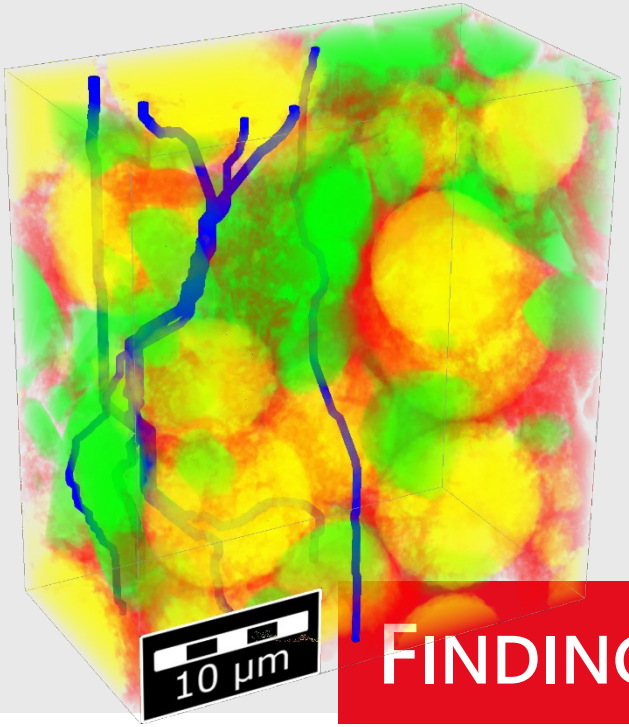


GeoDict
The Digital Material Laboratory

Finding the optimum amount of binder

Ilona Glatt; F. Biebl; C. Wagner – Math2Market

