

How does the micro-structure of the cathode material influence the performance of Batteries?

Speaker: Dr. Ilona Glatt

Authors: F. Biebl, T. Hofmann, S. Schwichow, J. Zausch & many more

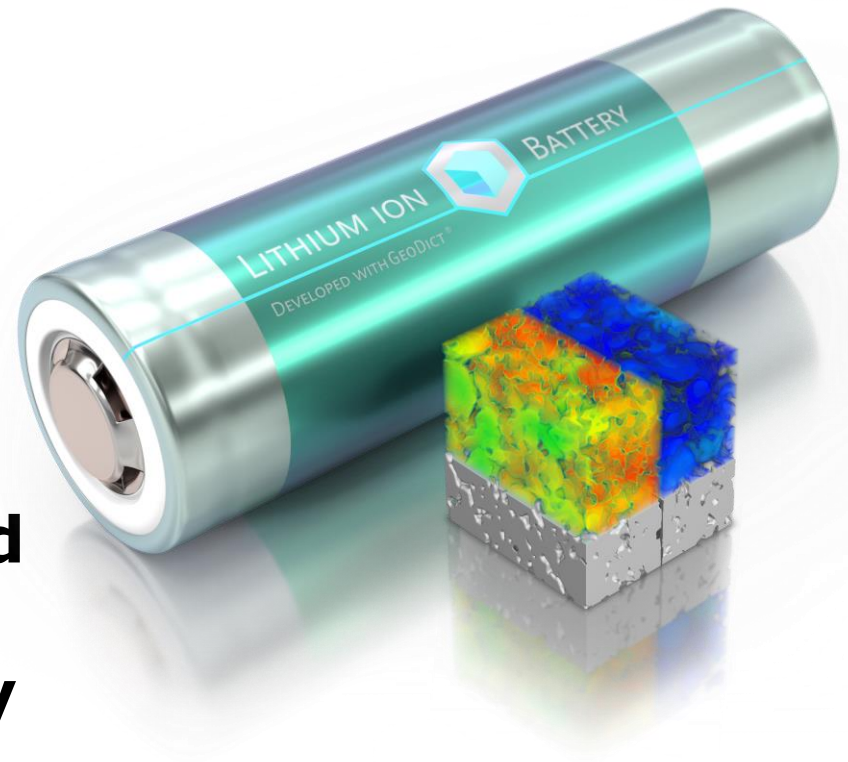


USER MEETING 2017

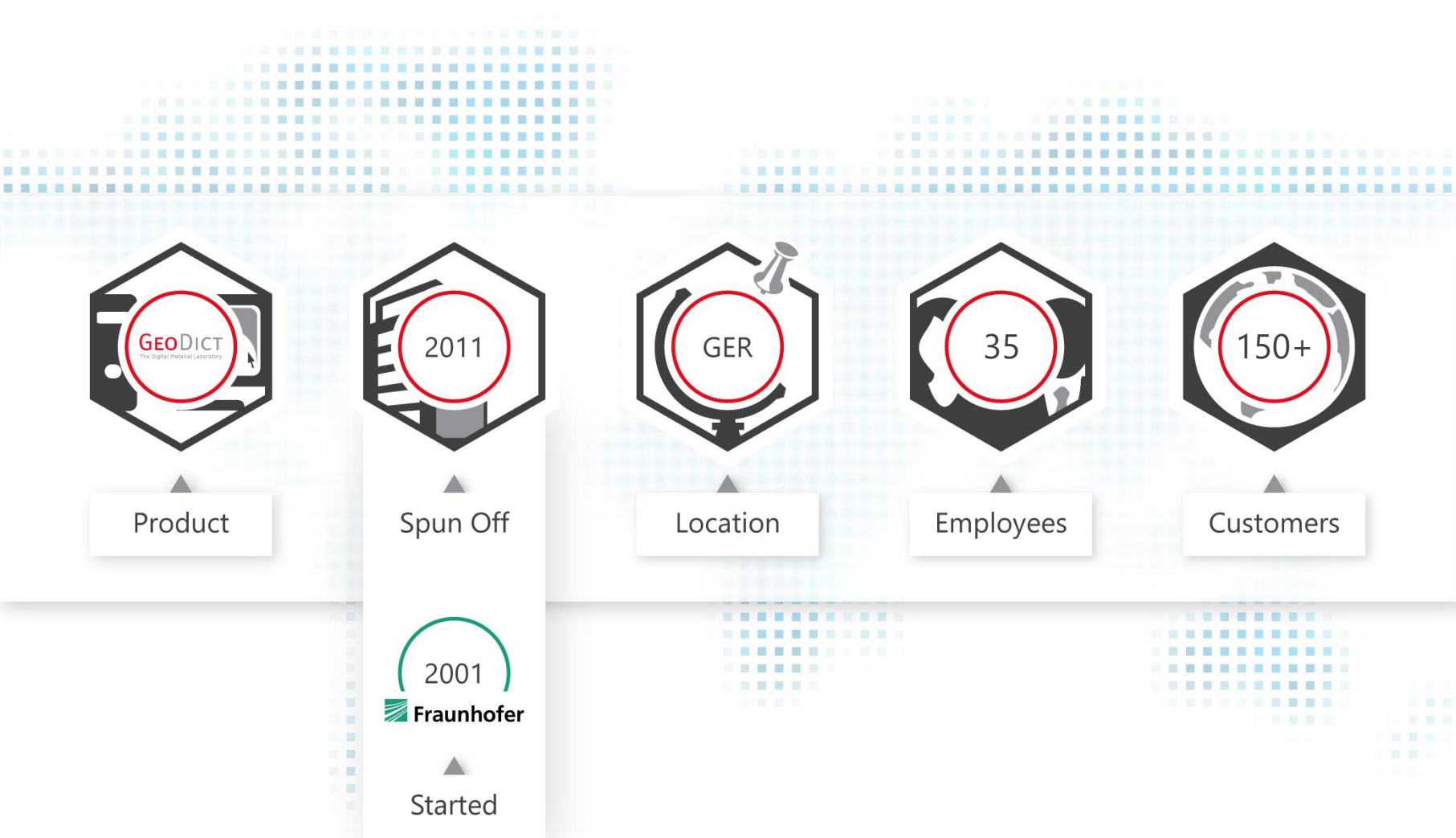
September 26-27 in Kaiserslautern

Overview

- Who are we?
- Analyses of the microstructure
- Testing the analyzed material in a battery



