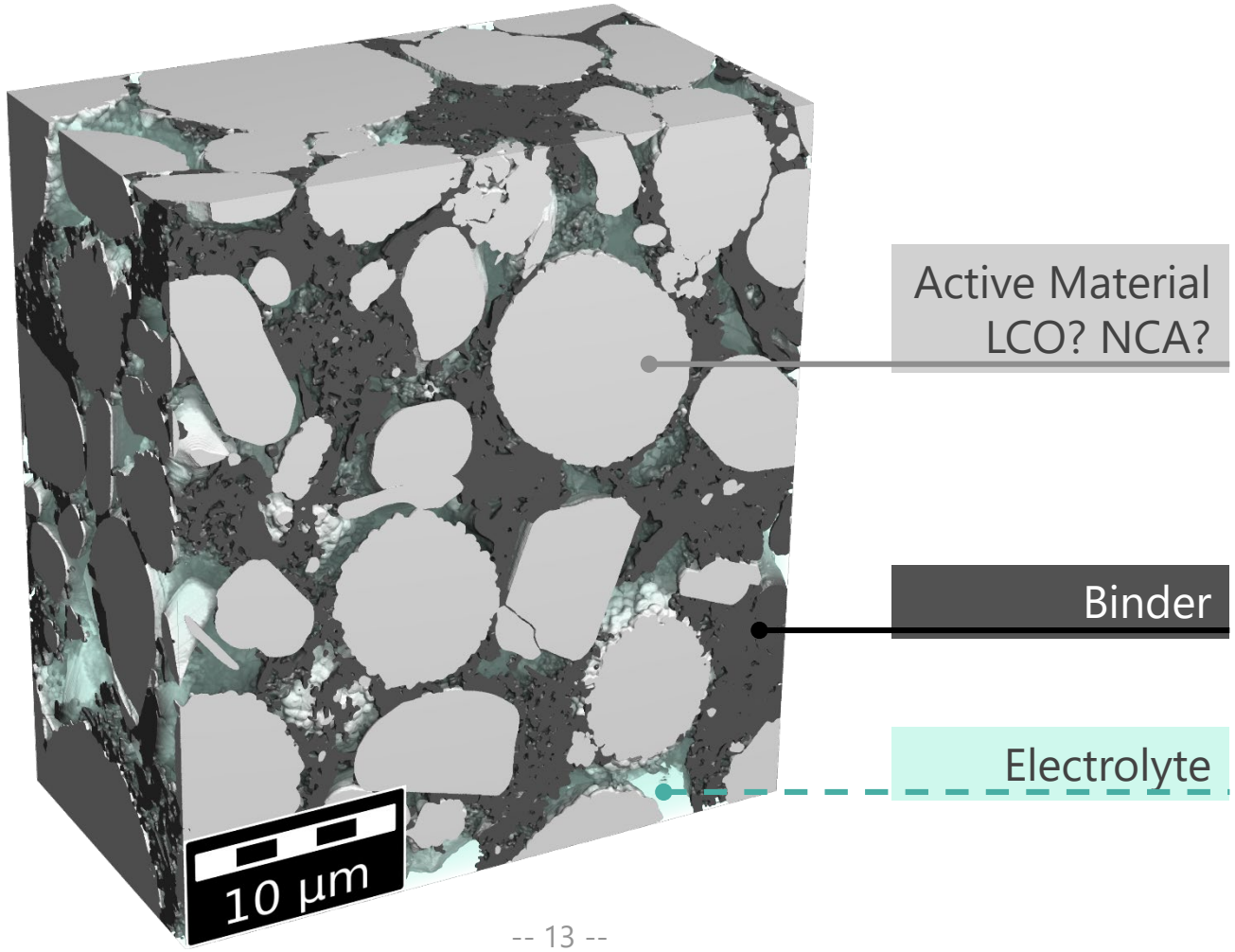
Cathode sample provided by KIT.
NCA: Lithium Nickel Cobalt Aluminum Oxide ($LiNiCoAlO_2$)
LCO: Lithium Cobalt Oxide ($LiCoO_2$)



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Separation of the active materials

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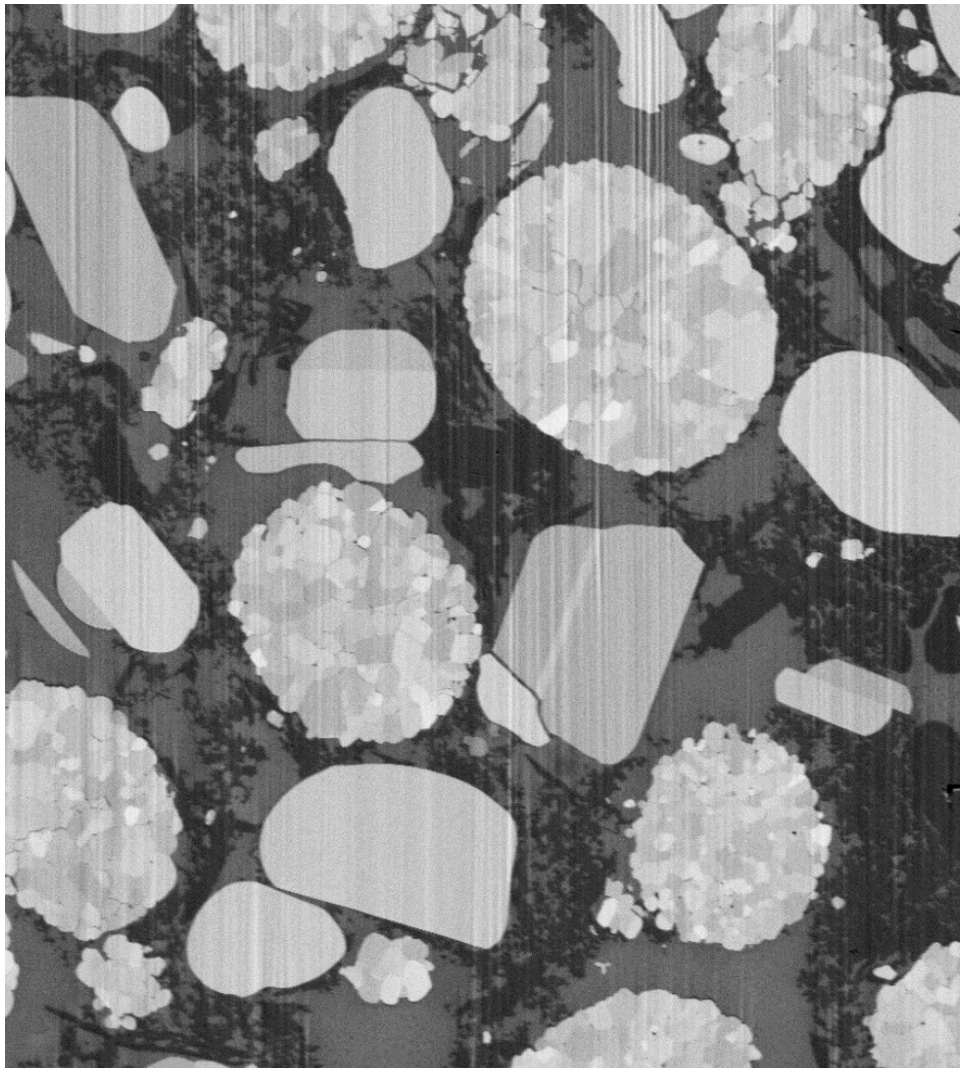
- Why separate LCO and NCA?
  - Different charging behavior of LCO and NCA
  - Need correct materials for accurate charging simulation
- Why no direct segmentation of LCO and NCA via global thresholding?
  - Gray values are too similar