J. Joos – Karlsruhe Institute of Technology

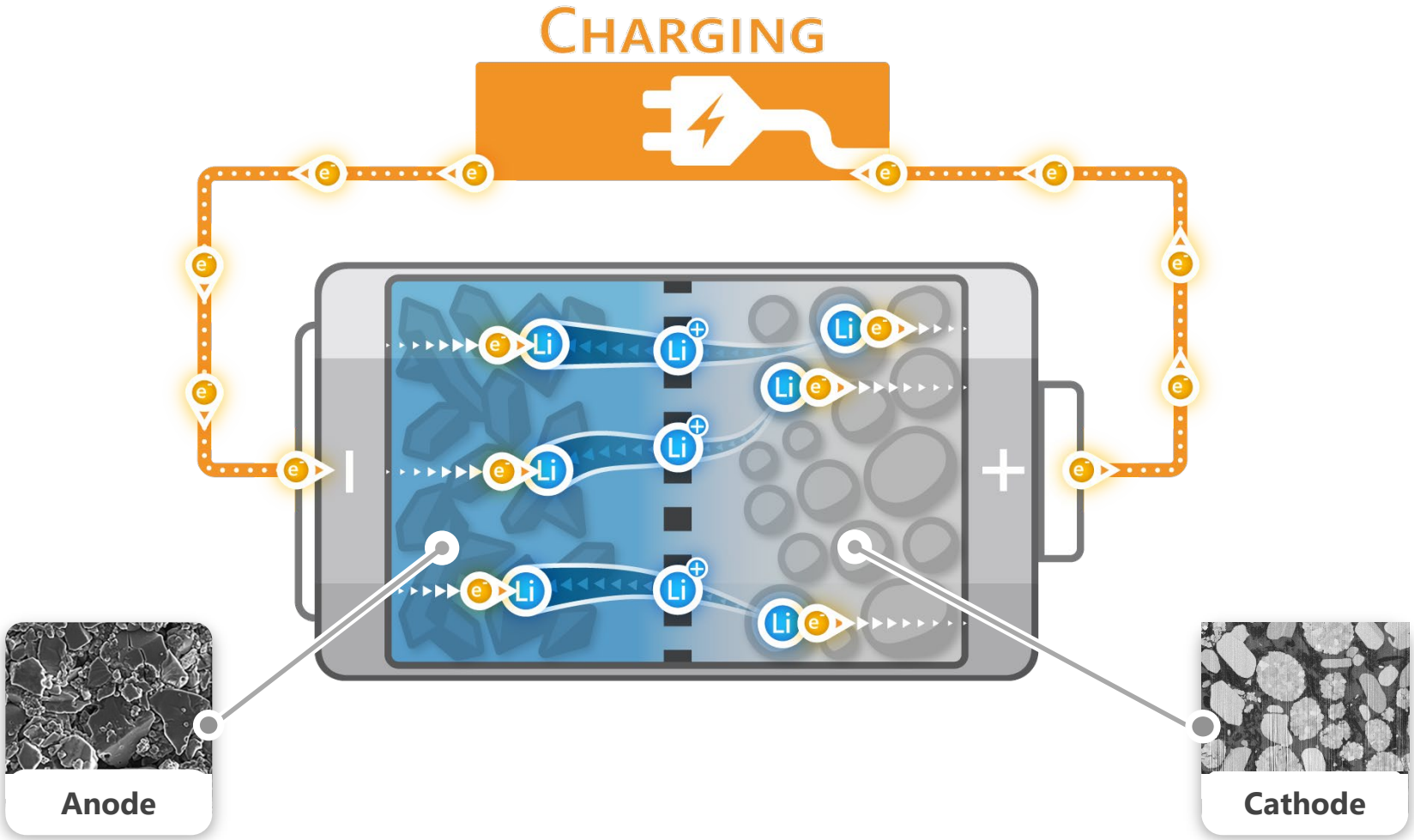
MATH
2 MARKET

Do-It-Yourself

- Most talks at DPG: front-end research
- Now: solve your own questions fast and easy-to-handle