Math2Market GmbH Company Overview



Math2Market GmbH

Location and Contact

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Germany

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Fax + 49 631 / 205 605 99

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Development of Materials



Development of materials by Digital Material Design

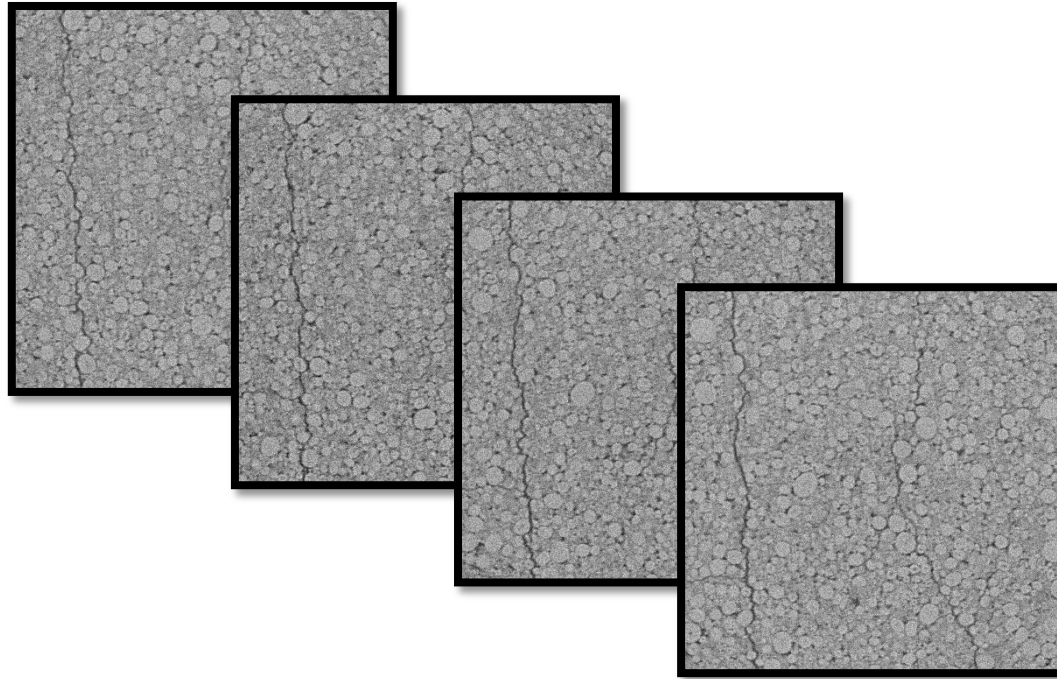


Image Acquisition



Development of Materials



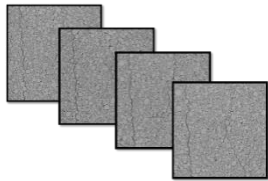


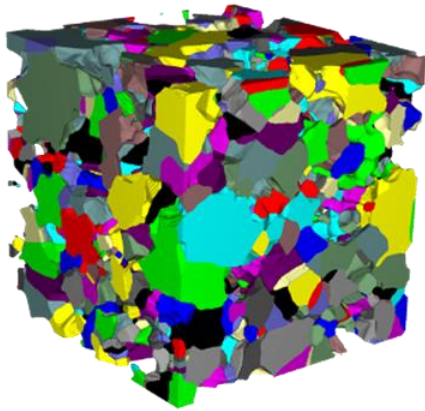
Image Acquisition



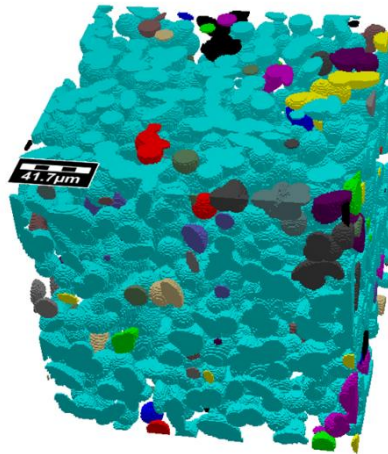
Development of Materials



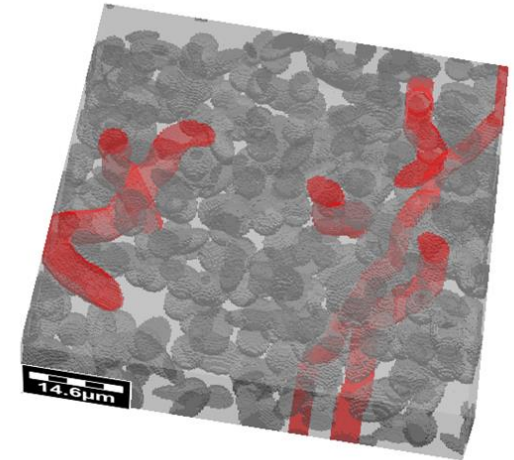
Development of materials by Digital Material Design



pore analysis



grain analysis



tortuosity

Image Analysis



Development of Materials



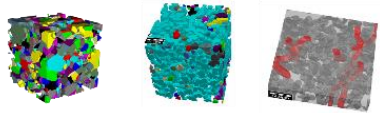


Image Analysis

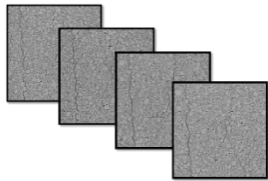


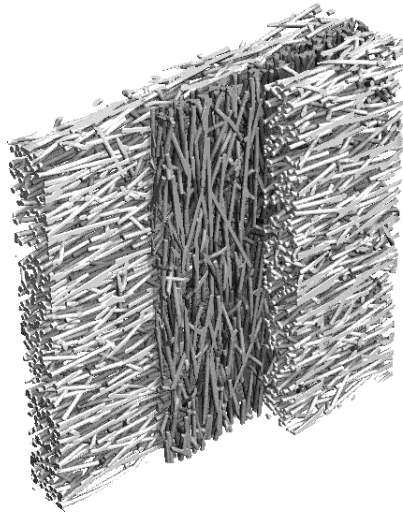
Image Acquisition



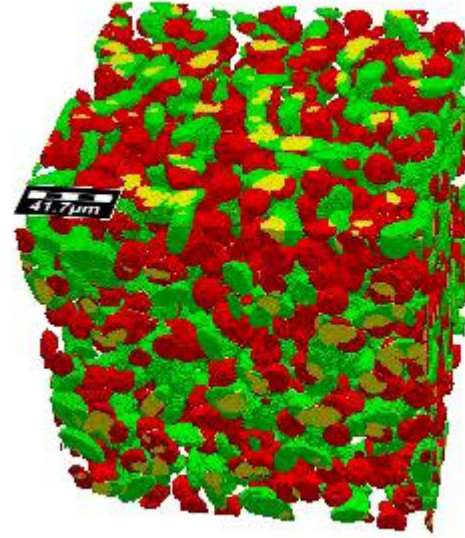
Development of Materials



Development of materials by Digital Material Design



fiber structures



grain structures

Modelling
Microstructures



Development of Materials



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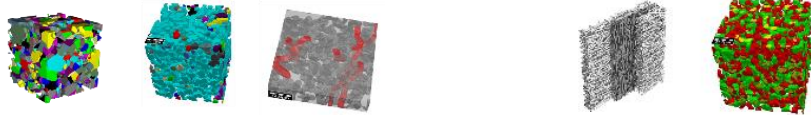


Image Analysis

Modelling
Microstructures

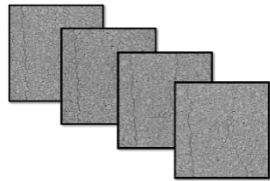


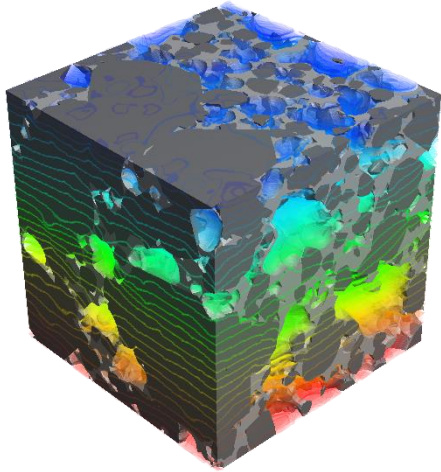
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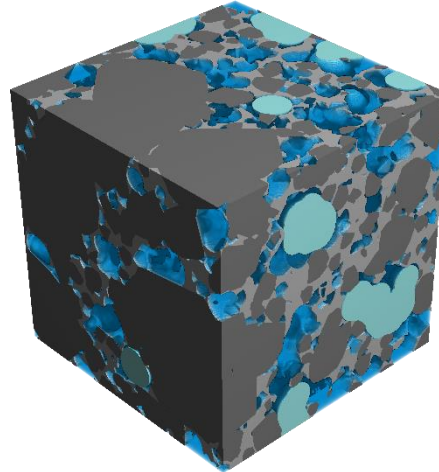
Development of Materials



