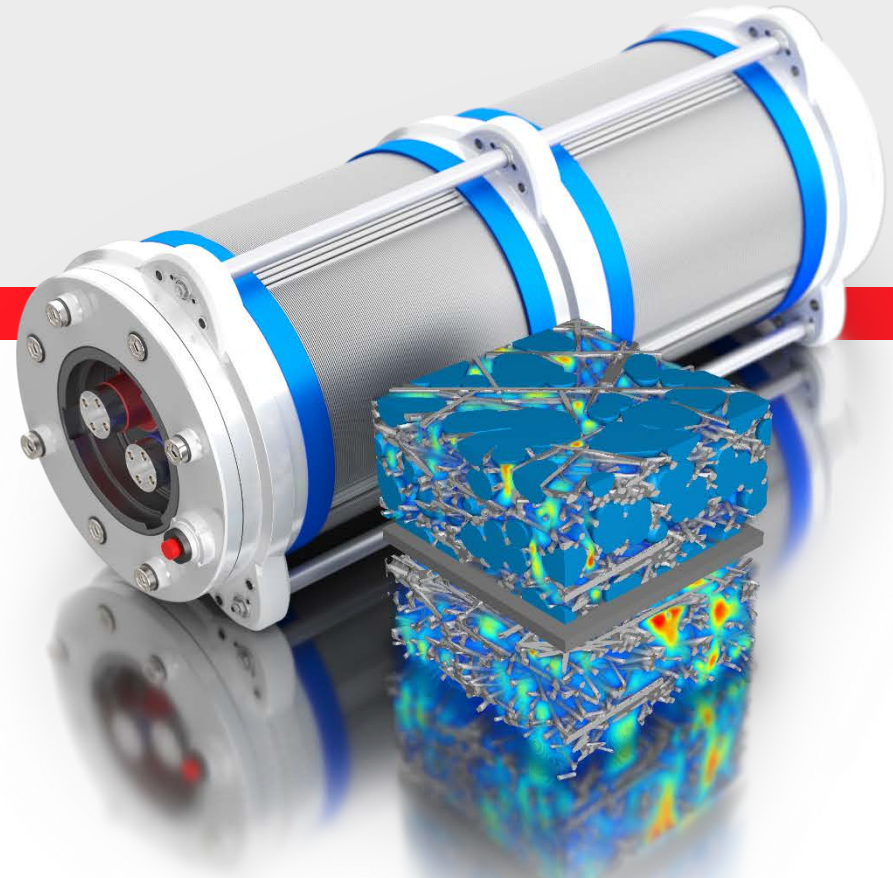


How does the micro-structure of the cathode material influence the performance of Batteries?