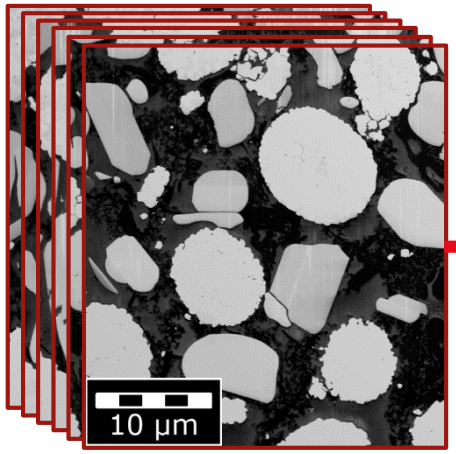
Schematic of a Li-Ion Battery

GeoDict

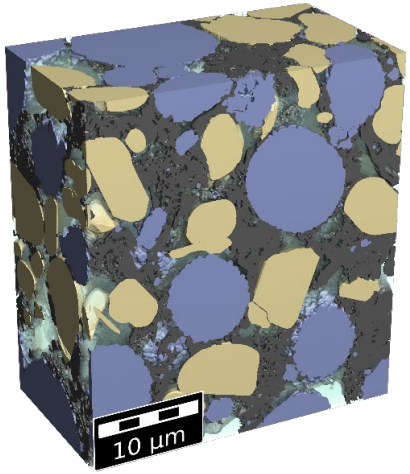


MATH 2 MARKET

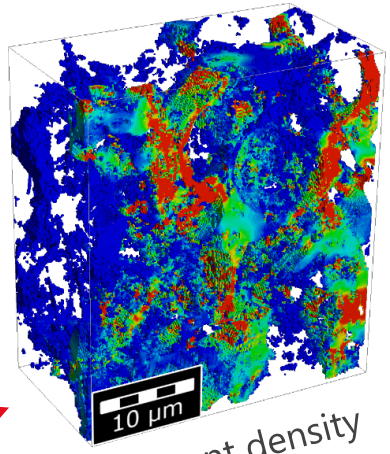
Example GeoDict Workflow



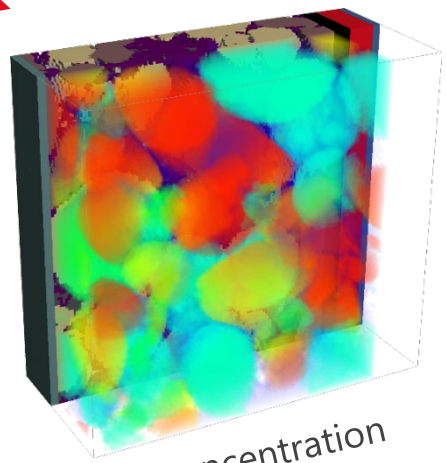
FIB-SEM image stack



3d-model



Current density



Li^+-concentration

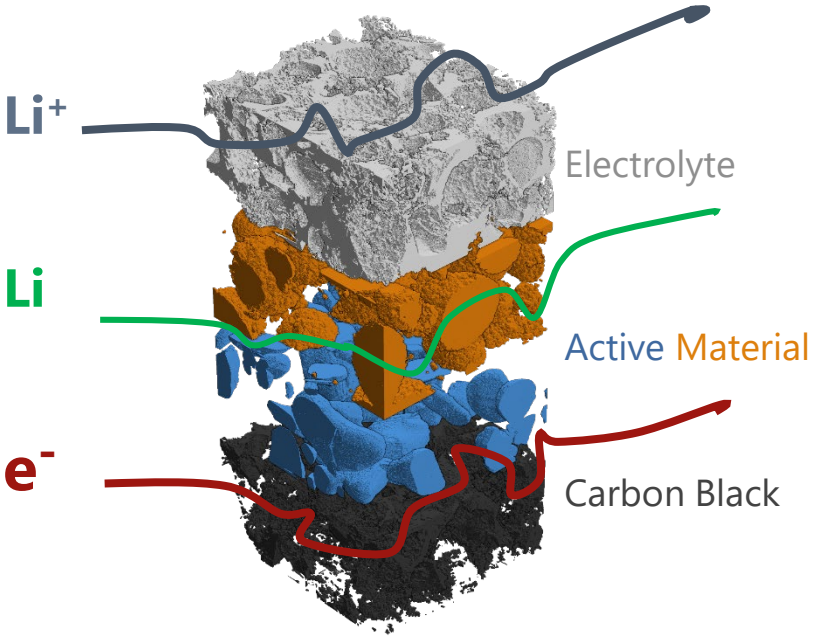