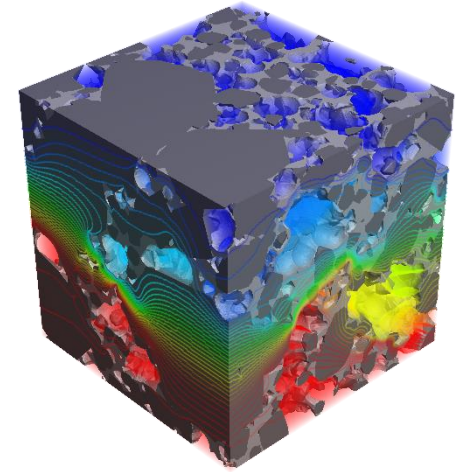
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conductivity simulation



saturation simulation



flow simulation

Microstructure
Simulation



Development of Materials



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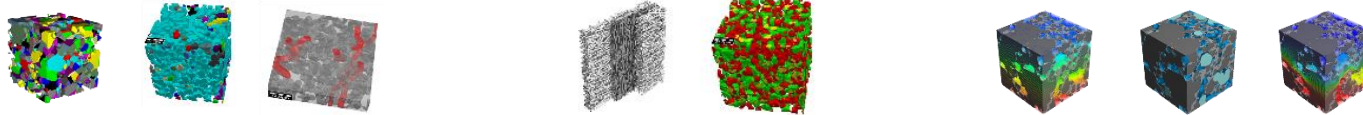


Image Analysis

Modelling
Microstructures

Microstructure
Simulation

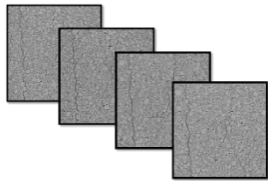


Image Acquisition



Development of Materials



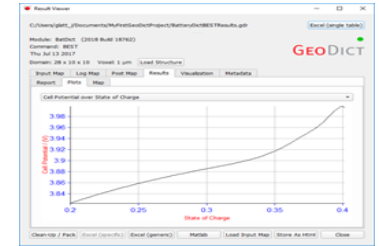
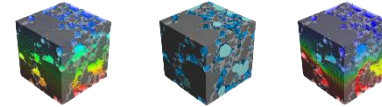
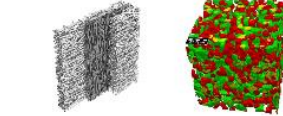
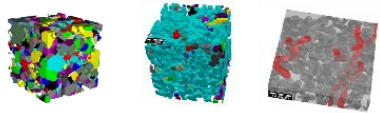
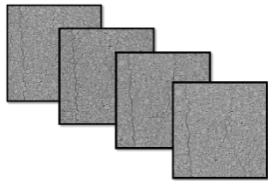


Image Analysis

Modelling
Microstructures

Microstructure
Simulation

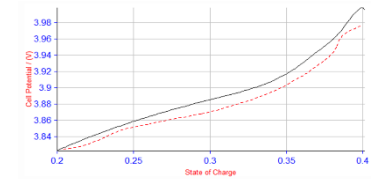
Macroscopic Material
Parameters



Change Geometry

Material Property

Image Acquisition



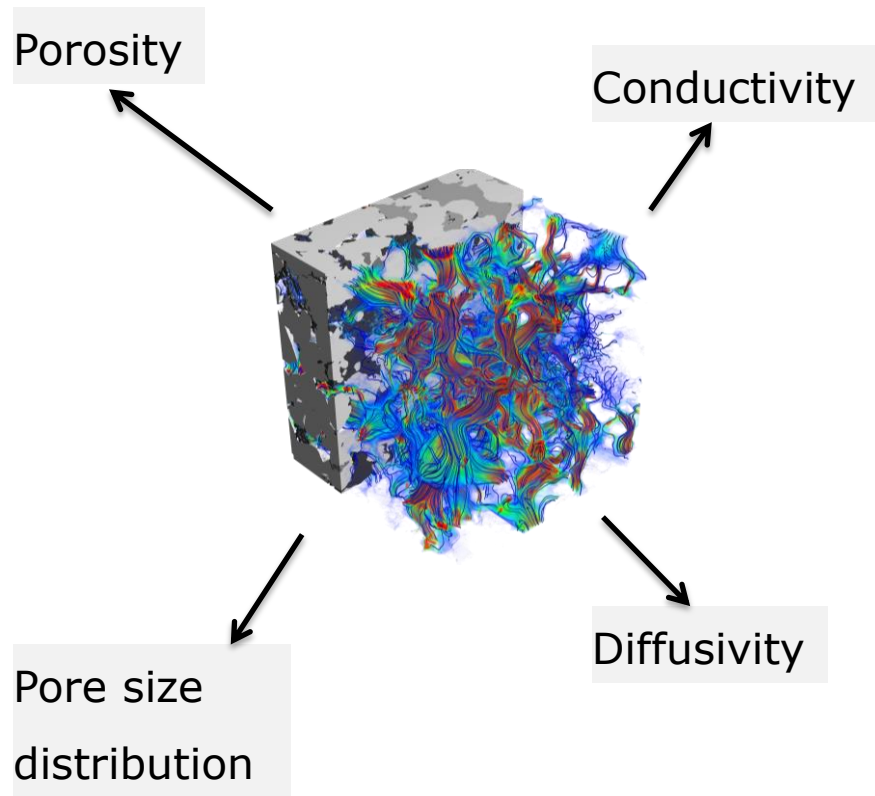
Experimental
Verification



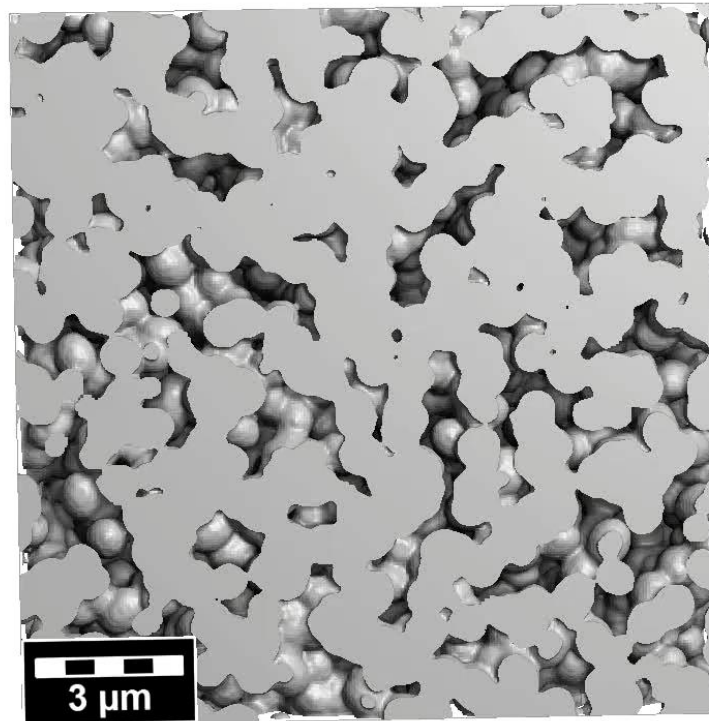
Development of Materials



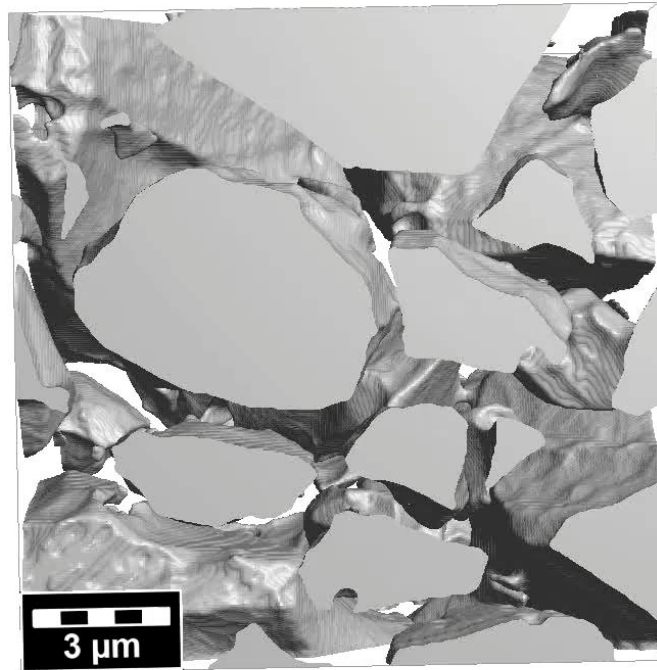
BatteryDict



Anode



Cathode



BatteryDict GUI

Design Battery

GEODICT

Result File Name (*.gdr)