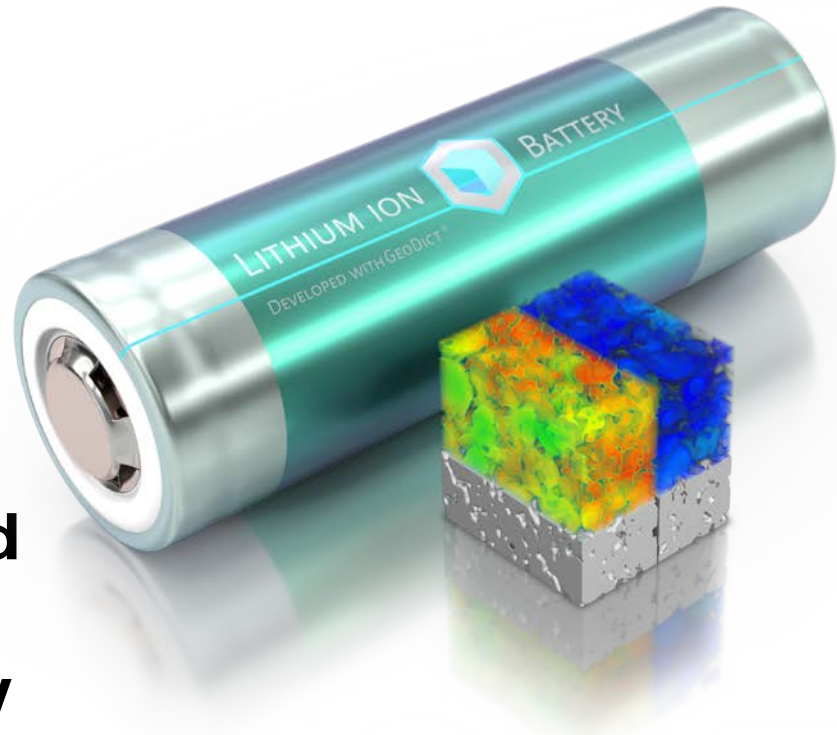
Dr. Ilona Glatt

■ EVS30, Stuttgart, 10.10.2017

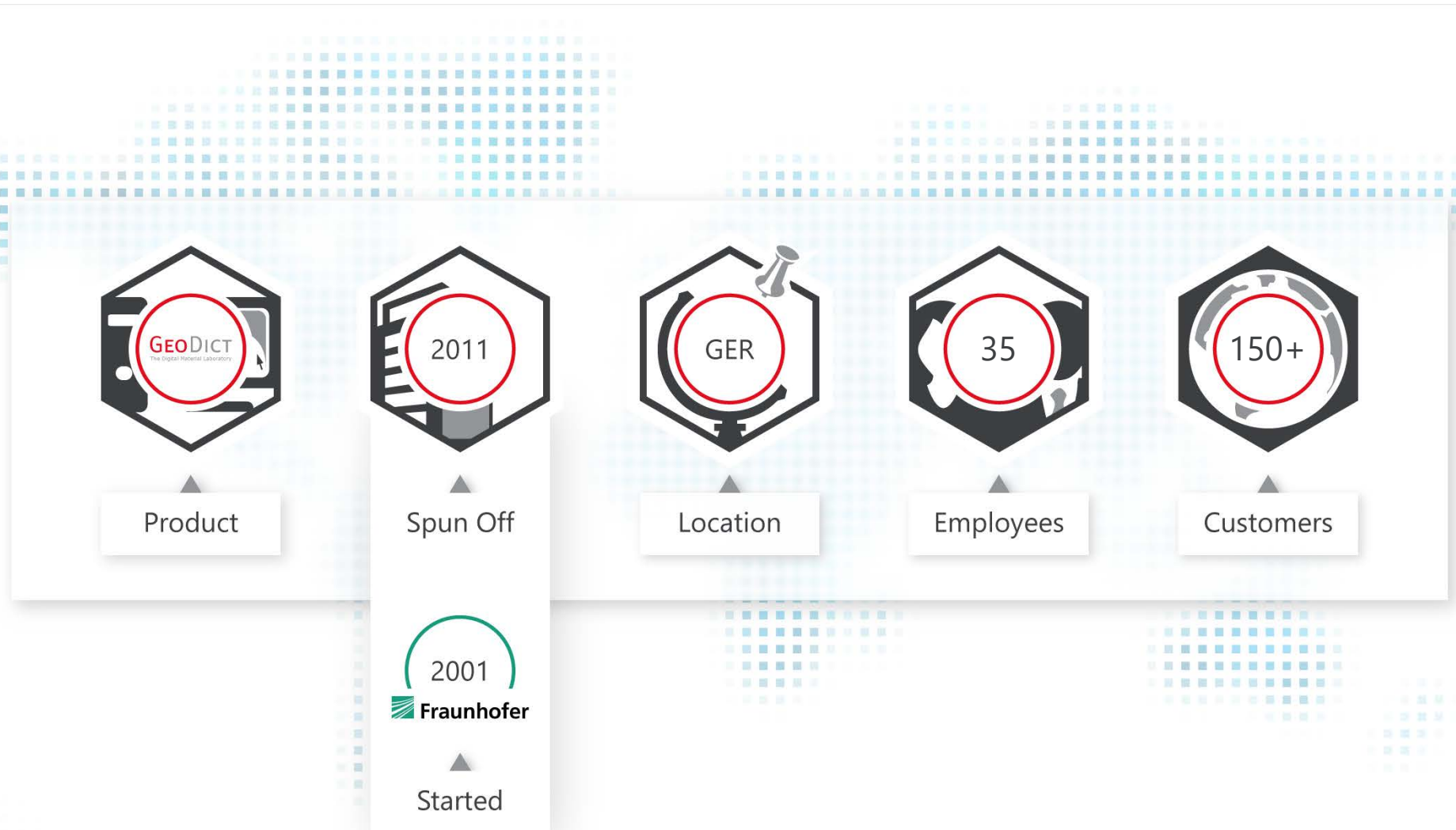


Overview

- 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

Phone + 49 631 / 205 605 0
Fax + 49 631 / 205 605 99

www.geodict.com





Development of Materials



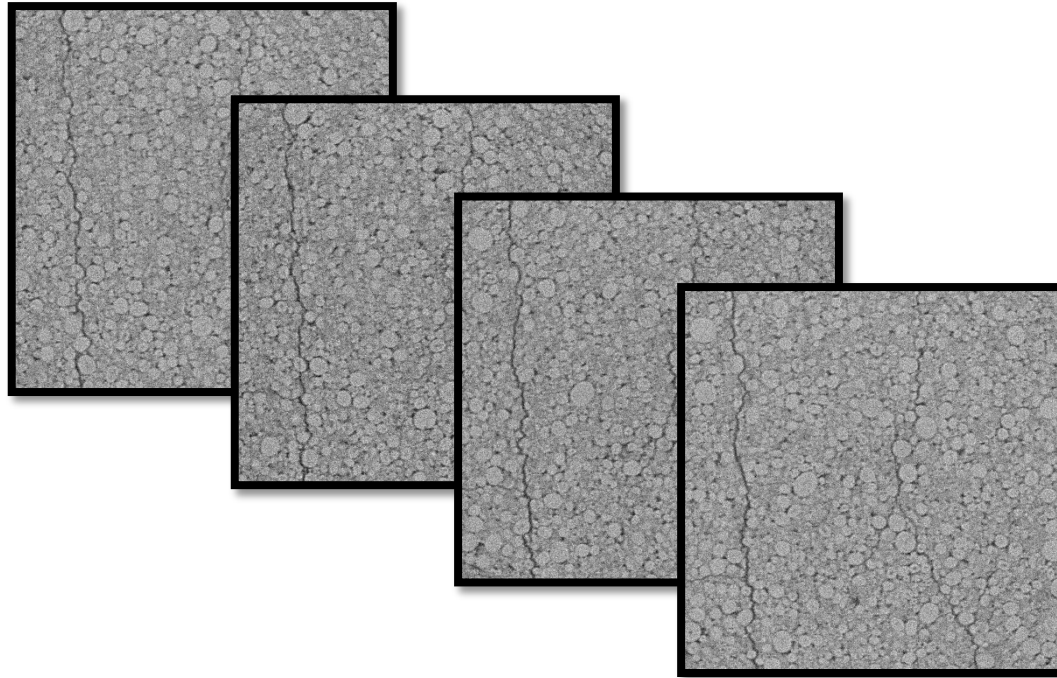


Image Acquisition



Development of Materials



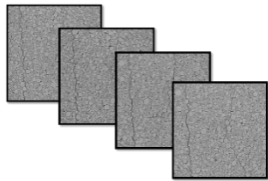
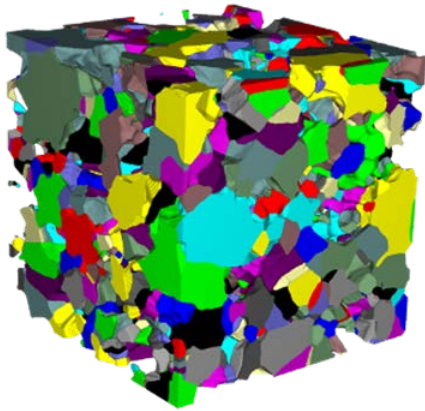


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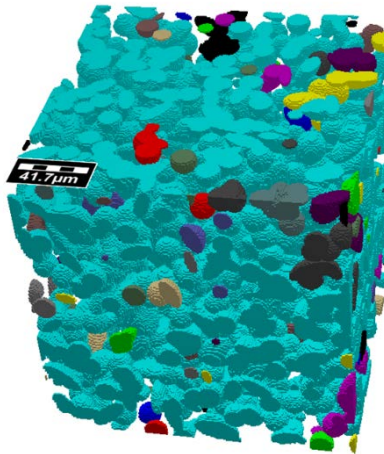


Development of Materials

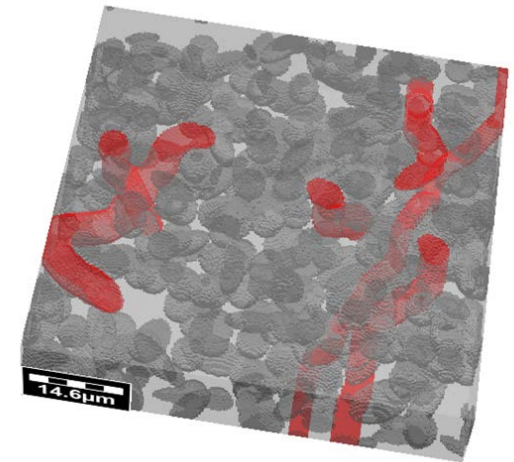




pore analysis



grain analysis



tortuosity

Image Analysis



Development of Materials



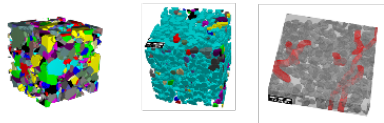


Image Analysis

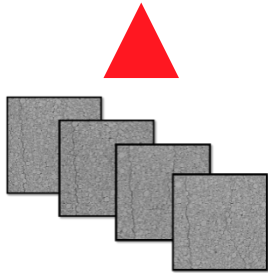


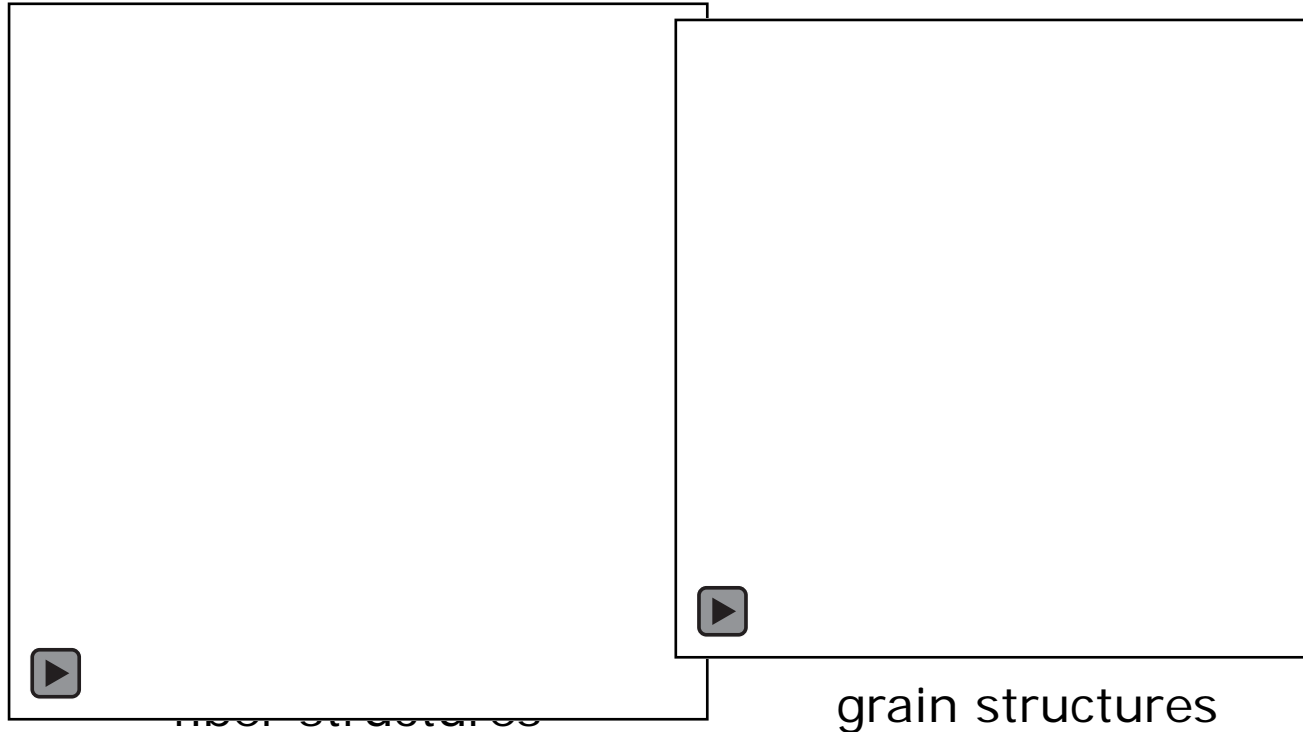
Image Acquisition



Development of Materials



Development of materials by Digital Material Design



Modelling
Microstructures



Development of Materials





Image Analysis

Modelling
Microstructures

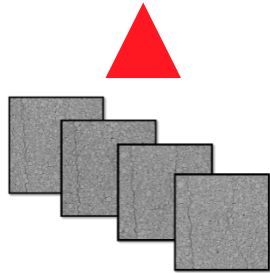


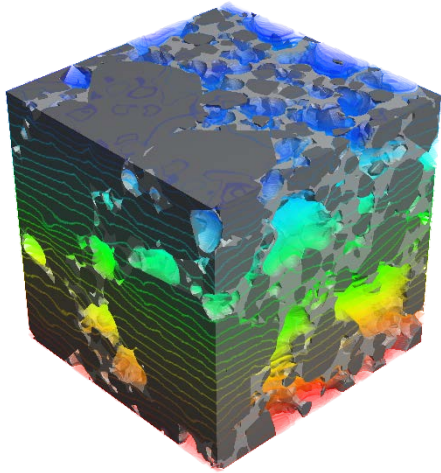
Image Acquisition



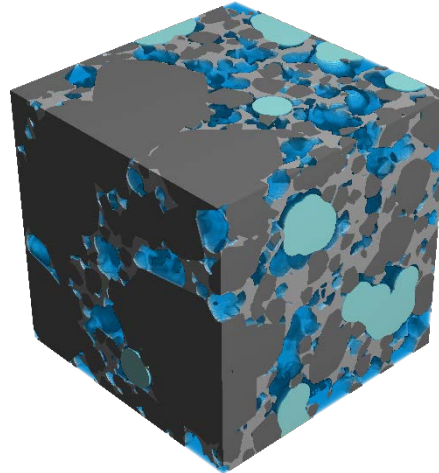
Development of Materials



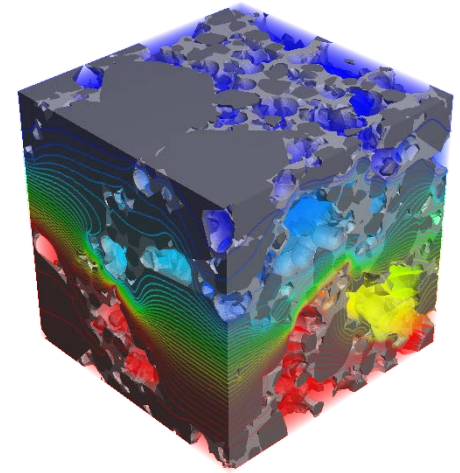
Development of materials by Digital Material Design