NCA: Lithium Nickel Cobalt Aluminum Oxide ($LiNiCoAlO_2$)
LCO: Lithium Cobalt Oxide ($LiCoO_2$)

GeoDict

MATH 2 MARKET

Well organized Transport is key

GeoDict



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

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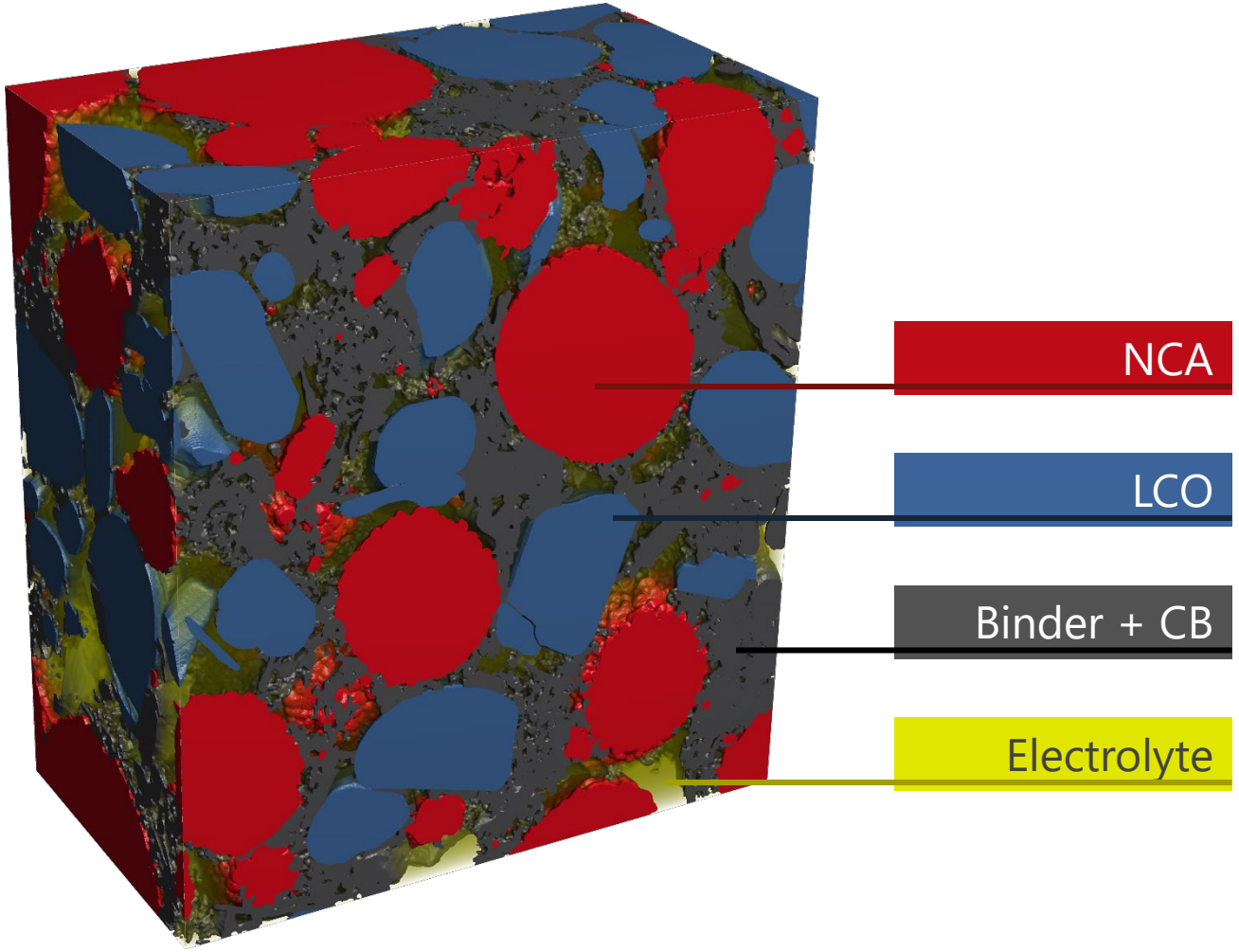
Cathode Material