Attachment of Electrodes in **x-Direction**: 513 Voxels, 31.806 μm

y-Direction
256 Voxels
15.872 μm

z-Direction
256 Voxels
15.872 μm

Anode Current Collector
3 Voxels
0.186 μm

Anode
Voxel Length: 62 nm
Size: 252x256x256 Voxels
Anode File (*.gad, *.gdt)

Separator / (Voxels)

0.186 μm

Cathode
Voxel Length: 62 nm
Size: 252x256x256 Voxels
Cathode File (*.gad, *.gdt)

Cathode Current Collector
3 Voxels
0.186 μm

Boundary Conditions in Tangential Direction
 periodic
 symmetric

Rotate around

Rotate around

Result Viewer

File path: //m2mnas/home/Anoden und Macro/BatteryDictBESTmicroFFT_10.gdr
 C:/Users/glatt/Desktop/CaseStudy BatteryDict/BatteryDictDesigner.gdr

Module: BatteryDict (2018 Build 20353)
 Command: DesignBattery
 Wed Sep 20 2017

Domain: 513 x 256 x 256 Voxel: 62 nm

GEODICT

Input Map Log Map Results Metadata

Report Map

BatteryGeo

In the following, the central properties of the battery geometry are shown. A more detailed description can be found in the Tab 'Map'.

Battery

The volume fraction in the battery are as follows:

Volume Fractions	Anode	Cathode	Electrolyte
Active	34.3723 %	12.1451 %	39.0467 %
Inactive	0.013019 %	13.214 %	0.0393367 %
Current Collector	0.584795 %	0.584795 %	-
Separator	-	-	0.584795 %

Anode

The volume fraction within the Anode are as follows:

Volume Fractions	Solid	Electrolyte
Active	69.9721 %	29.9698 %
Inactive	0.0265031 %	0.0315954 %

Cathode

The volume fraction within the Cathode are as follows:

Volume Fractions	Solid	Electrolyte
Active	24.7239 %	48.3276 %
Inactive	26.9 %	0.048483 %

Battery

The volume fraction in the battery are as follows:










Volume Fractions	Anode	Cathode	Electrolyte
Active	34.3723 %	12.1451 %	39.0467 %
Inactive	0.013019 %	13.214 %	0.0393367 %
Current Collector	0.584795 %	0.584795 %	-
Separator	-	-	0.584795 %

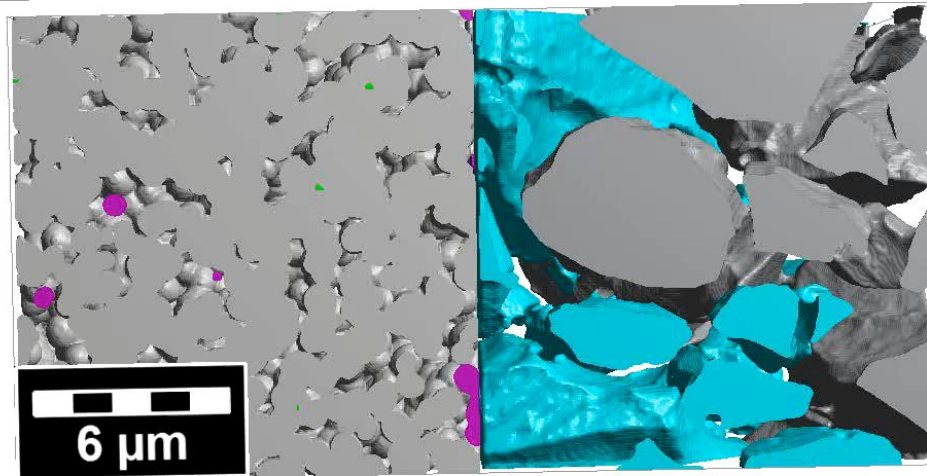
Anode

The volume fraction within the Anode are as follows:

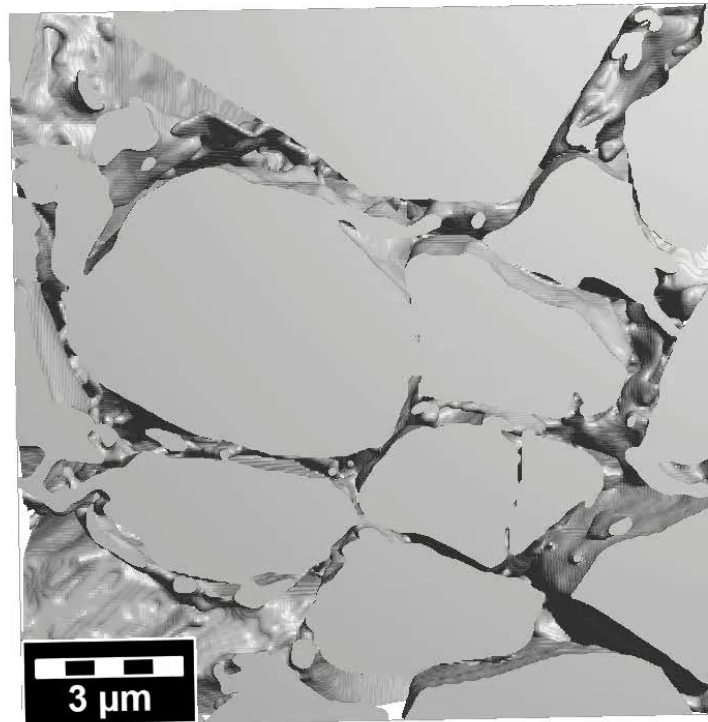
Volume Fractions	Solid	Electrolyte
Active	69.9721 %	29.9698 %
Inactive	0.0265031 %	0.0315954 %

Material Information:

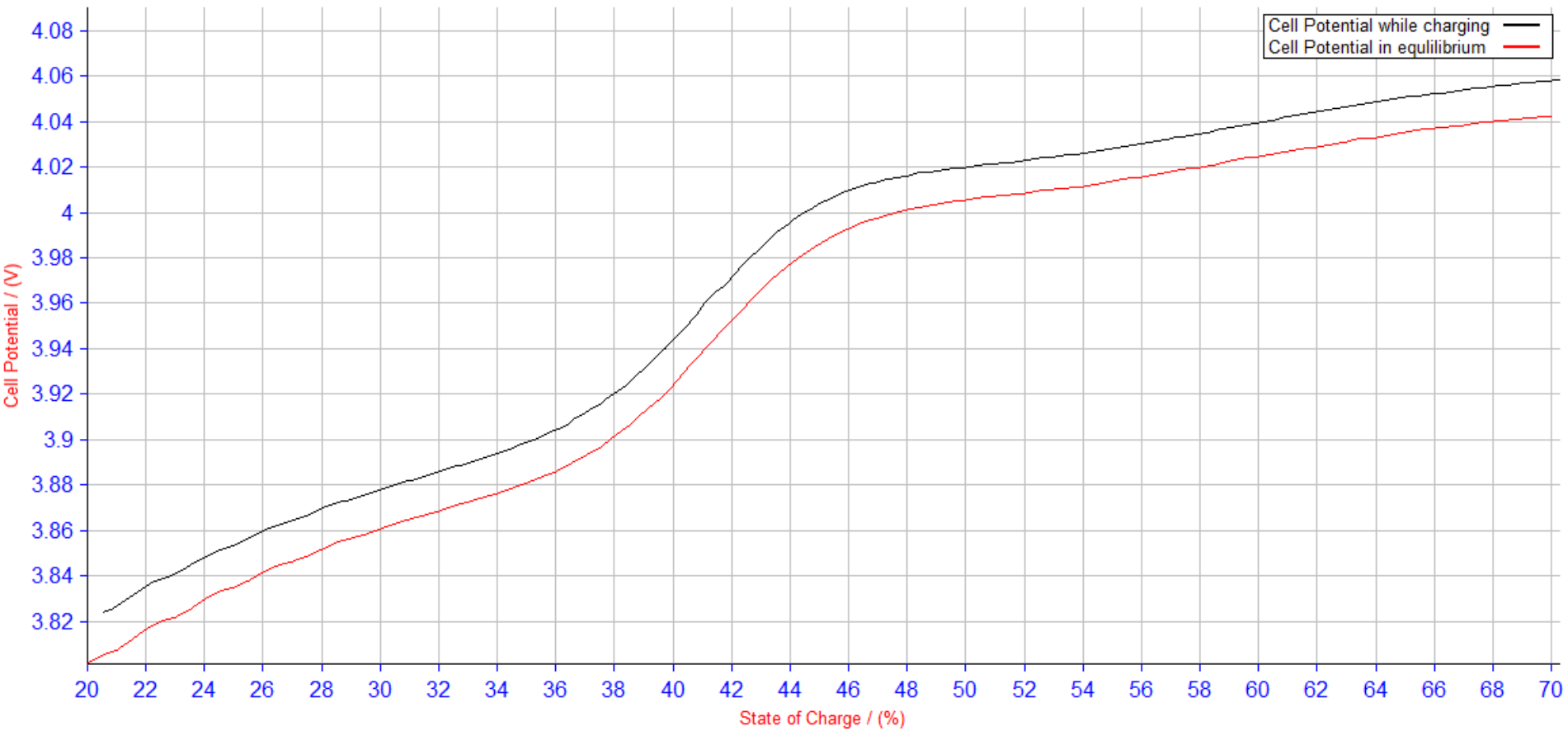
	ID 00: Electrolyte [invis.]
	ID 01: Anode Material
	ID 02: Cathode Material
	ID 03: Anode Current Collector [invis.]
	ID 04: Cathode Current Collector [invis.]
	ID 05: Inactive Anode Material
	ID 06: Inactive Cathode Material
	ID 07: Inactive Electrolyte
	ID 08: Separator [invis.]