Grain identification

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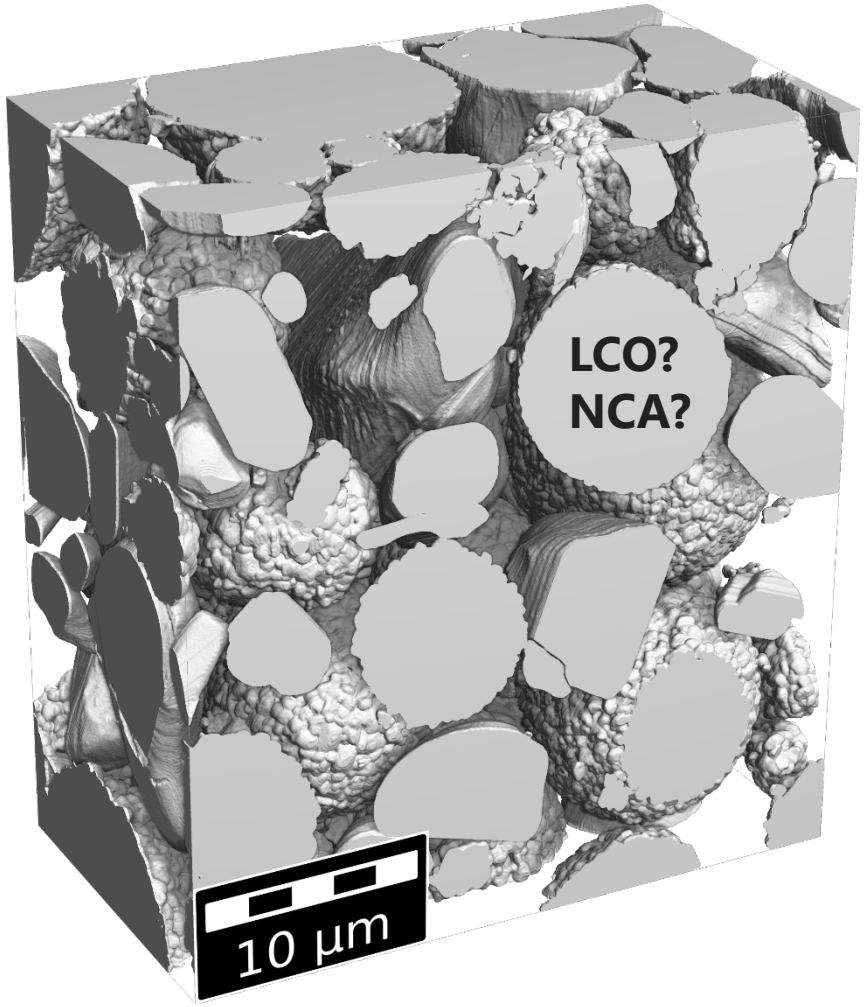
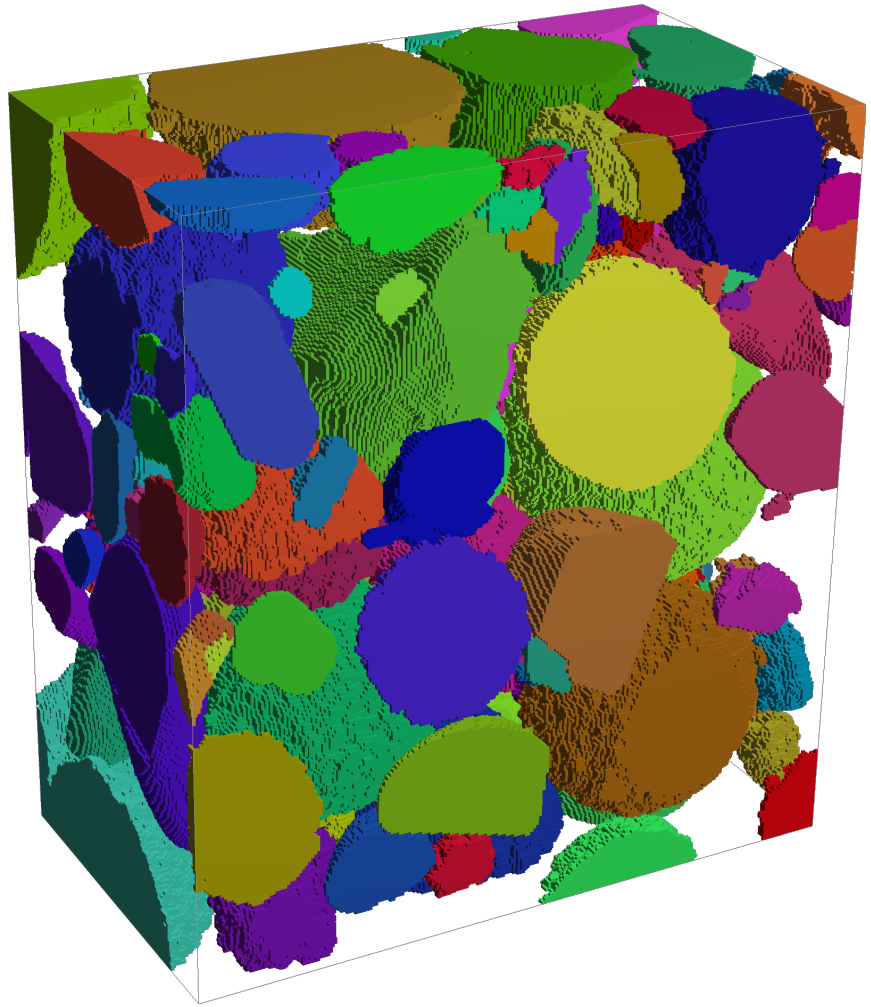
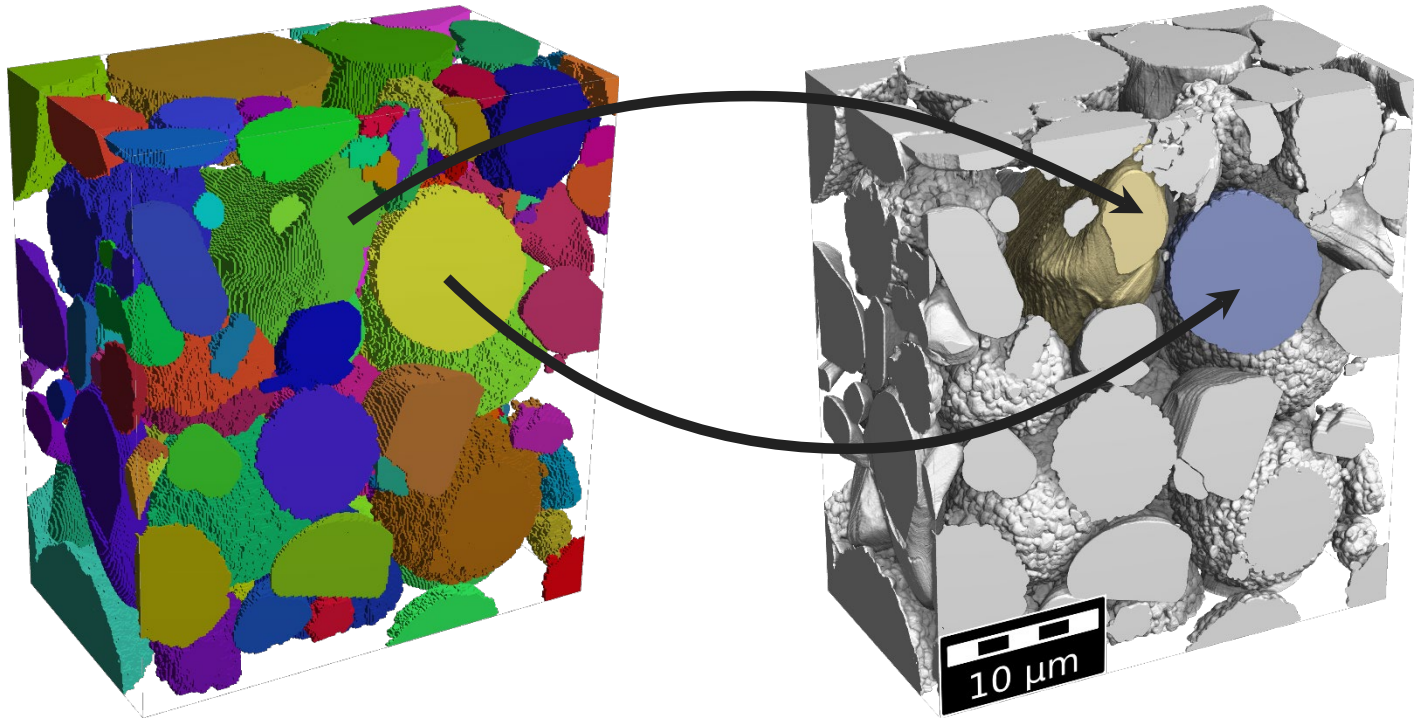