GeoDict



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Hot Research Topic: How much binder is optimal?

GeoDict

Not enough binder:

https://steiermark.orf.at/news

e^- have to take detours

Too much binder:

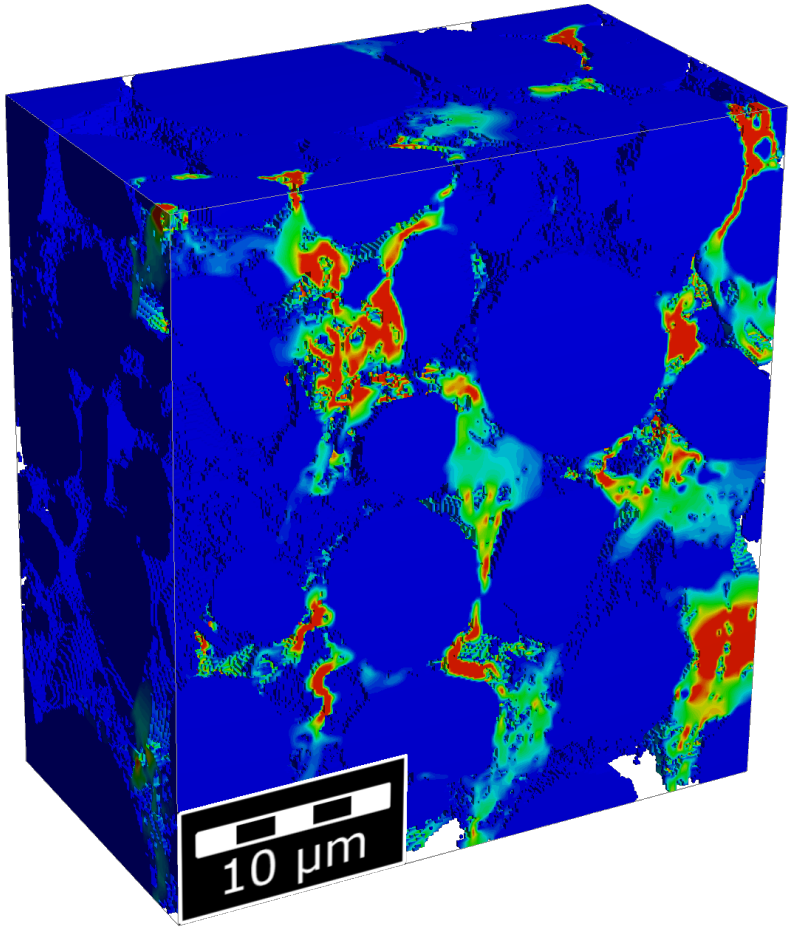
https://www.deinfuehrerschein.de

Li^+ cannot enter electrolyte

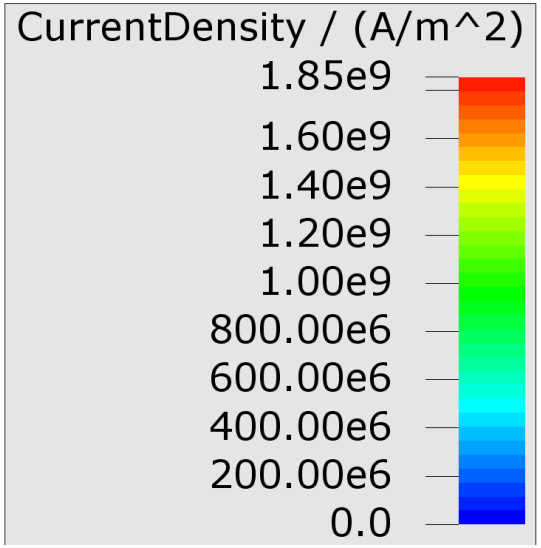
MATH 2 MARKET