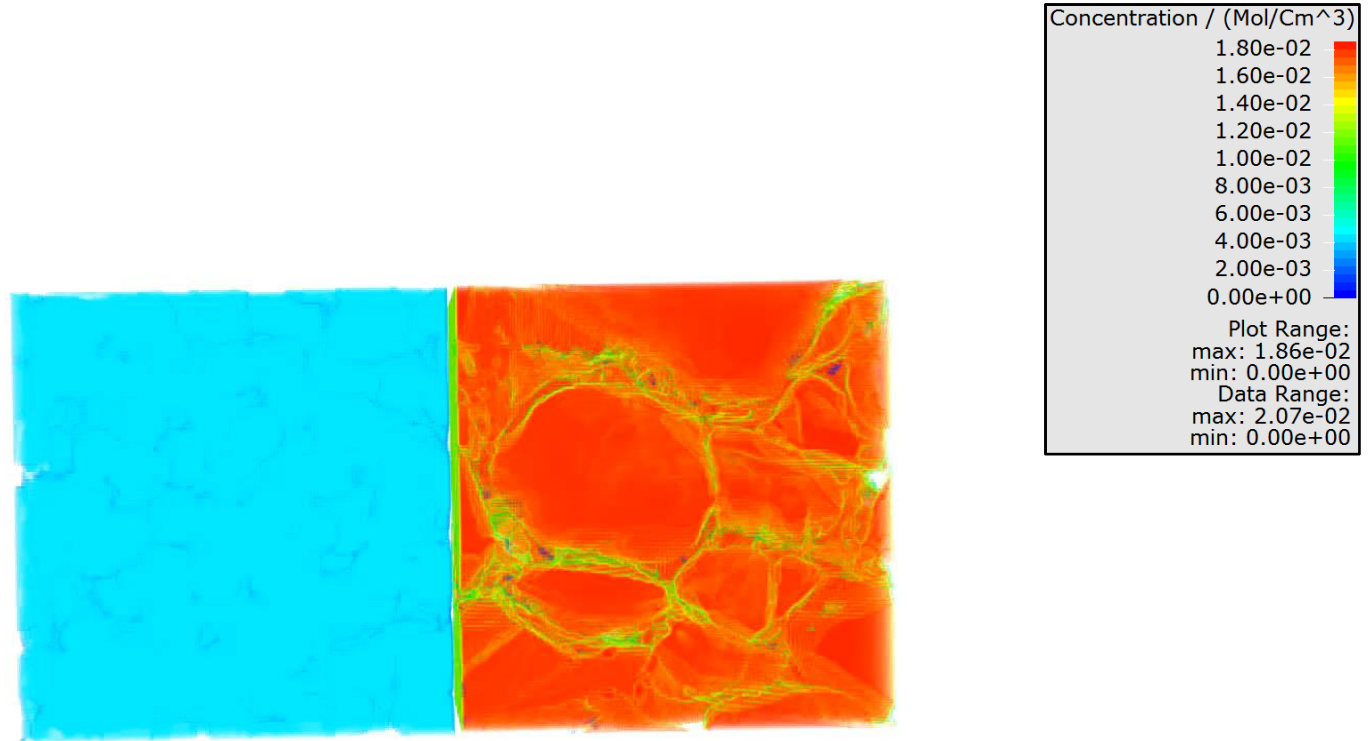
Cathode



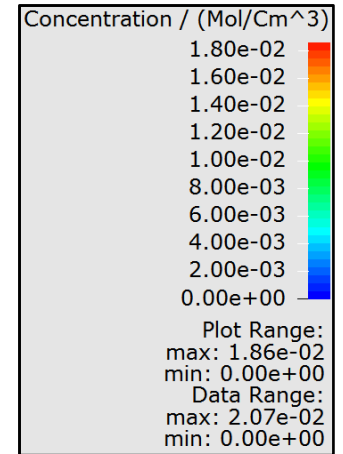
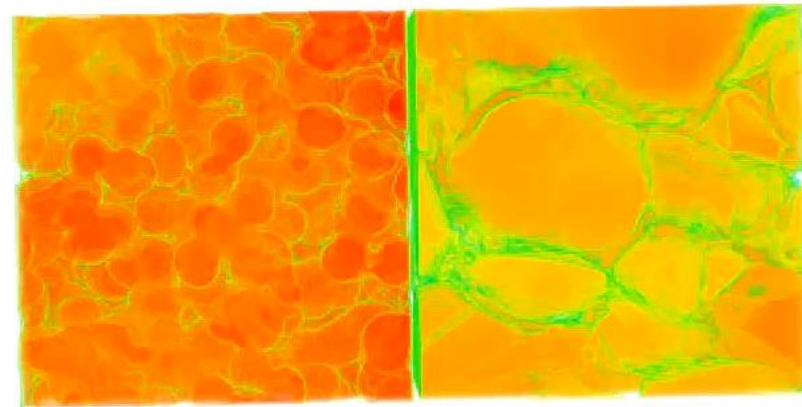
BatteryDict Result