Active material



Identified grains

Material assignment for each grain



- Selection of one voxel of the grains.
- Automatic assignment of active material per grain.

Cathode after material assignment

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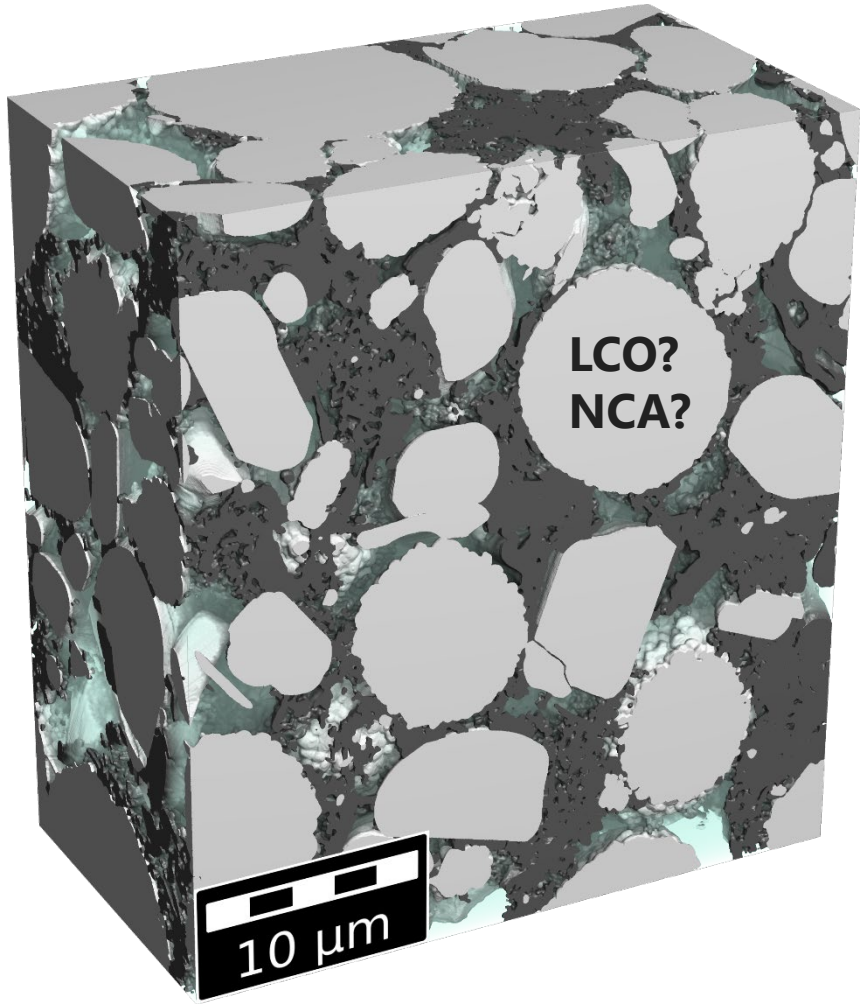
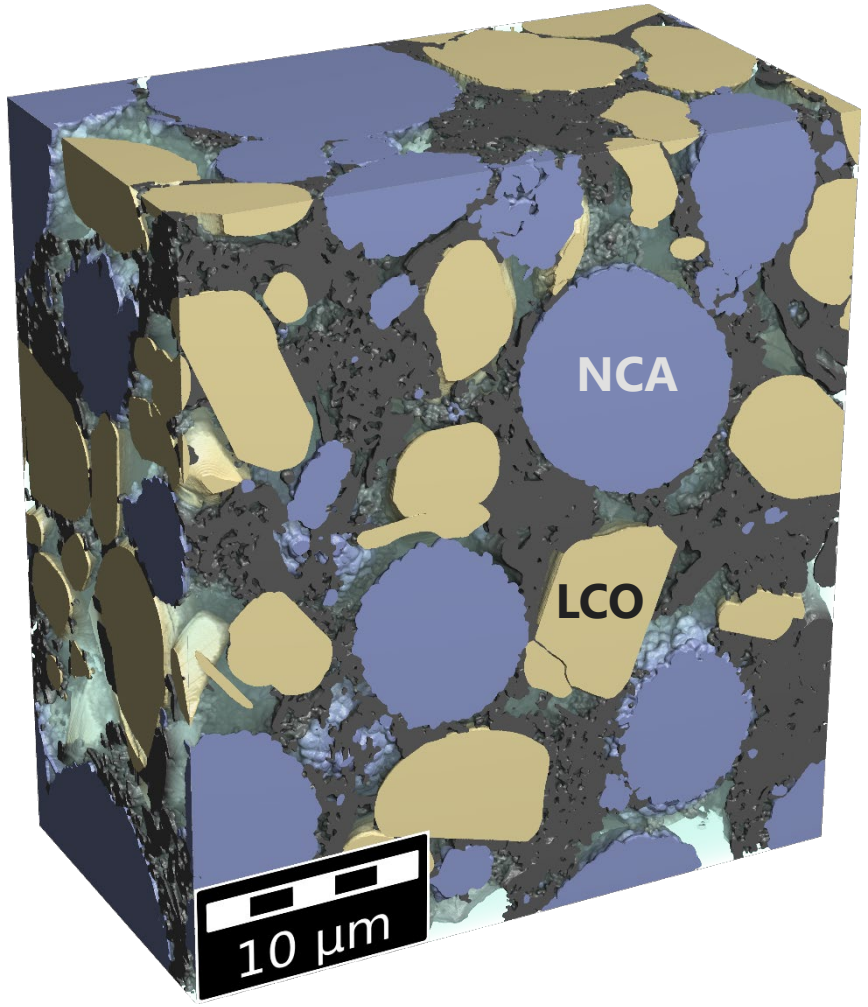