Current Density in all solid materials

GeoDict

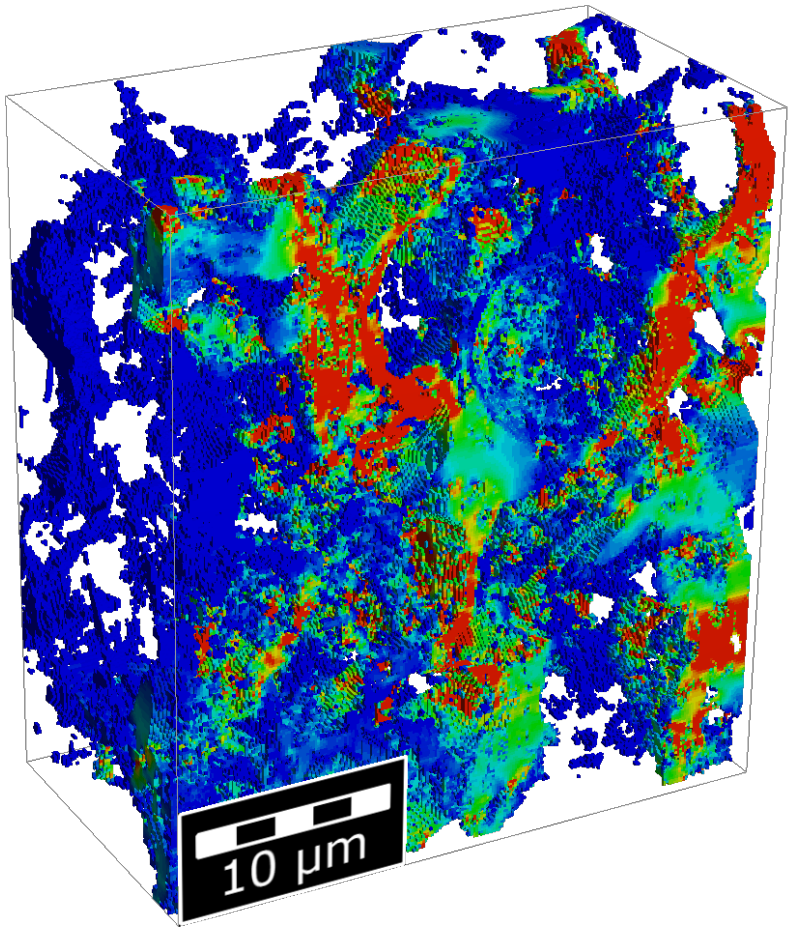


- Almost all current goes through the binder + carbon black

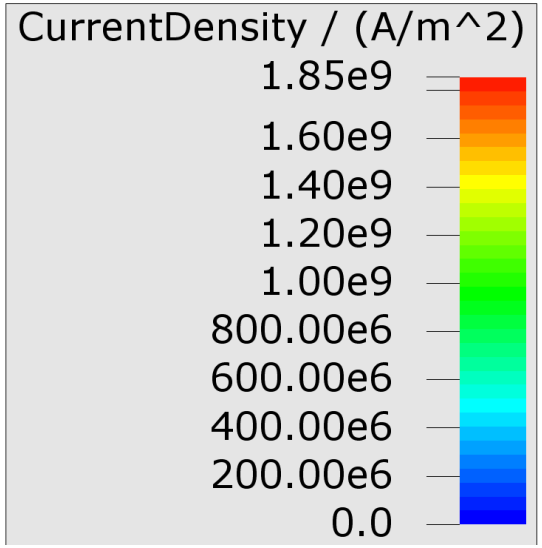


MATH 2 MARKET

Current Density in Binder

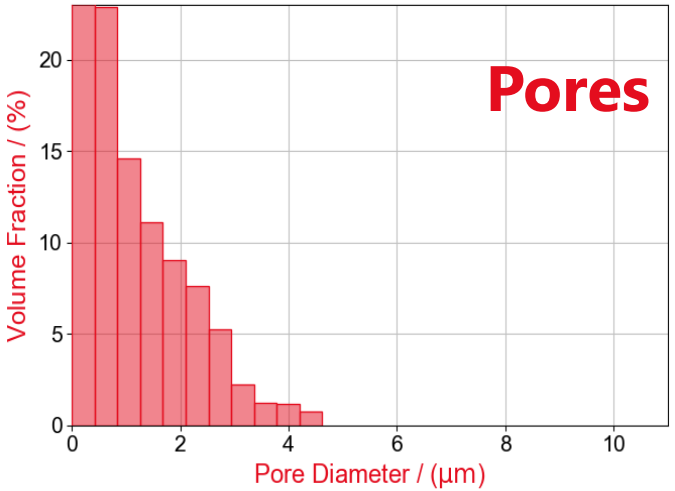


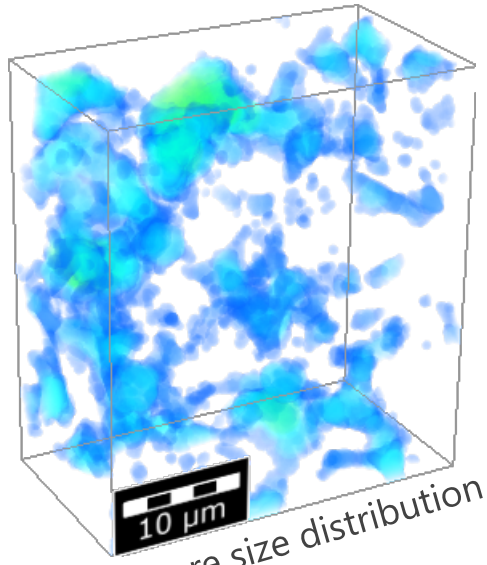
- Even the binder has only few local throughpaths
  - -> high risk of traffic jam