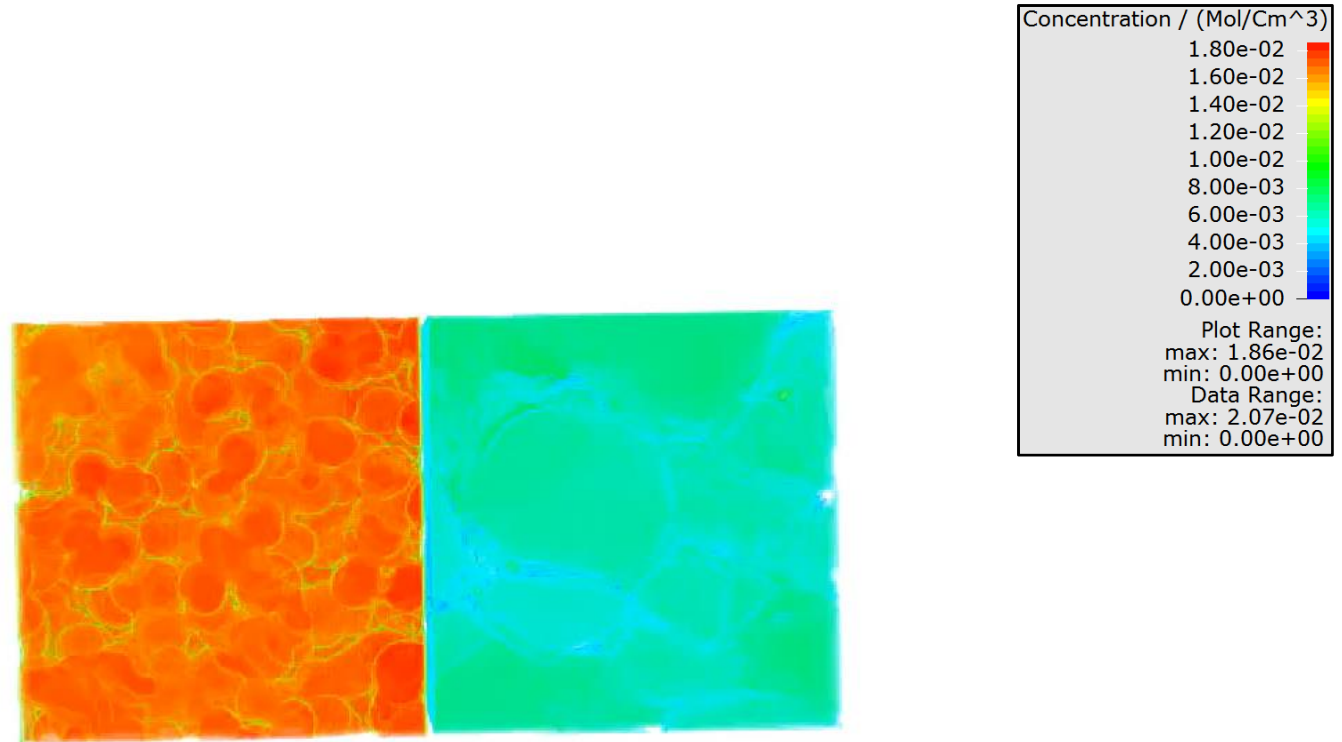
Concentration of Li-Ions at 20% SOC



Concentration of Li-Ions at 50% SOC

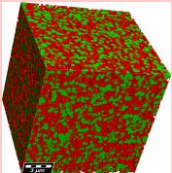
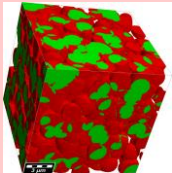
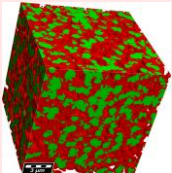
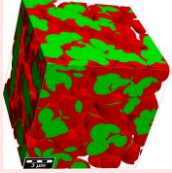
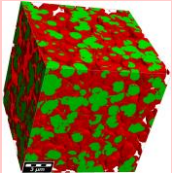
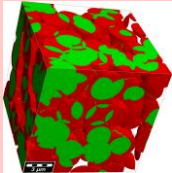
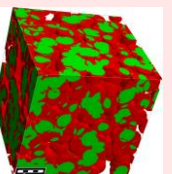
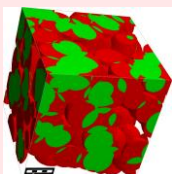


Concentration of Li-Ions at 70% SOC

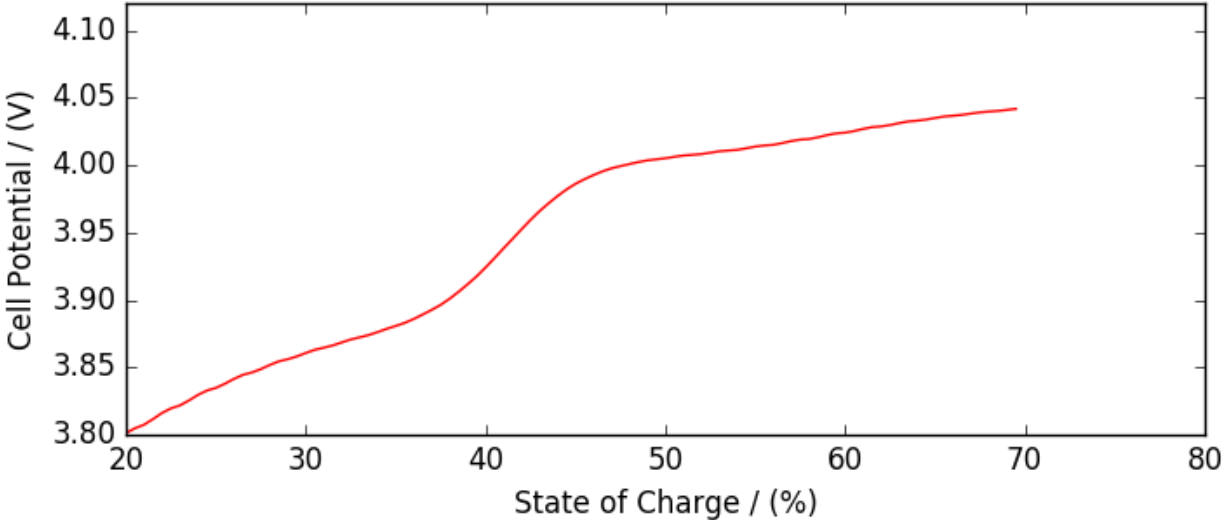


Case Study

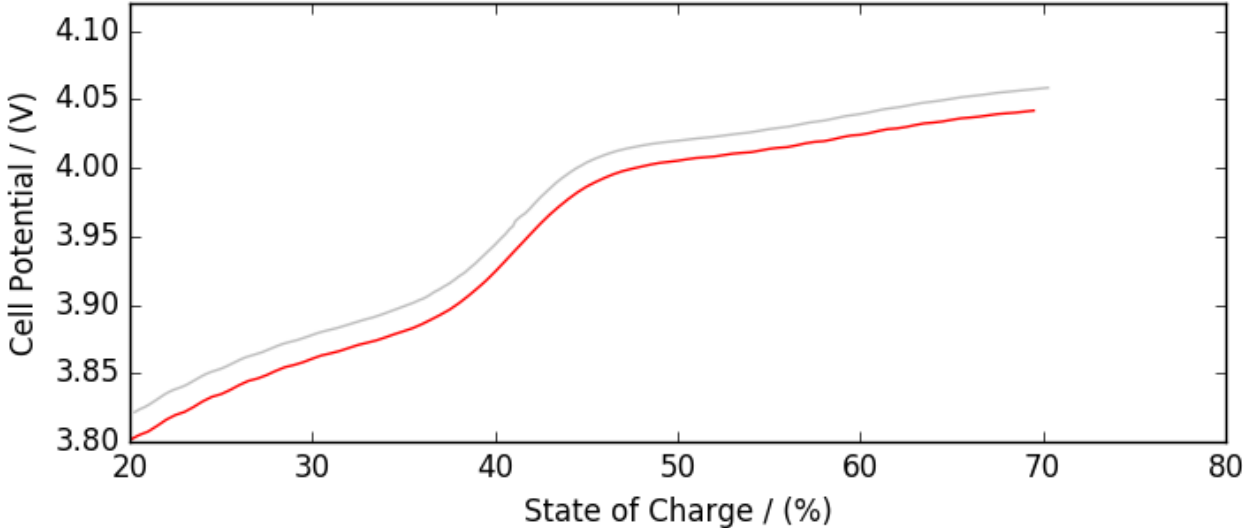
- Linking microstructural properties to macroscopic performance
- Simple test: different grain sizes for the anode material

10 voxel $\triangleq 0.62 \mu\text{m}$		50 voxel $\triangleq 3.10 \mu\text{m}$	
20 voxel $\triangleq 1.24 \mu\text{m}$		60 voxel $\triangleq 3.72 \mu\text{m}$	
30 voxel $\triangleq 1.86 \mu\text{m}$		70 voxel $\triangleq 4.34 \mu\text{m}$	
40 voxel $\triangleq 2.48 \mu\text{m}$		80 voxel $\triangleq 4.96 \mu\text{m}$	