conductivity simulation



saturation simulation



flow simulation

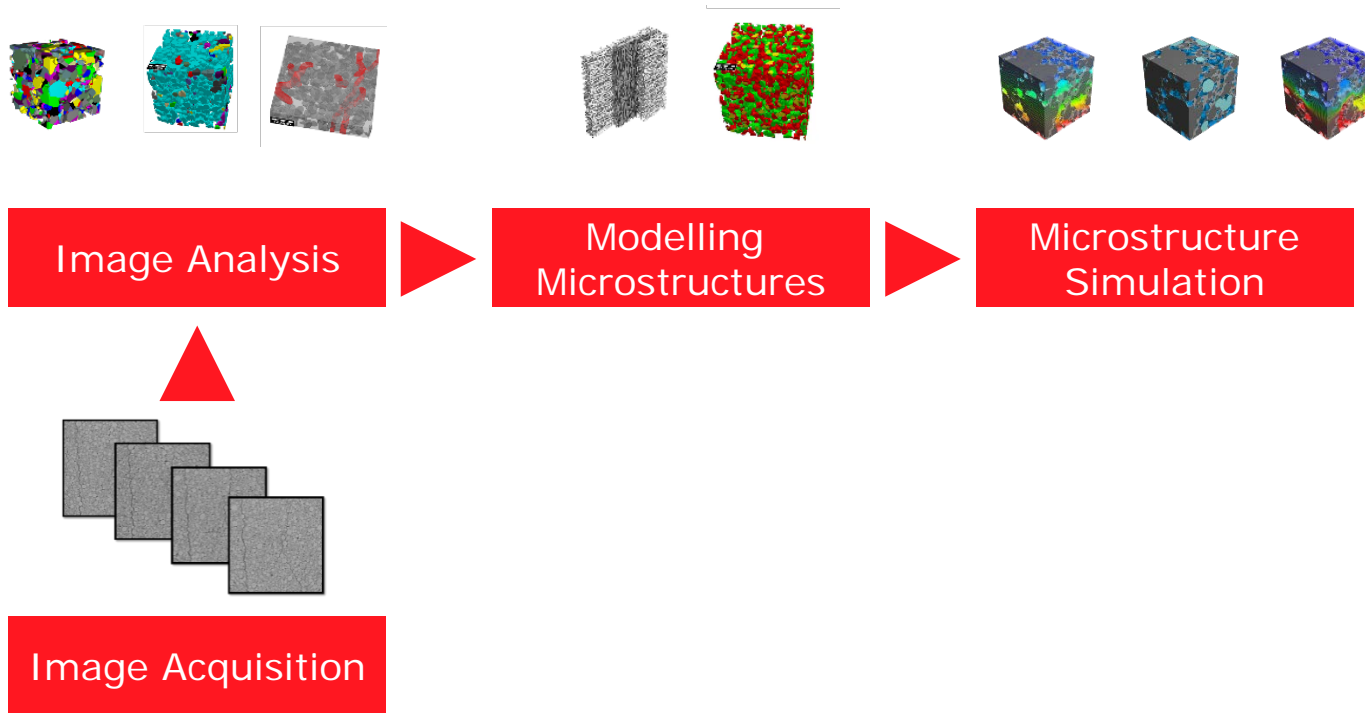
Microstructure
Simulation



Development of Materials

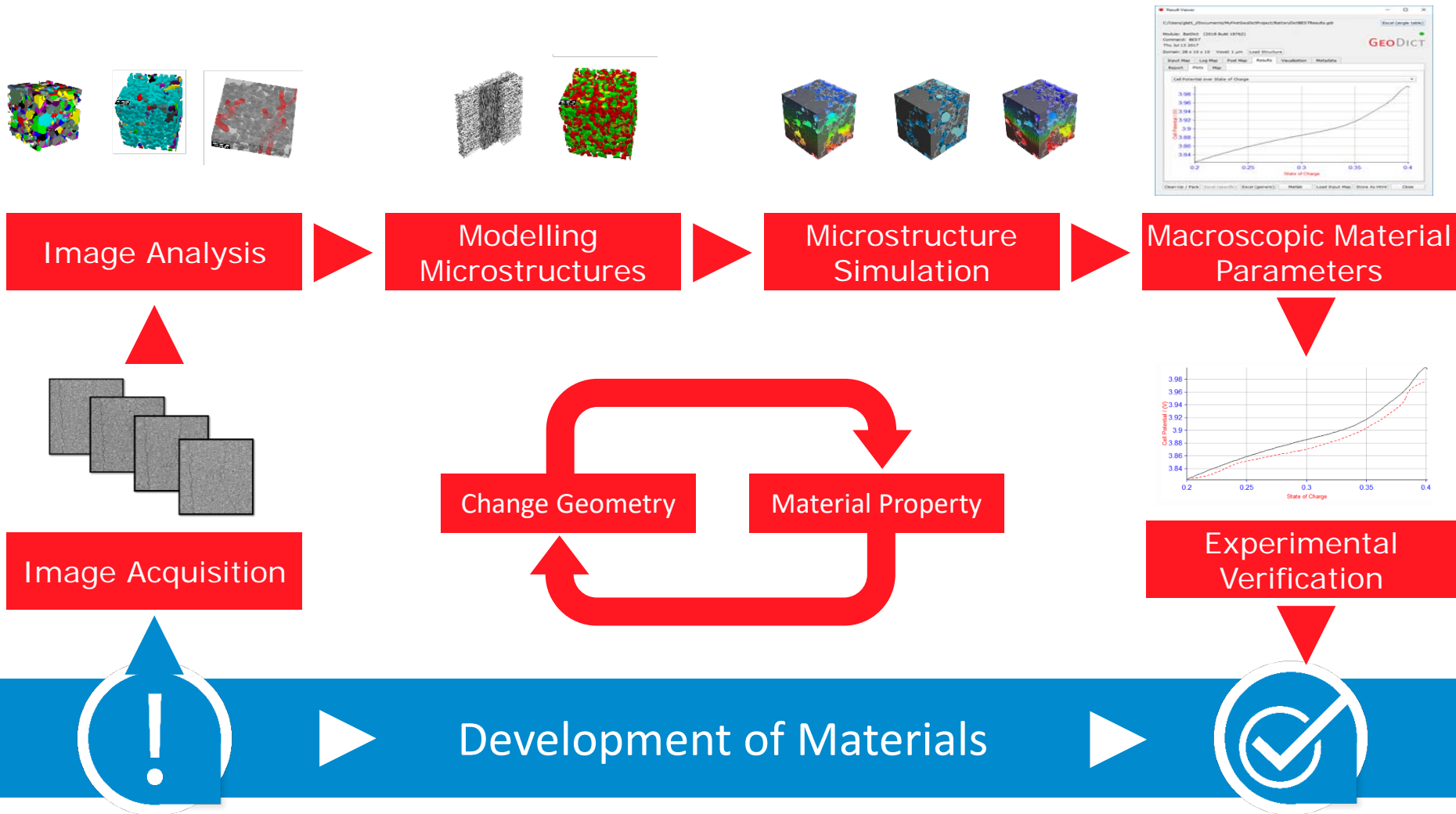


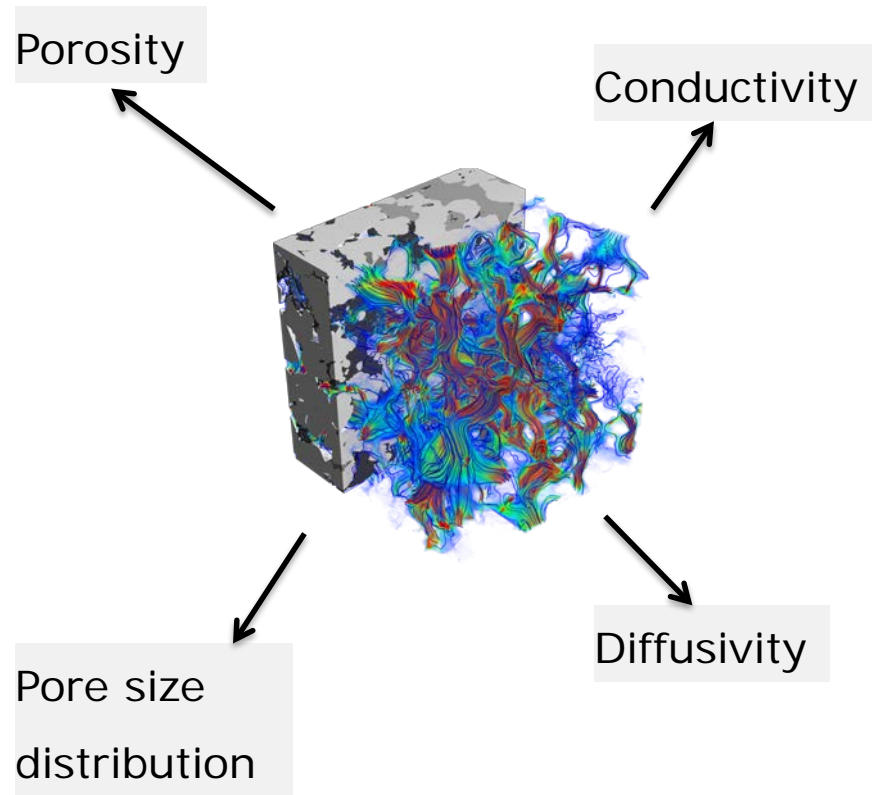
Development of materials by Digital Material Design