Pore Space

GeoDict

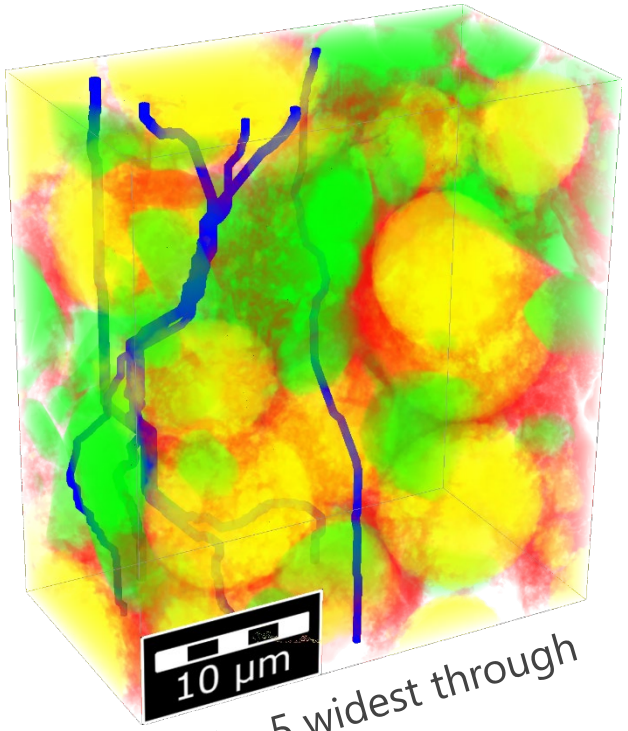




3D pore size distribution

Tortuosity factor: 3.5

Diffusivity: 7.4



The 5 widest through paths

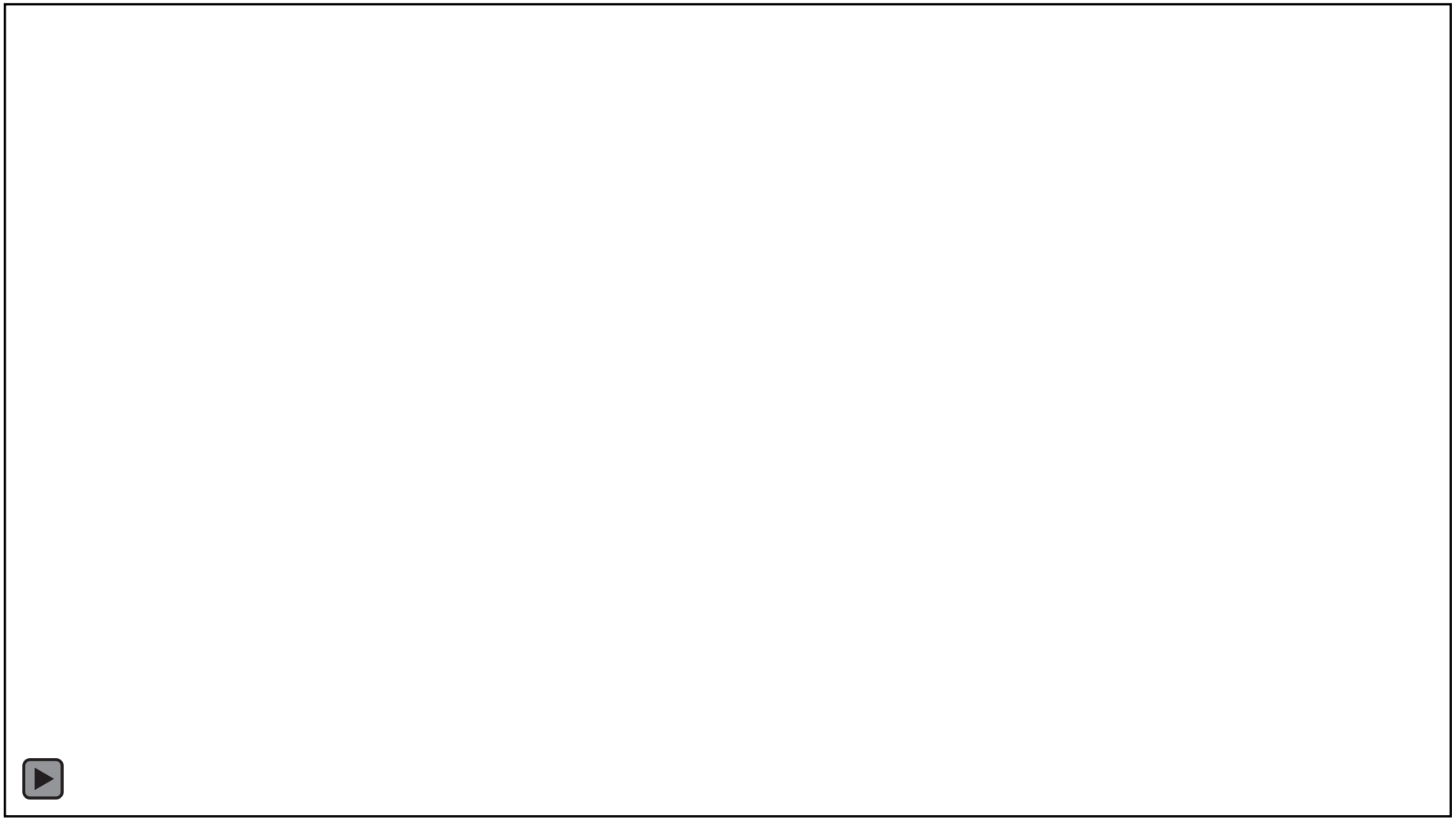
3 of the 5 largest through paths pass the same bottleneck