(Pre-)segmented cathode with electrolyte, binder, and combined active materials



Cathode with electrolyte, binder, LCO and NCA

Options for grain segmentation

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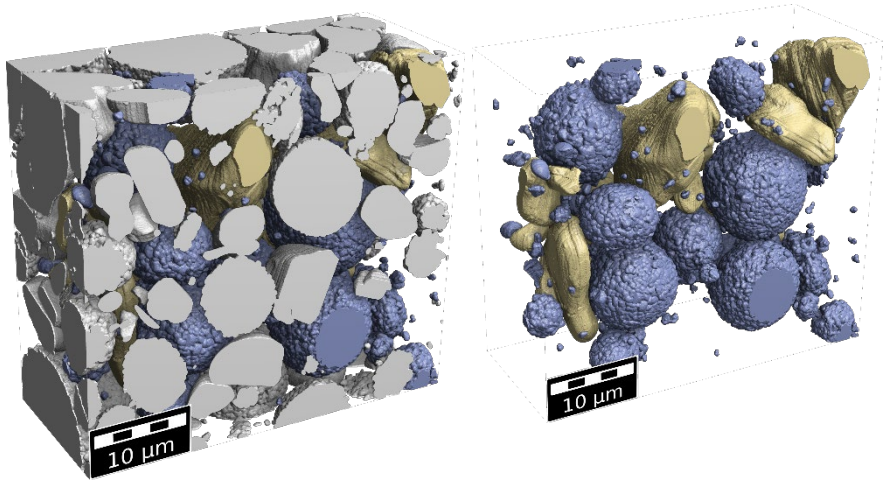
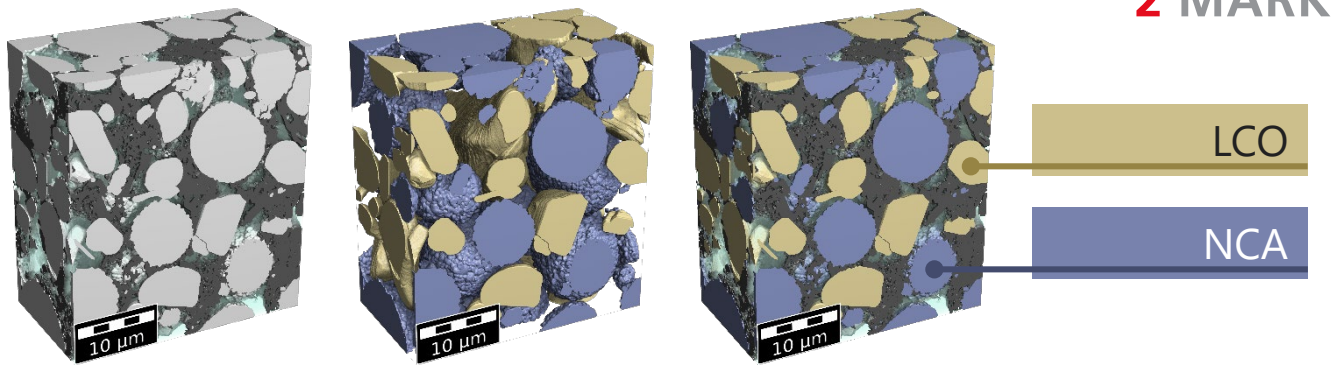
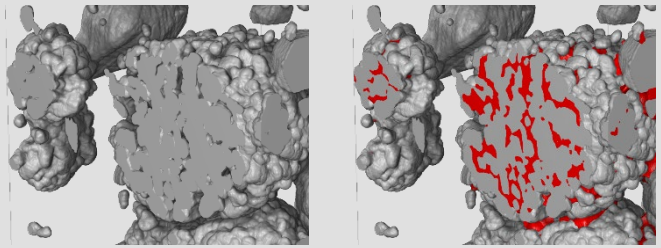
- Segmentation by selection
- Segmentation by shape