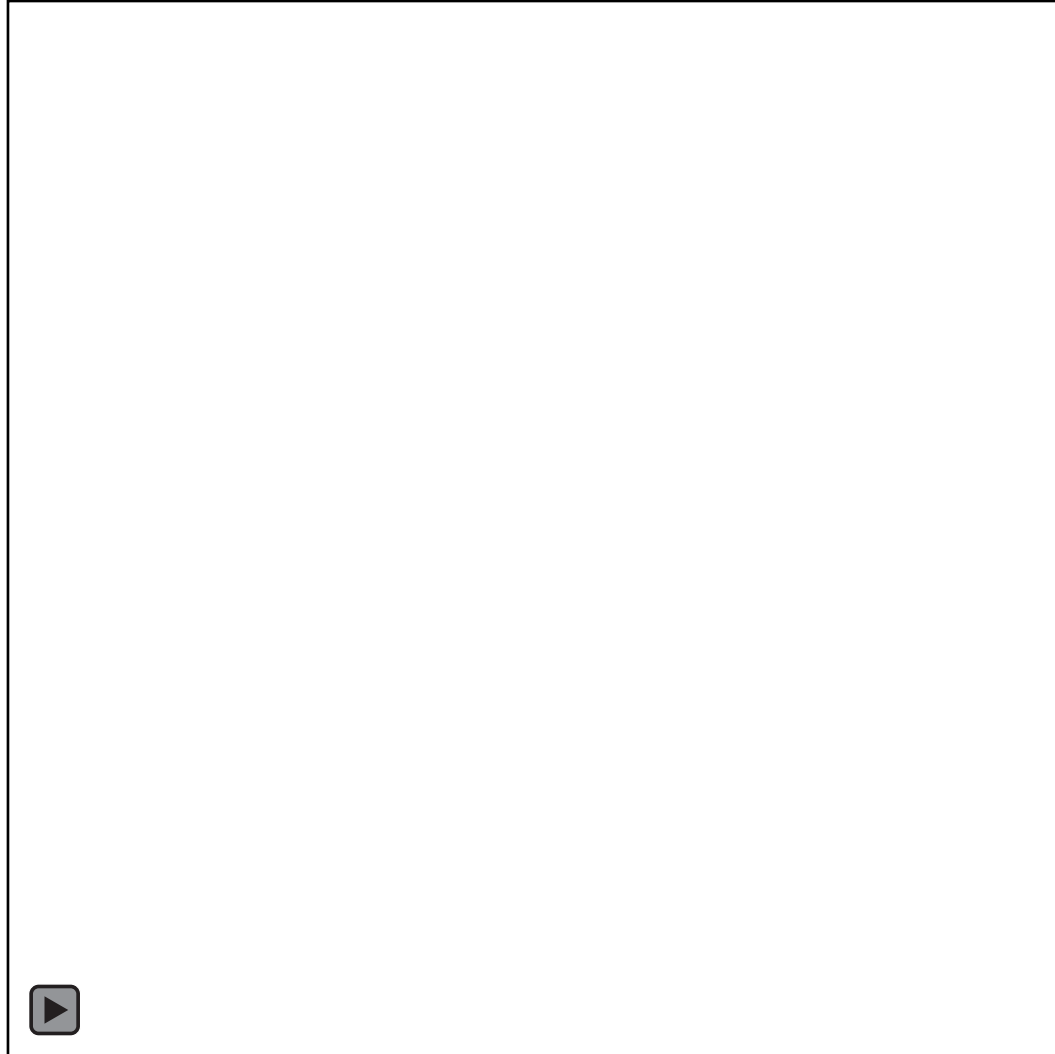
Development of Materials



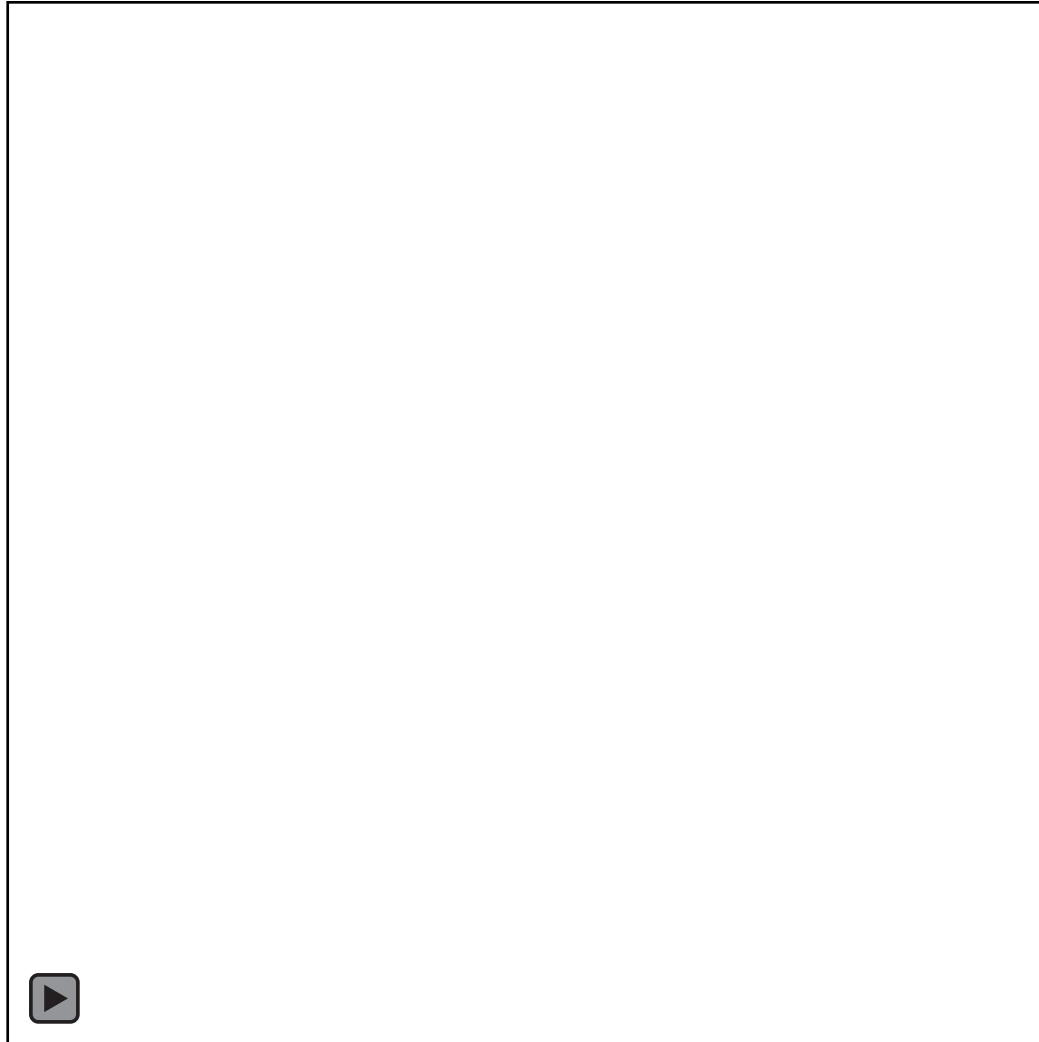




Anode

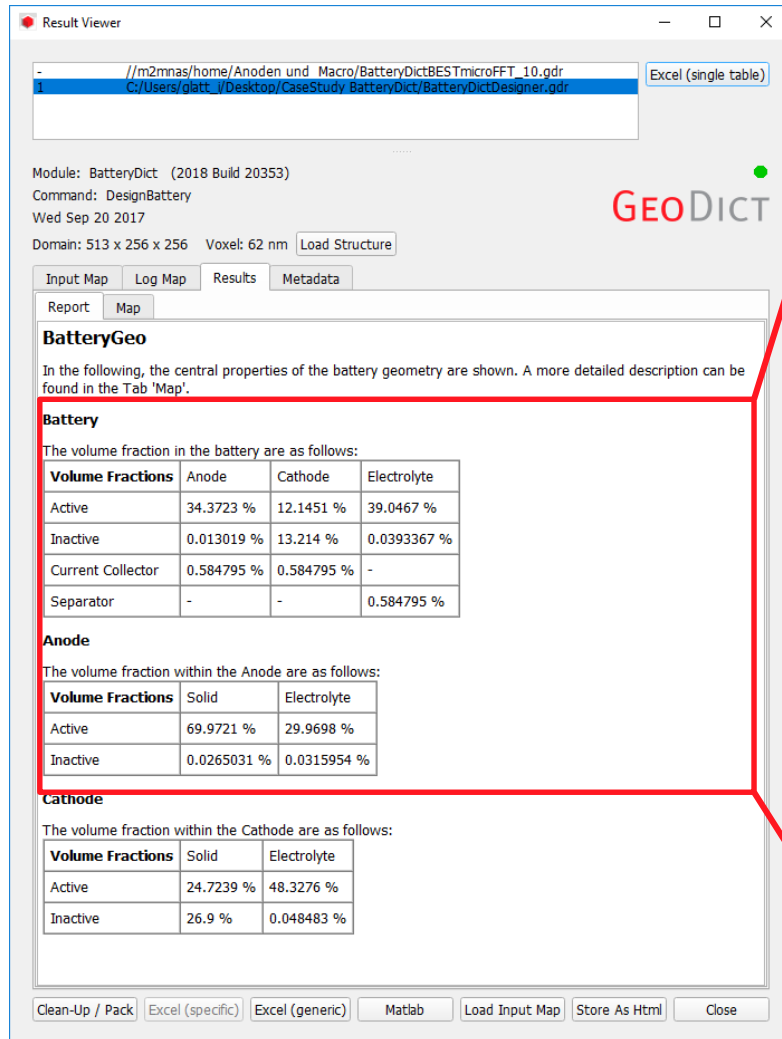


Cathode



BatteryDict GUI





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:

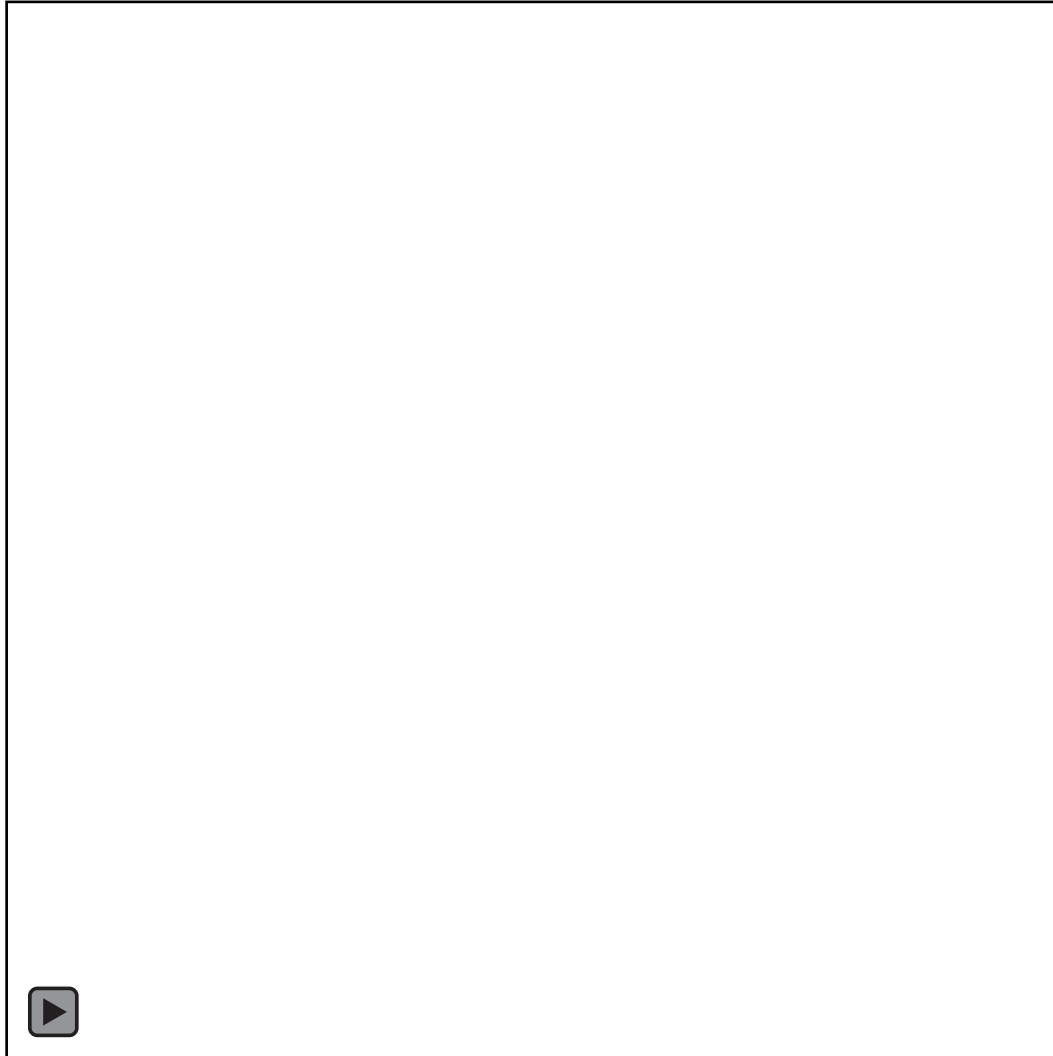
Volume Fractions	Solid	Electrolyte
Active	69.9721 %	29.9698 %
Inactive	0.0265031 %	0.0315954 %

Material Information:

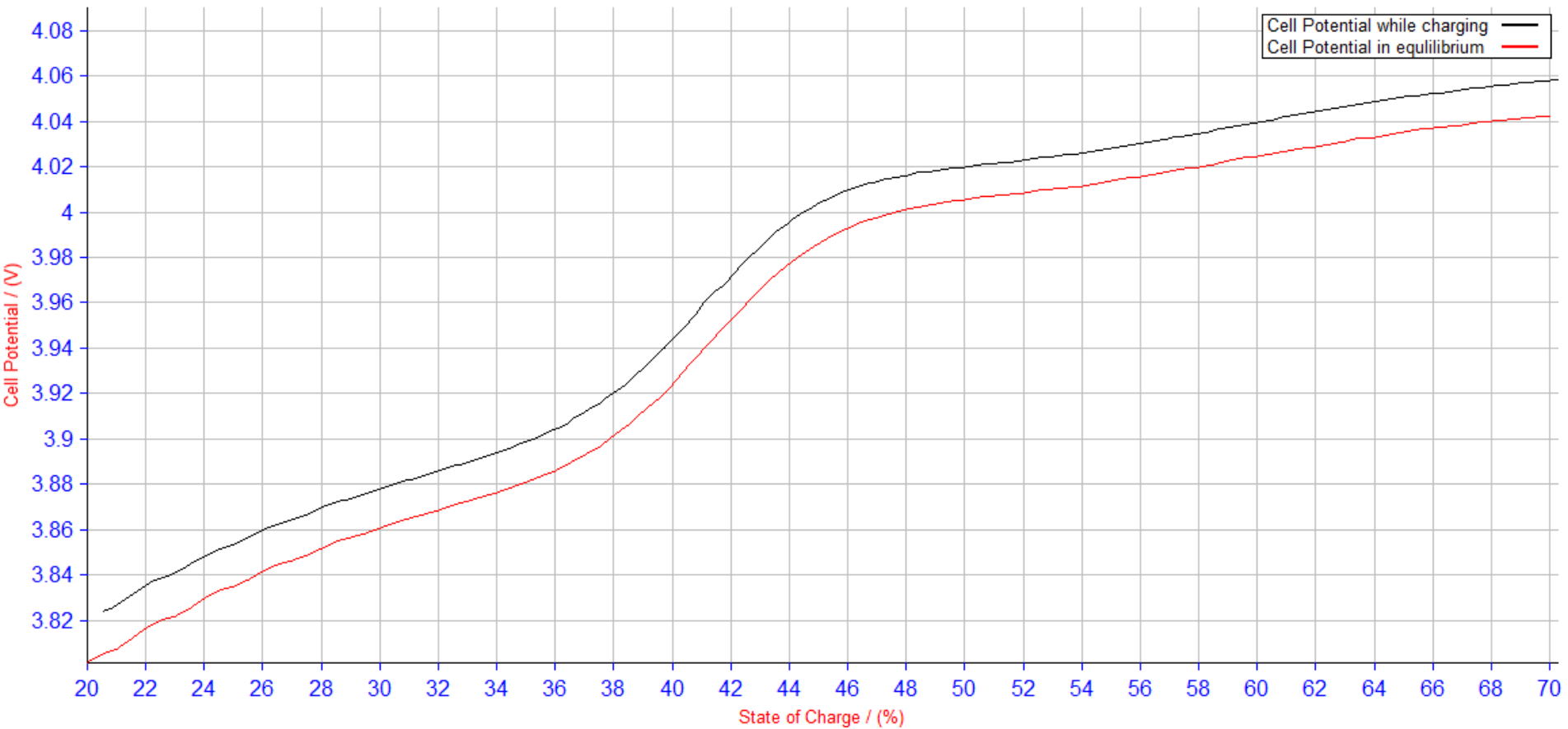
-  ID 00: Electrolyte [invis.]
-  ID 01: Anode Material
-  ID 02: Cathode Material
-  ID 03: Anode Current Collector [invis.]
-  ID 04: Cathode Current Collector [invis.]
-  ID 05: Inactive Anode Material
-  ID 06: Inactive Cathode Material
-  ID 07: Inactive Electrolyte
-  ID 08: Separator [invis.]