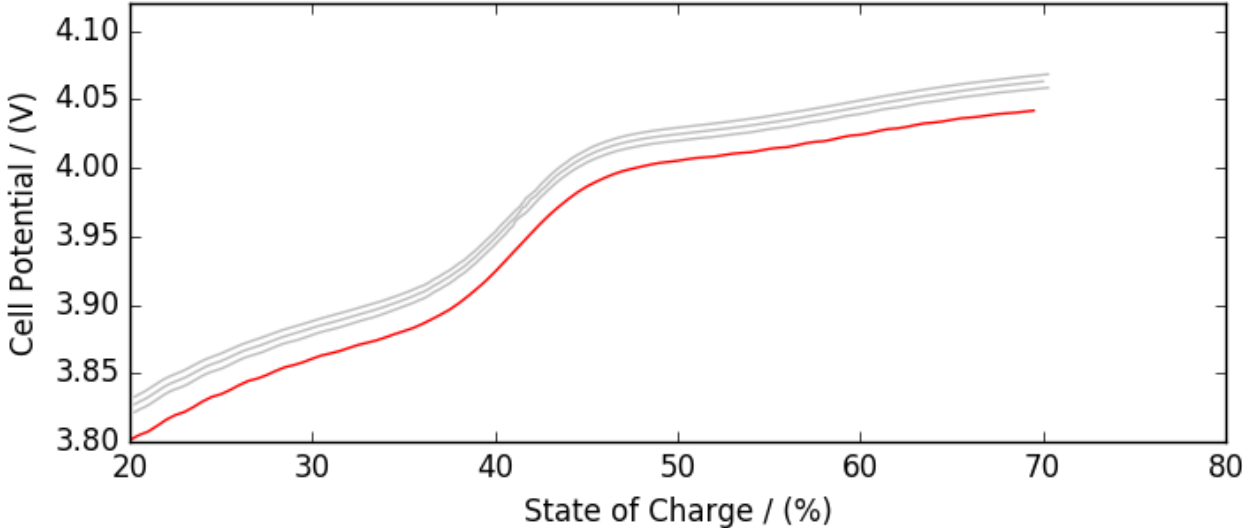
Results for several particle sizes



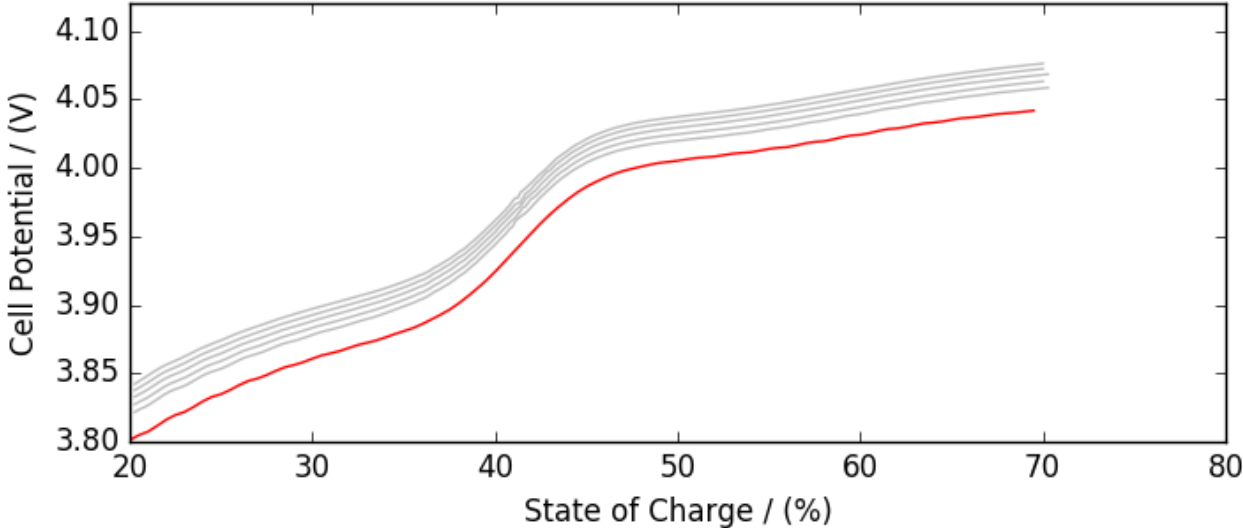
Results for several particle sizes



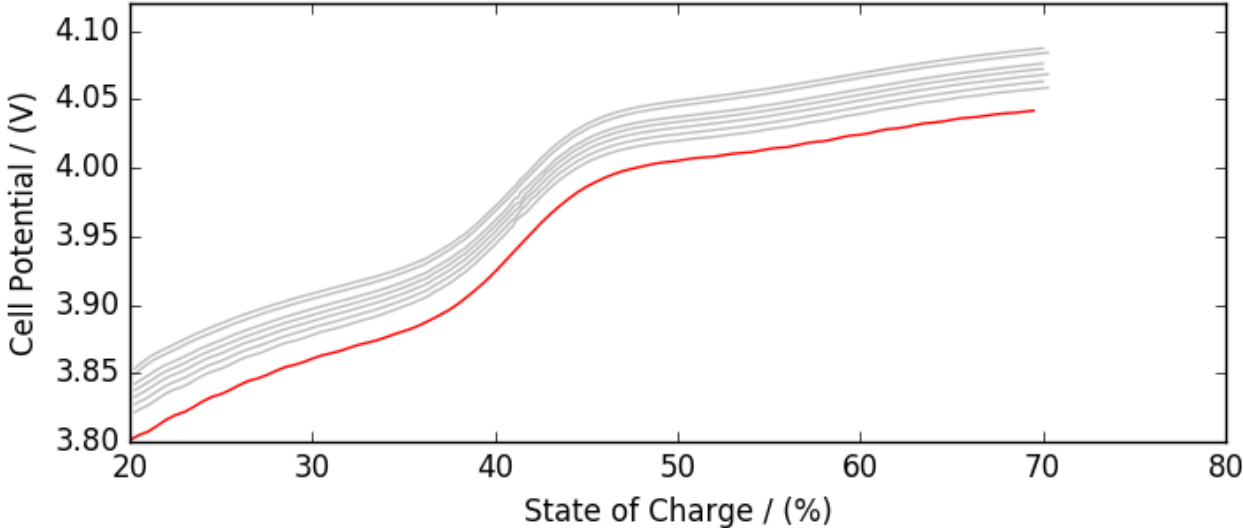
Results for several particle sizes



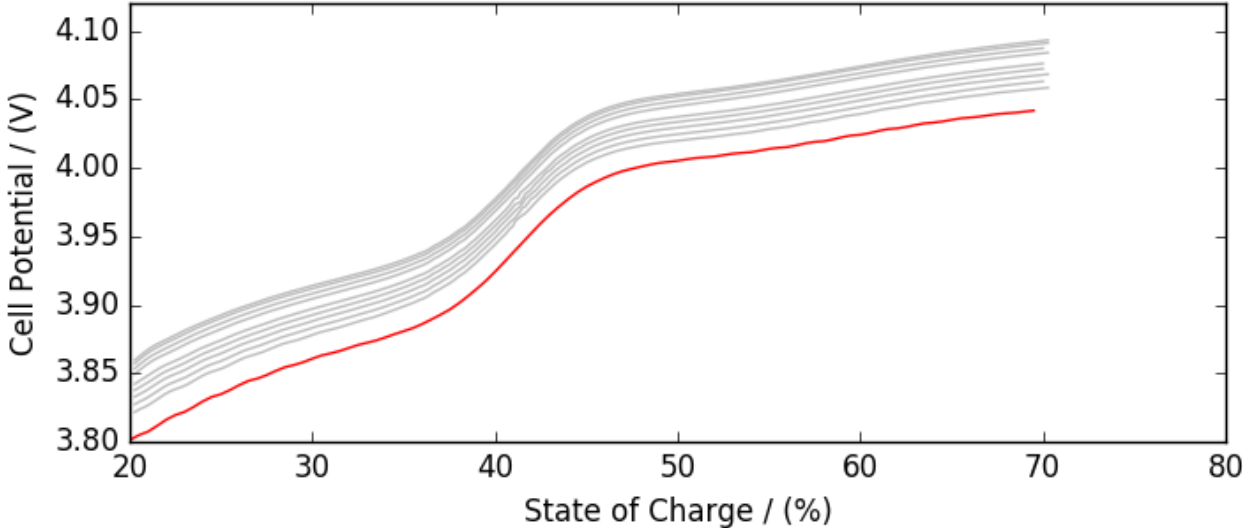
Results for several particle sizes



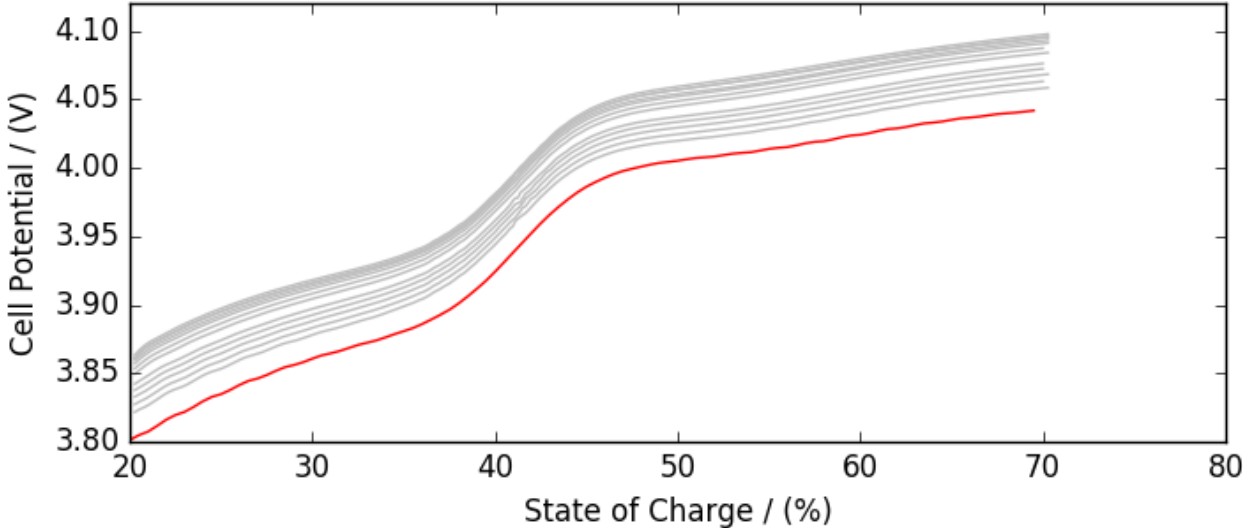