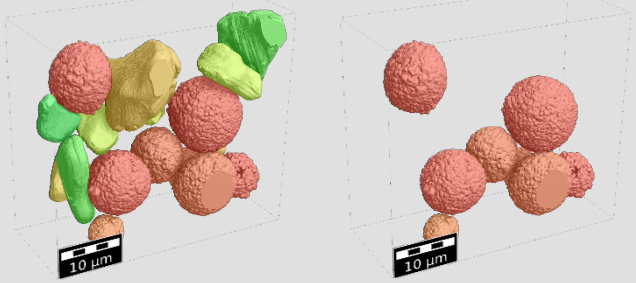




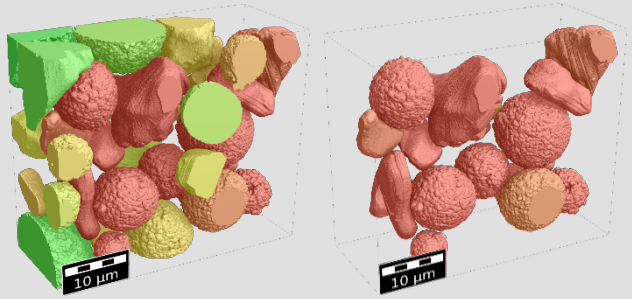
- Filling cracks



- Filtering by sphericity



- Filtering by boundary contact



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Hot research topic: how much binder is optimal?

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Not enough binder:

https://steiermark.orf.at/news

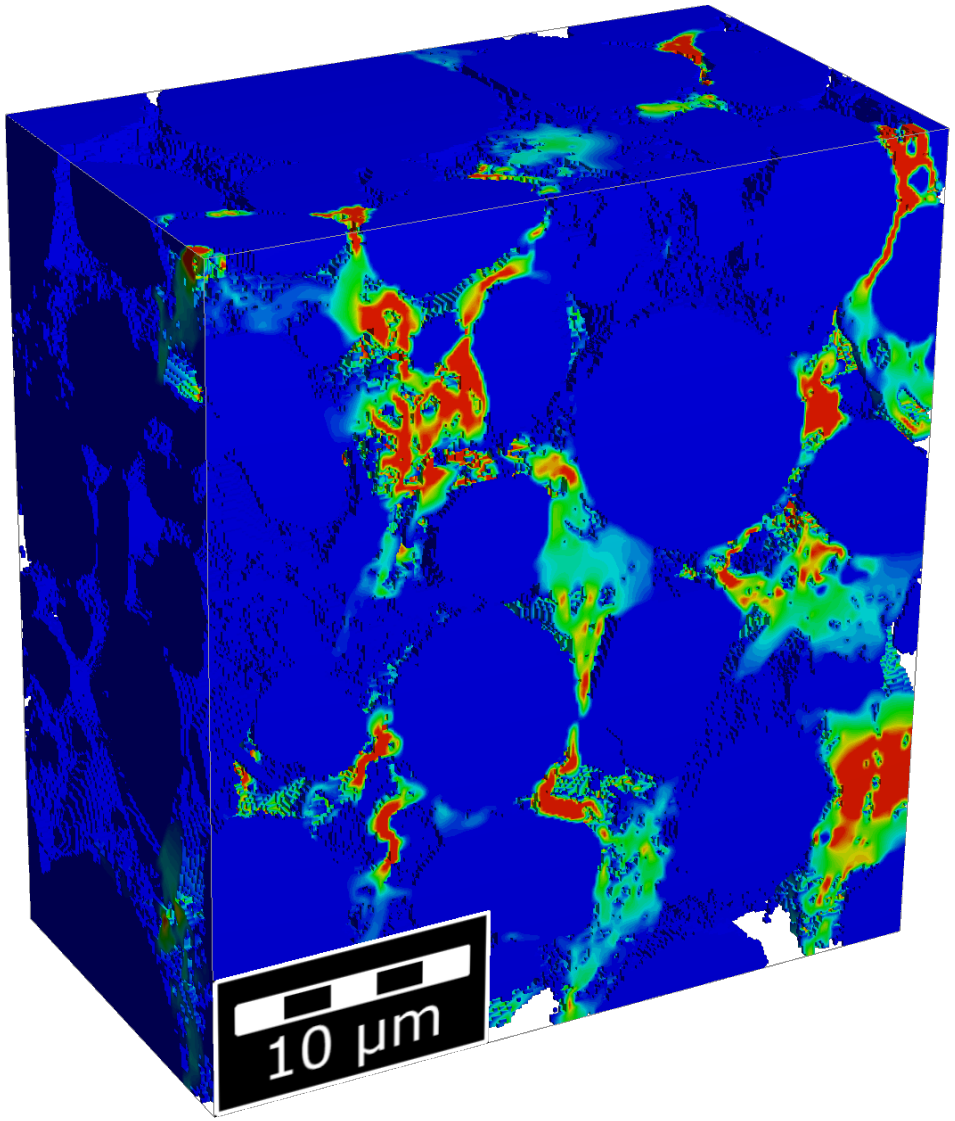
e^- have to take detours

Too much binder:

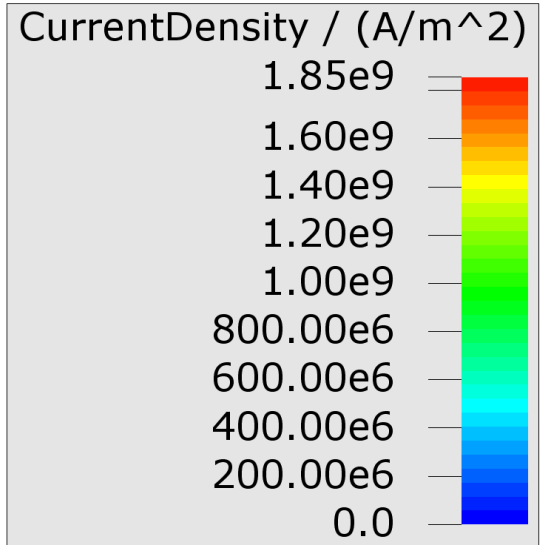
https://www.deinfuehrerschein.de

Li^+ cannot enter electrolyte

Current density in all solid materials



- Almost all current goes through the binder + carbon black



Li^+-CONCENTRATION IN THE CATHODE DURING CHARGING

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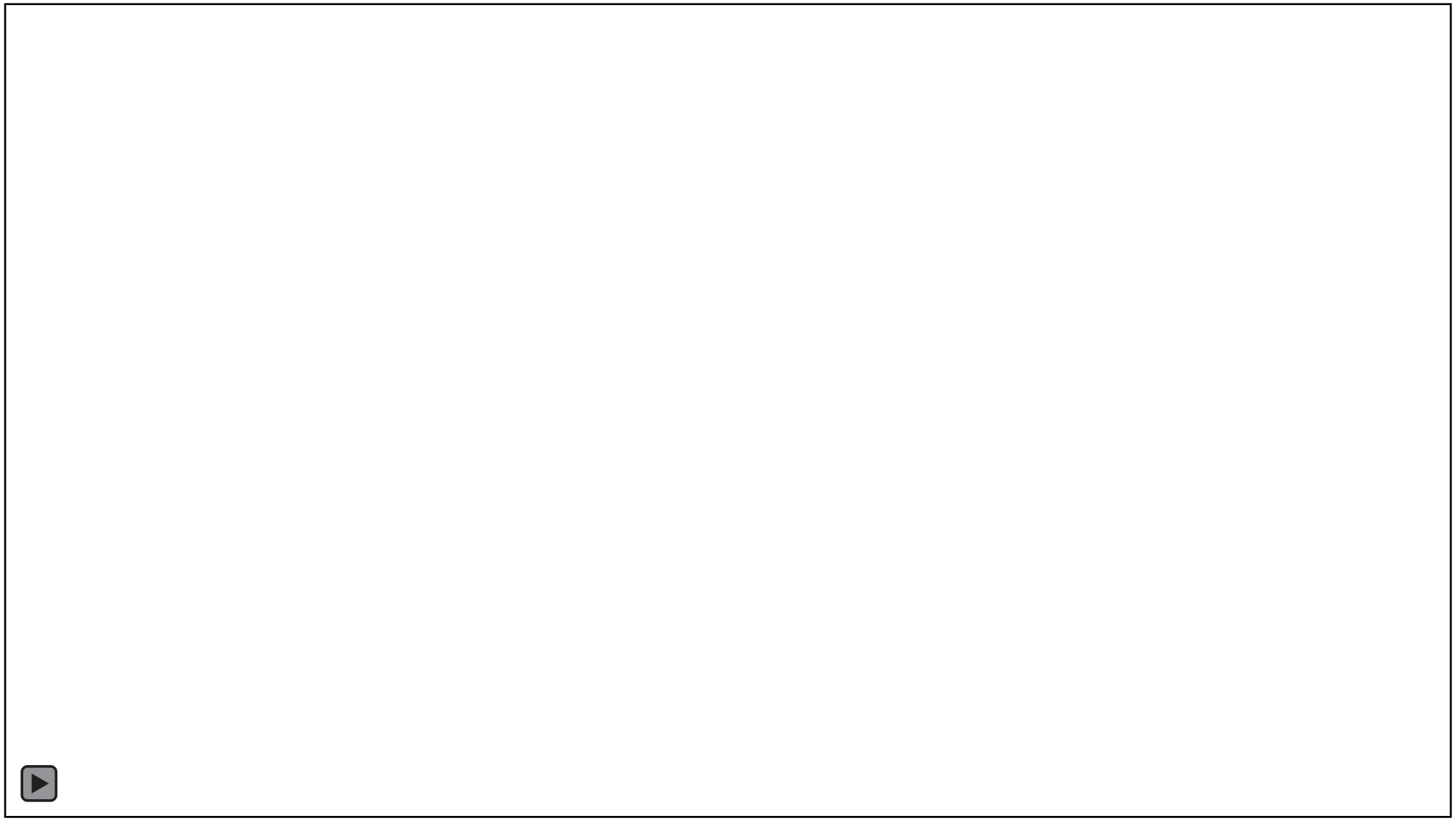

How much binder is optimal?