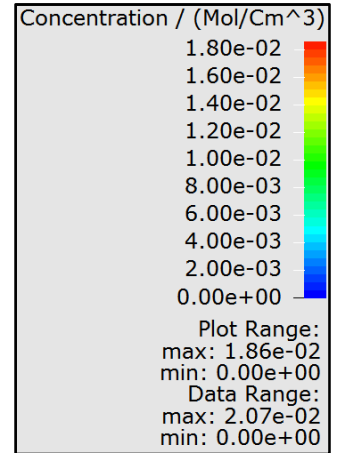
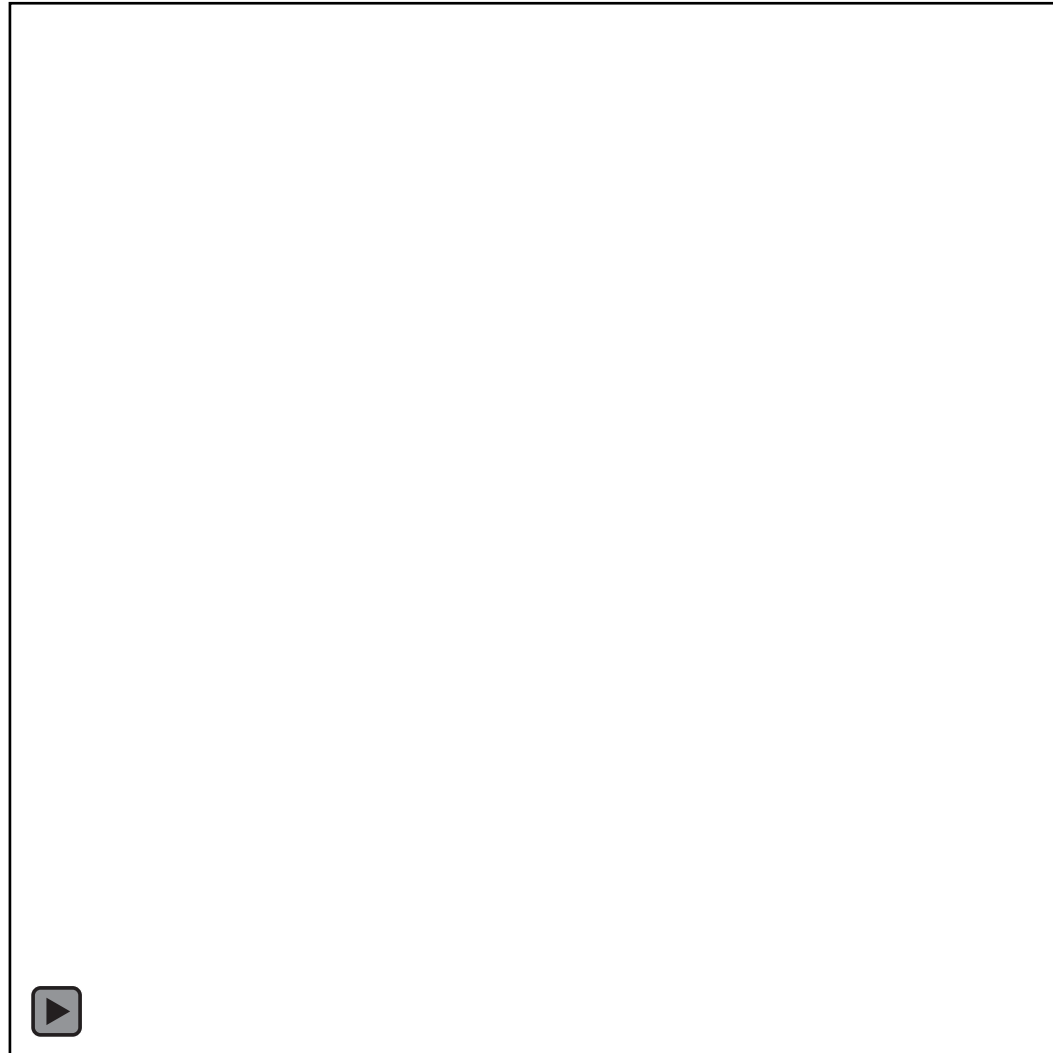
Cathode



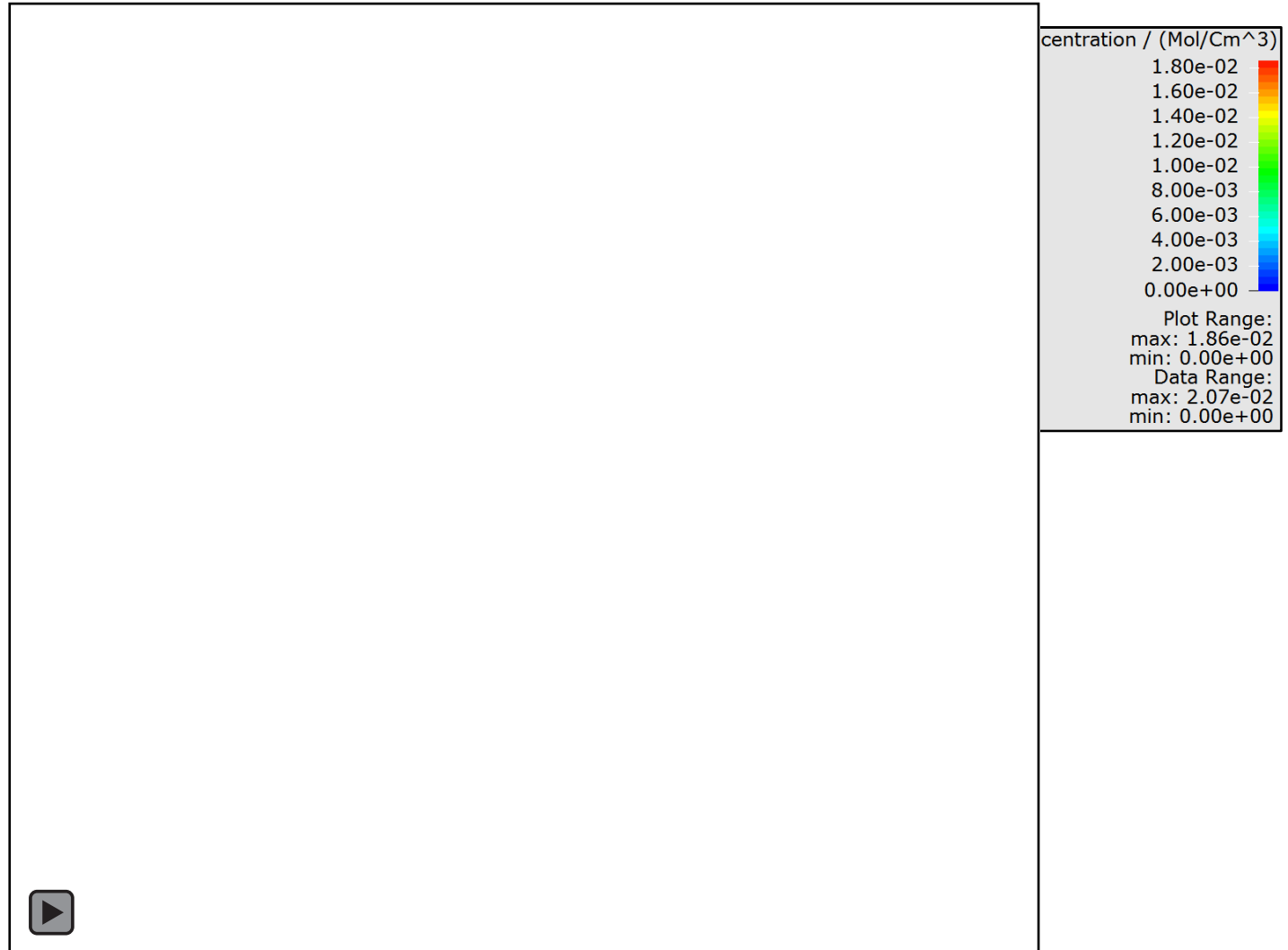
BatteryDict Result



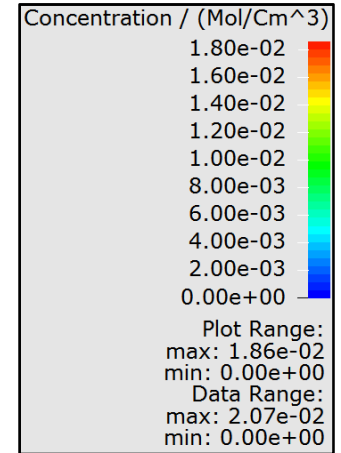
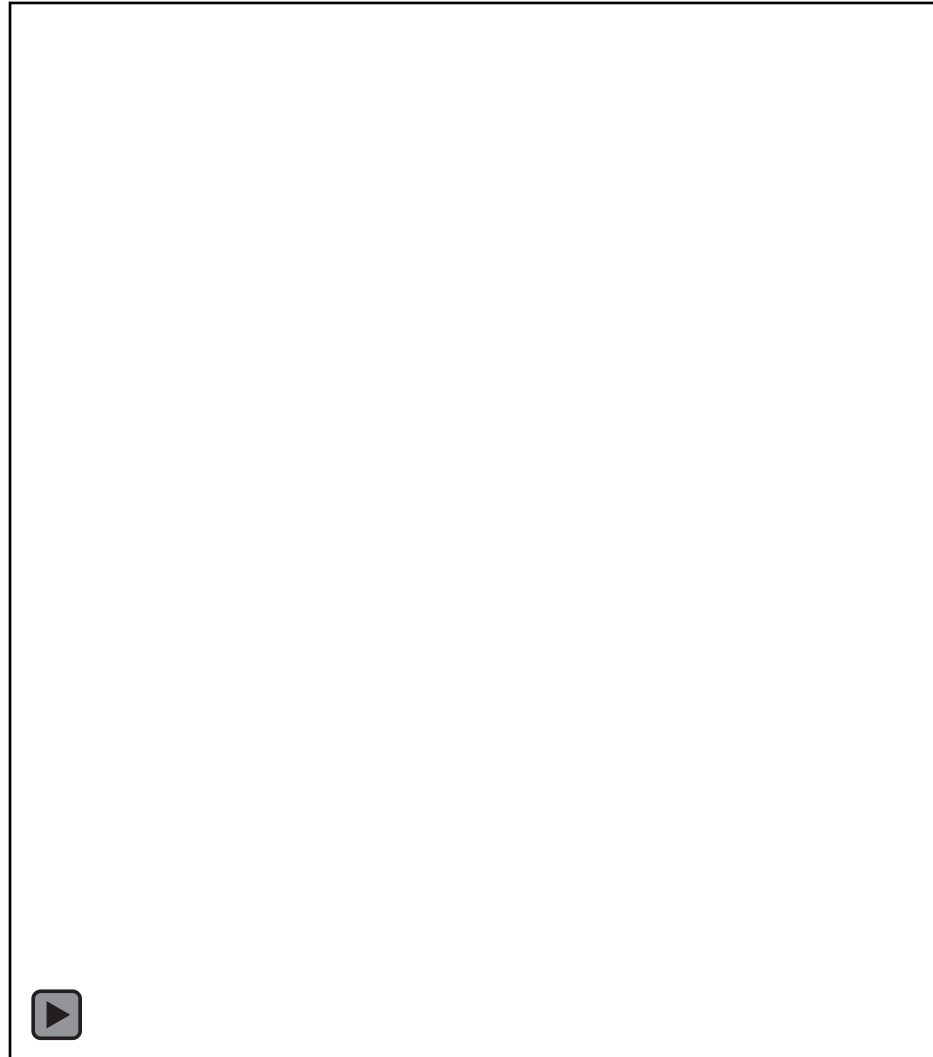
Concentration of Li-Ions at 20% SOC