Results for several particle sizes



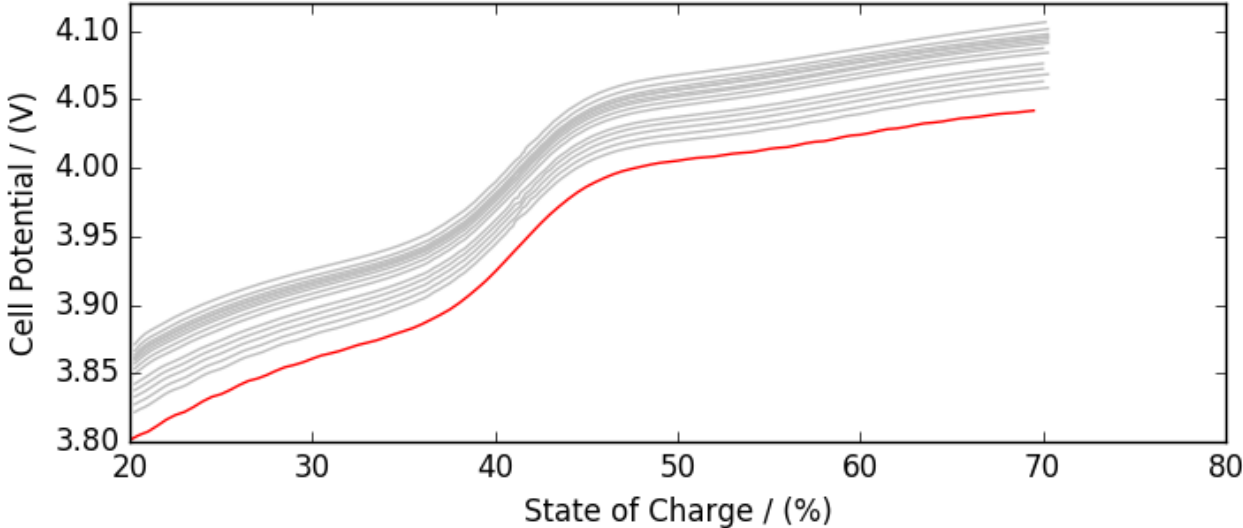
Results for several particle sizes



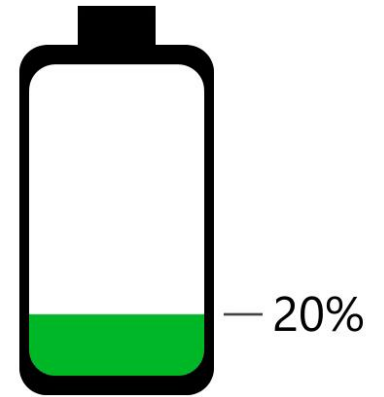
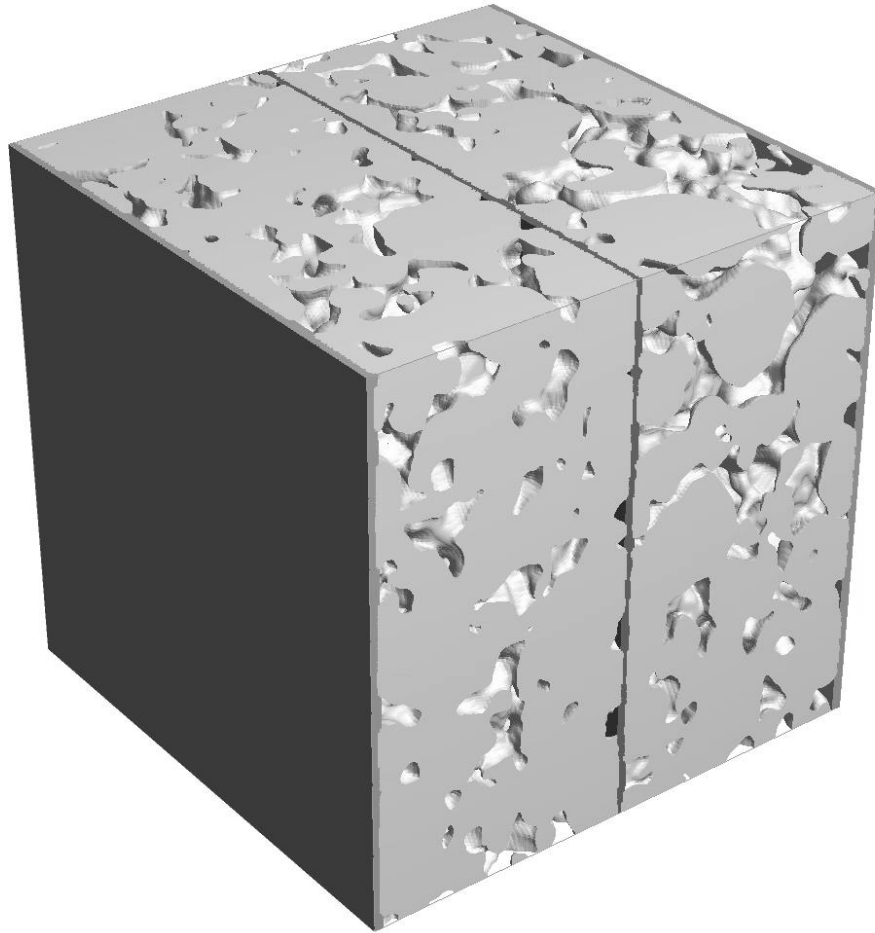
Results for several particle sizes



Results for several particle sizes



Charging Battery



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