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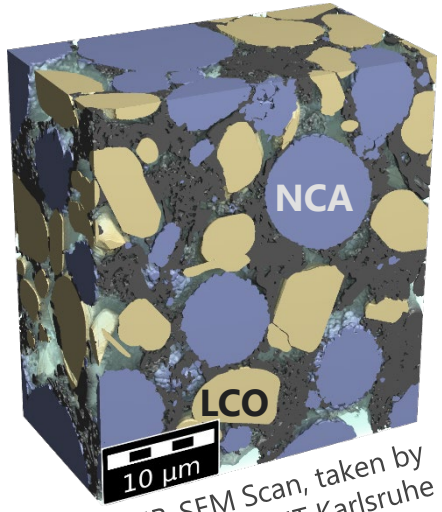
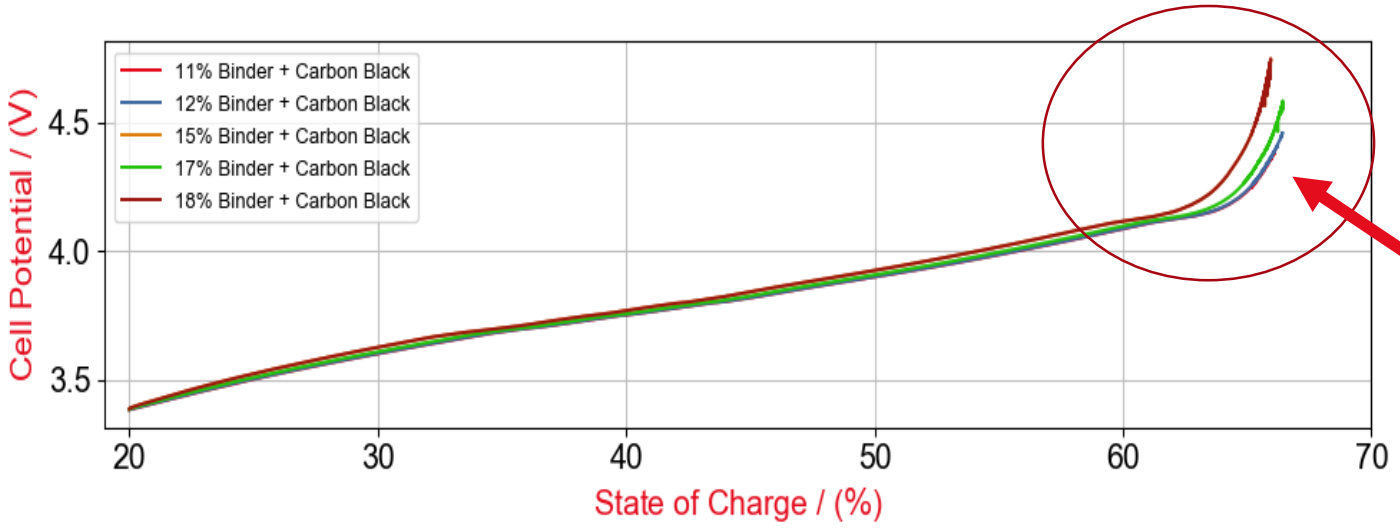
Binder $\%_{vol.}$	11%	12%	15%	17%	18%
Tortuosity Factor	2.7	3.1	3.5	3.9	4.4
Diffusivity	11.3	9.1	7.4	6.1	4.9

Good Cathode Configuration



FIB-SEM Scan, taken by Joos et al, KIT Karlsruhe

Flex point means, battery cannot be charged much further



More binder makes the cathode worse

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PARTICLE EXPANSION

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LITHIUM PLATING IN ANODE HALF-CELL SIMULATION

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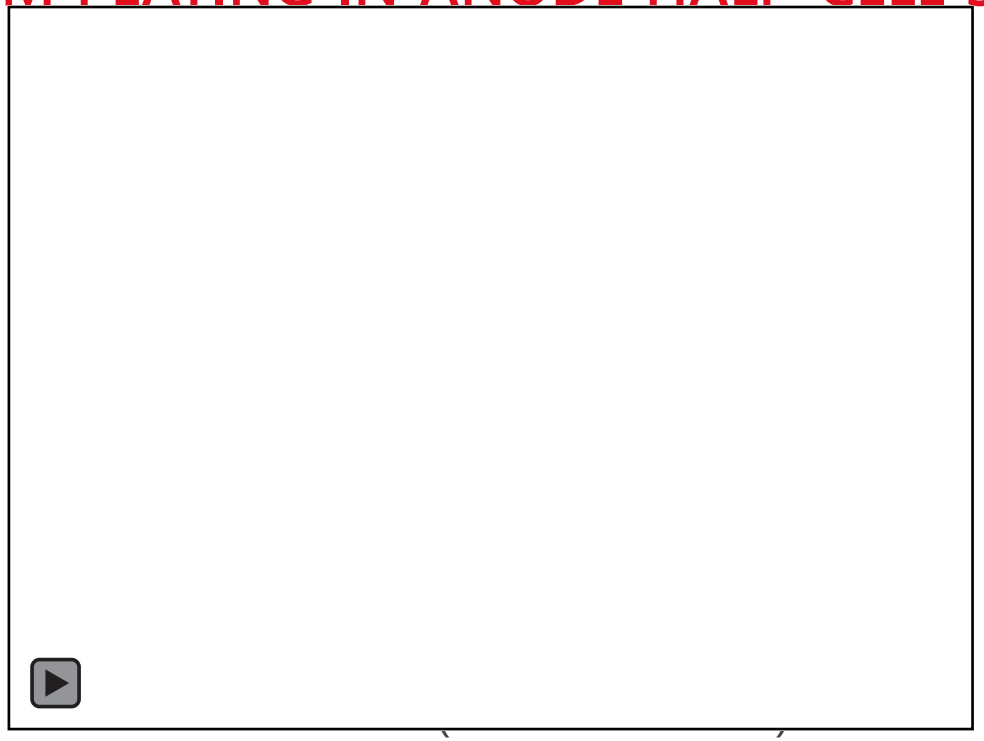
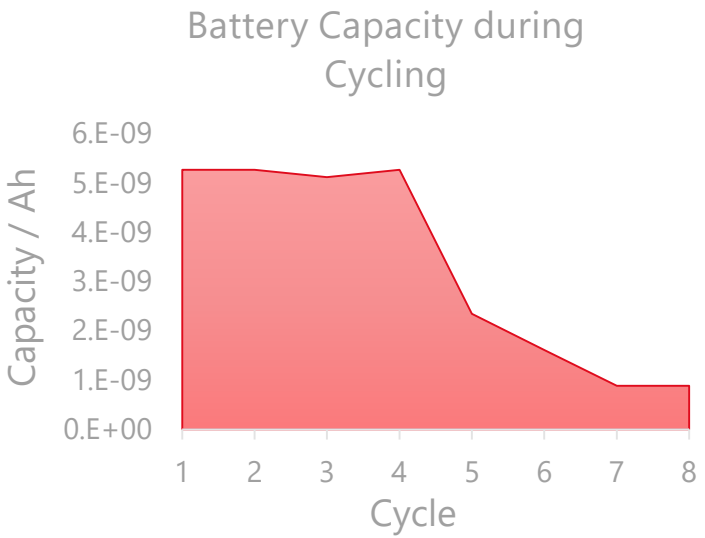
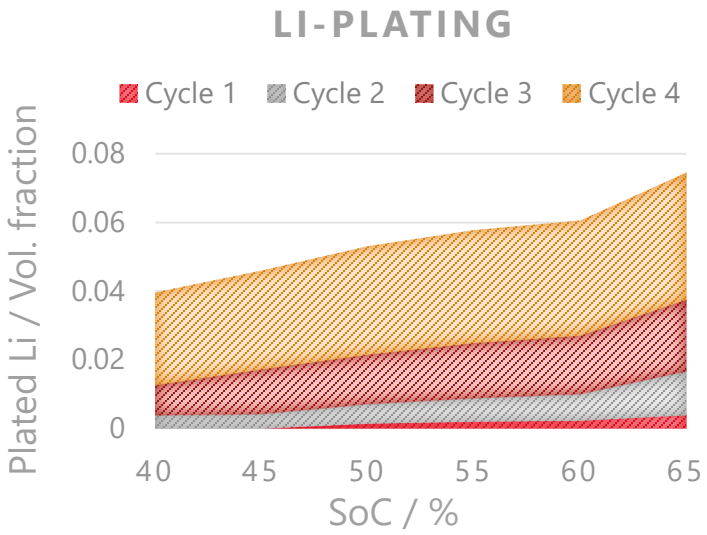