Concentration of Li-Ions at 50% SOC

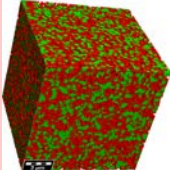
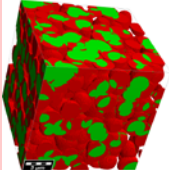
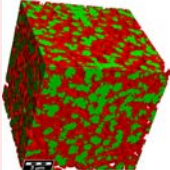
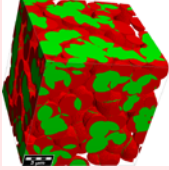
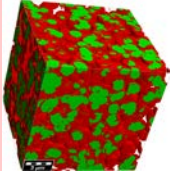
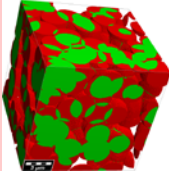
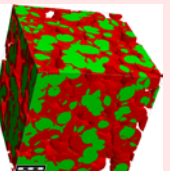
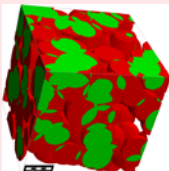


Concentration of Li-Ions at 70% SOC

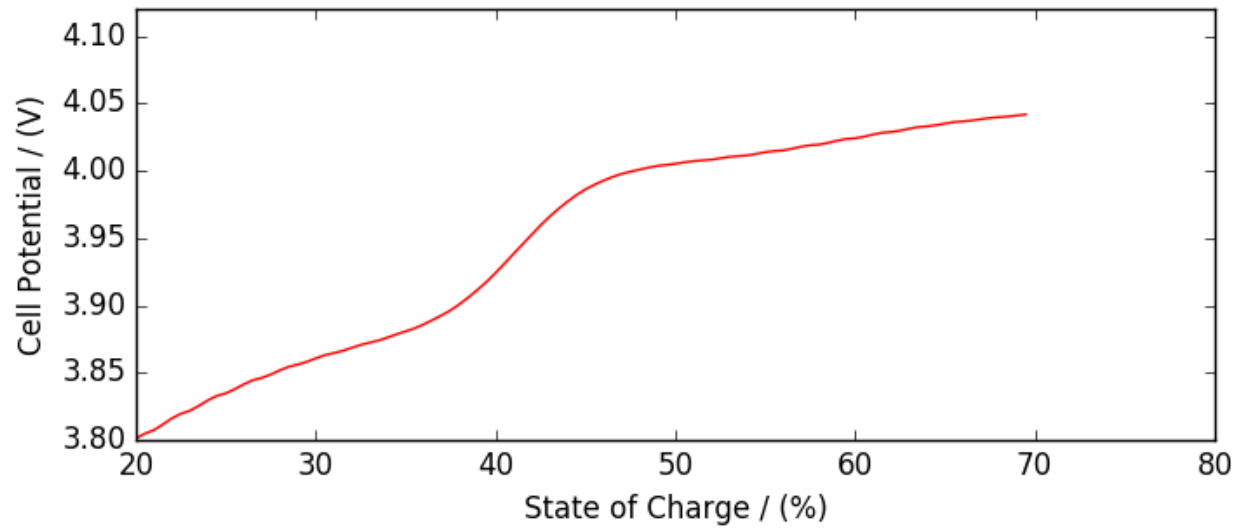


Case Study

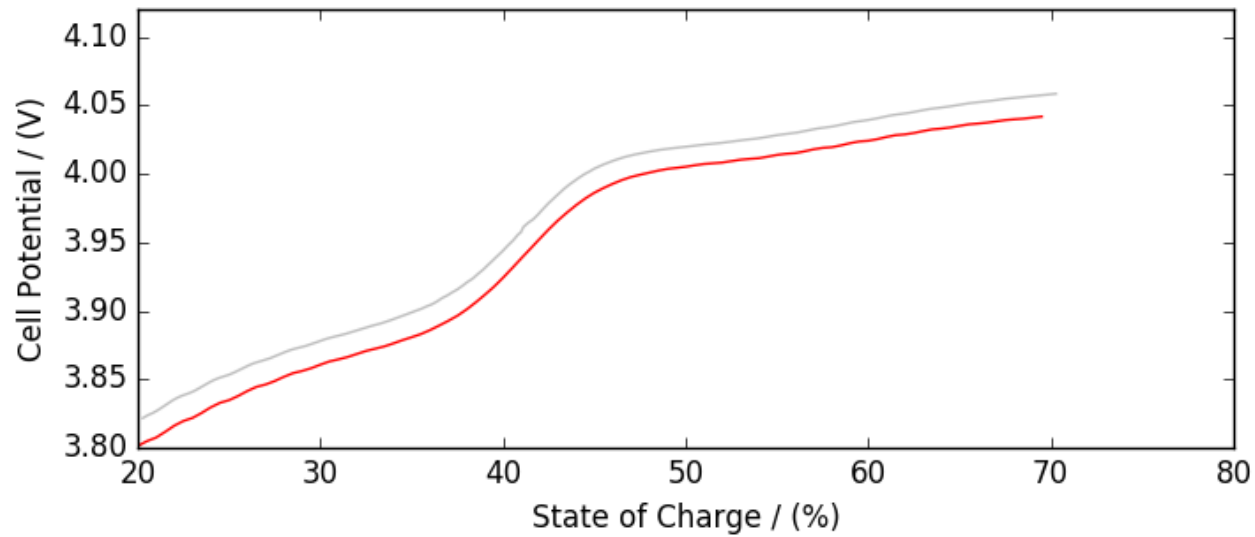
- Linking microstructural properties to macroscopic performance
- Simple test: different grain sizes for the anode material

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 $\triangleq 4.96 \mu\text{m}$	

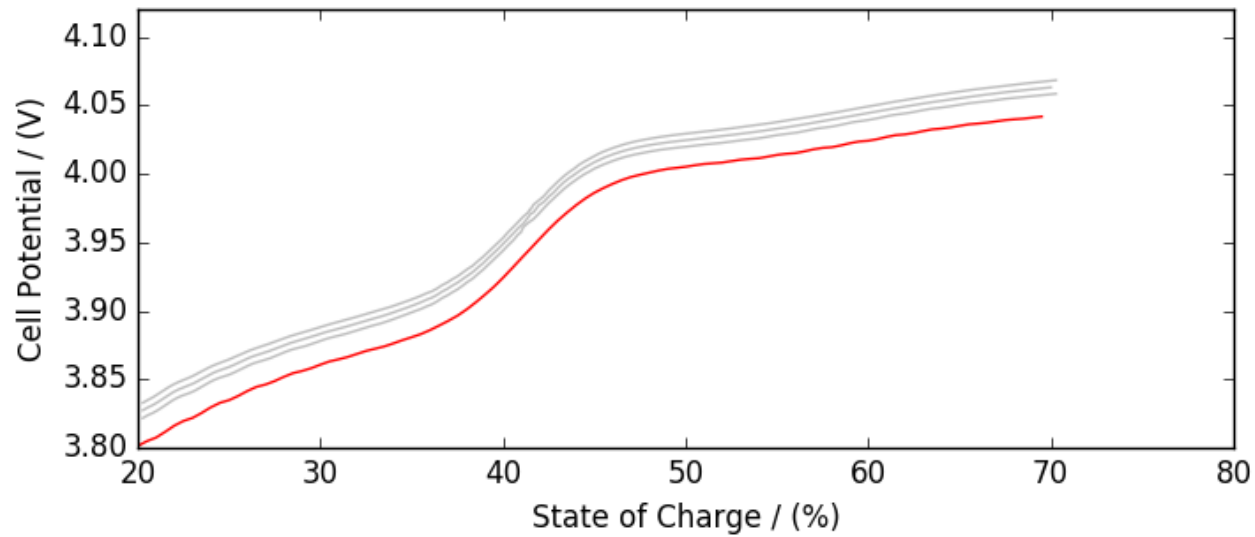
Results for several particle sizes



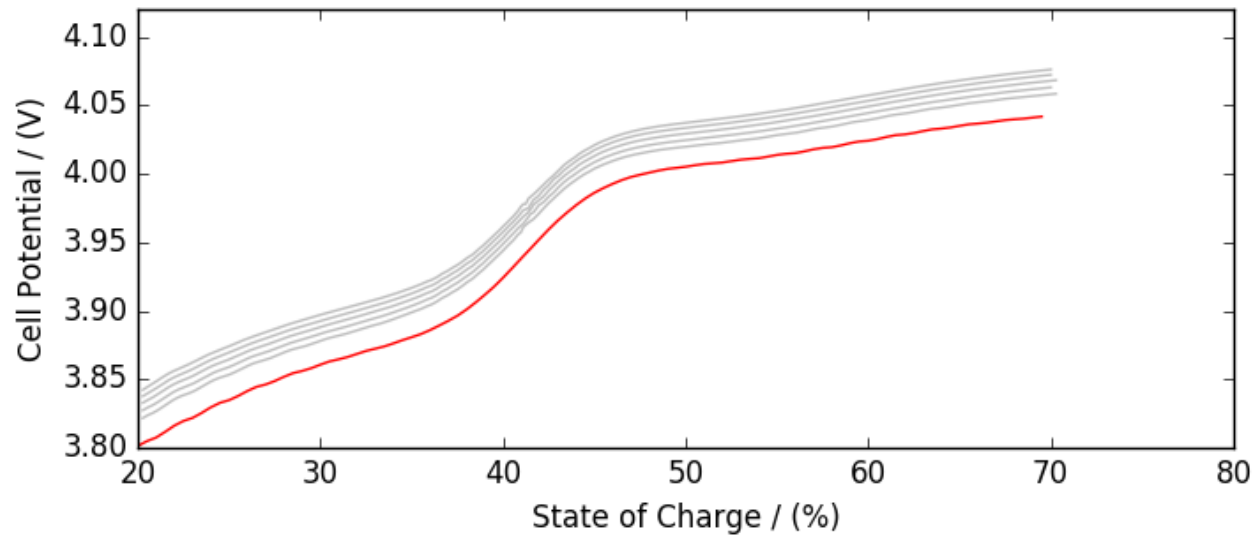
Results for several particle sizes



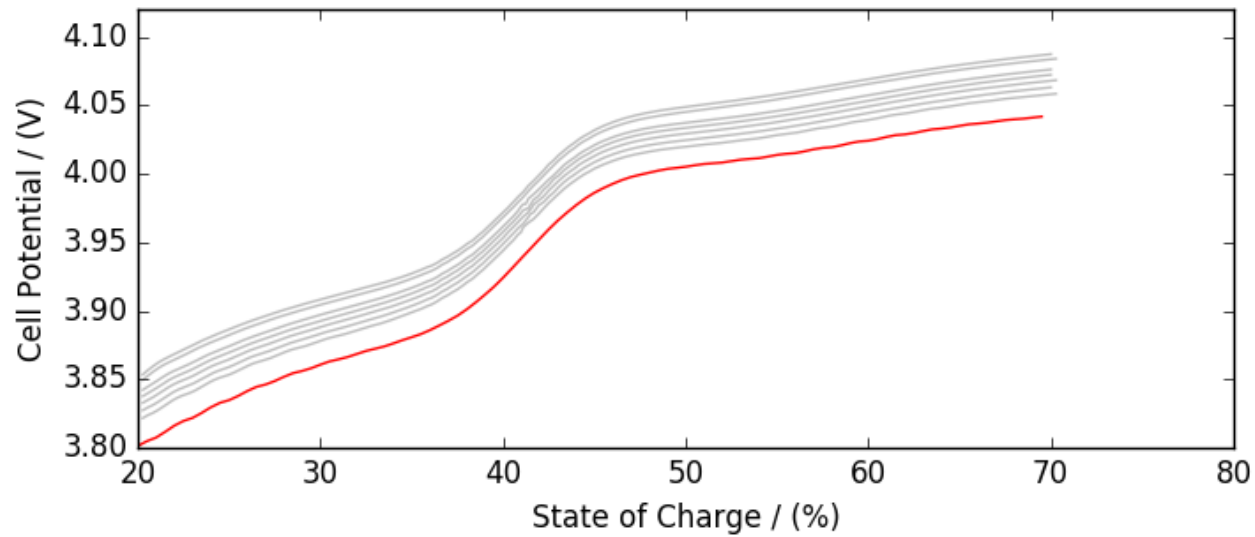
Results for several particle sizes



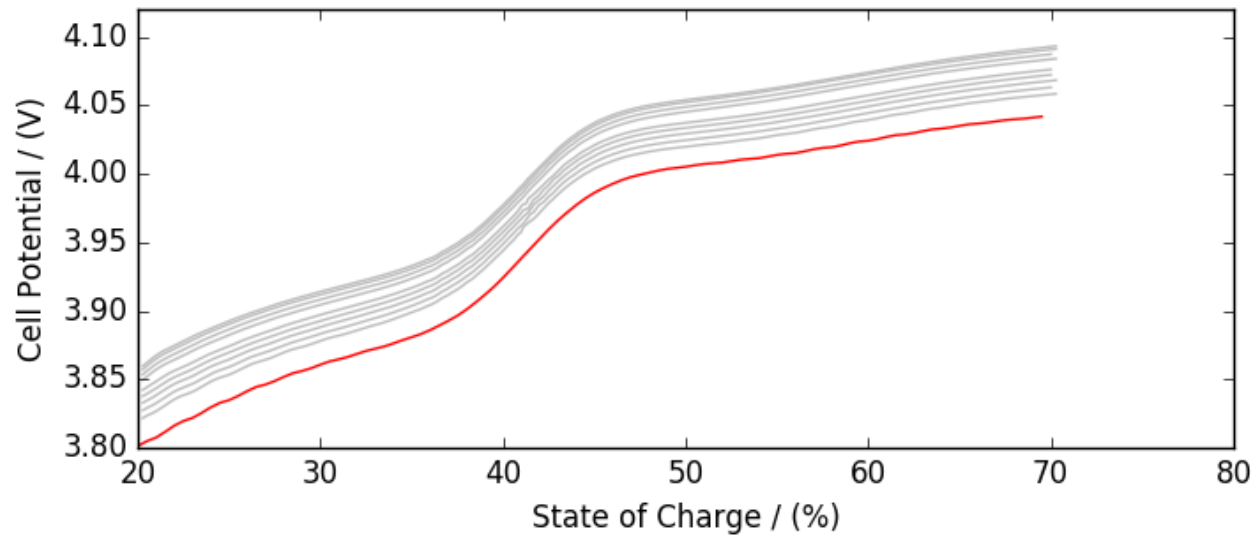
Results for several particle sizes



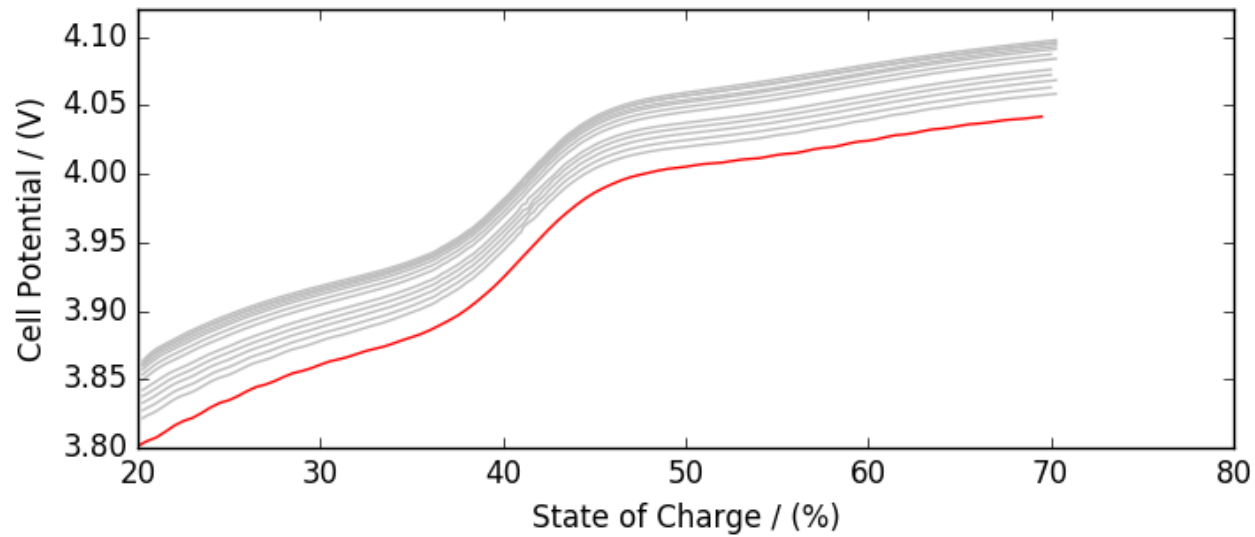
Results for several particle sizes



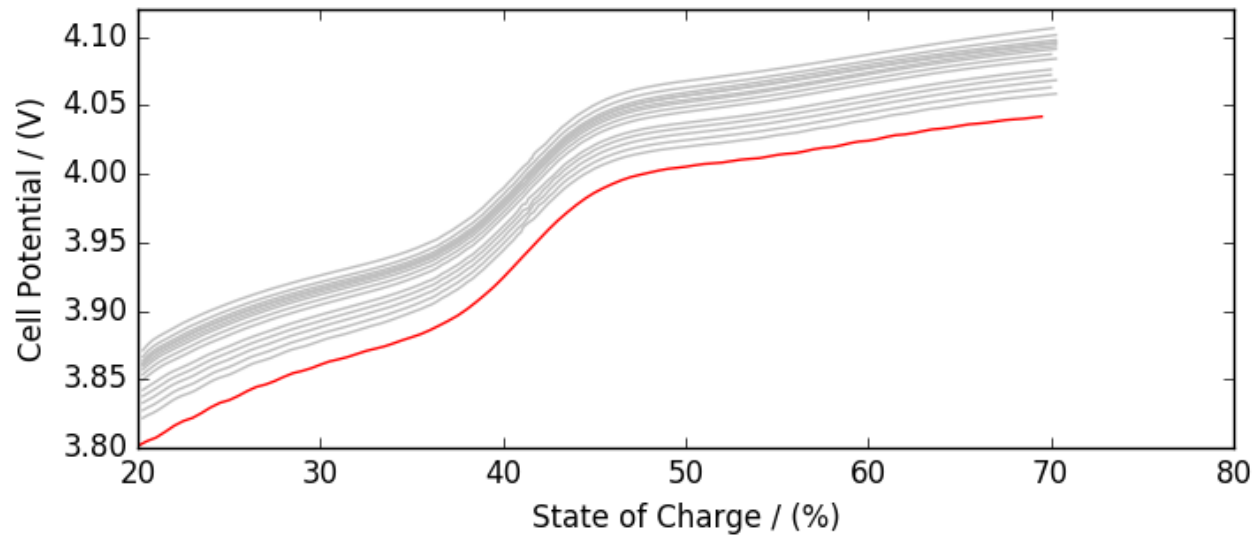
Results for several particle sizes



Results for several particle sizes



Results for several particle sizes



Charging Battery



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