charged with **3C** in BatteryDict

2. Executing Python-Script
3. Use updated anode for next cycle

- Plating sets in at 50 % SoC in the 1. cycle
- Capacity drops significantly after the 4. cycle





THANK YOU!

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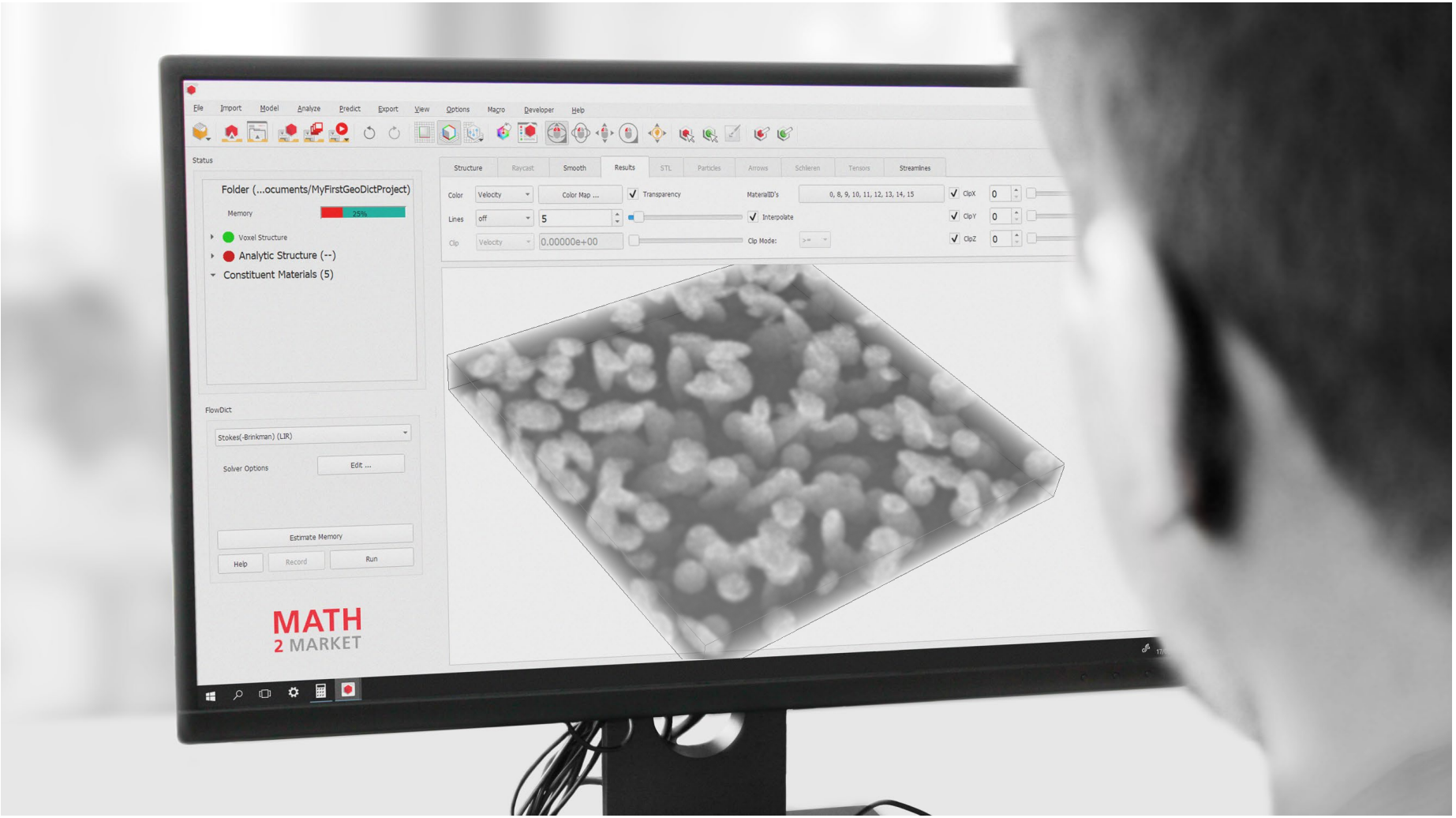

Meet us at BOOTH #6