Pores are much smaller than grains

MATH 2 MARKET

Li^+-concentration in the cathode during charging

GeoDict

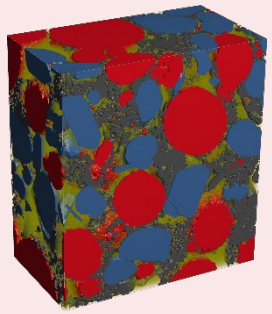
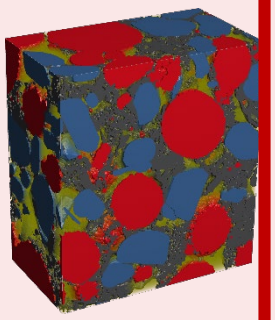
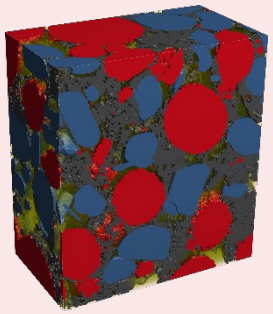
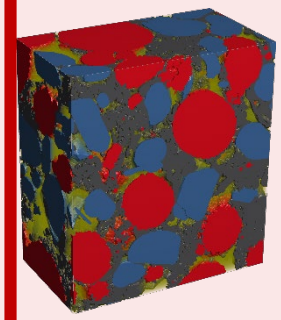
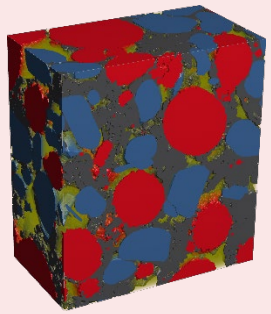


MATH 2 MARKET

Use several binder configurations

GeoDict

original

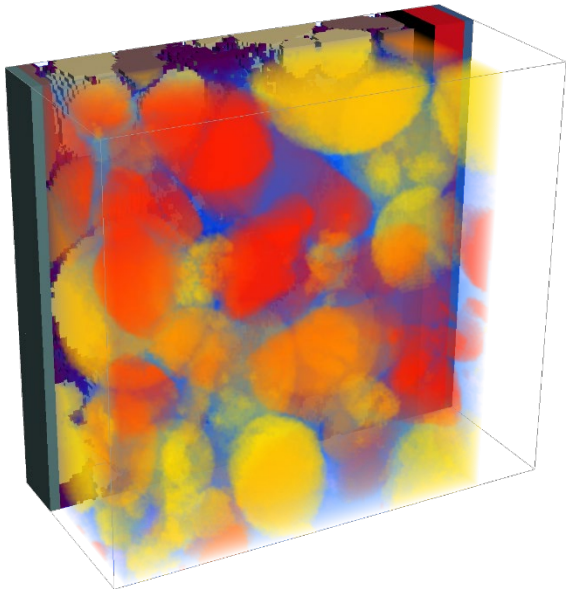
Binder $\%_{vol.}$	11%	12%	15%	17%	18%
Porosity %	31%	29%	26%	24%	22%
					

MATH 2 MARKET

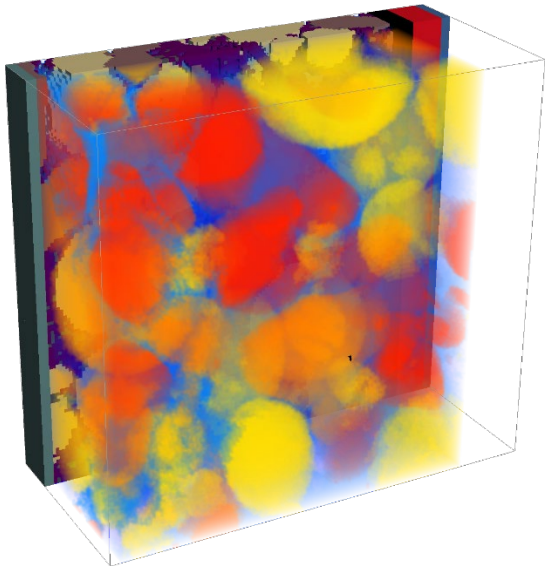
Li^+-concentration at 63% state of charge

GeoDict

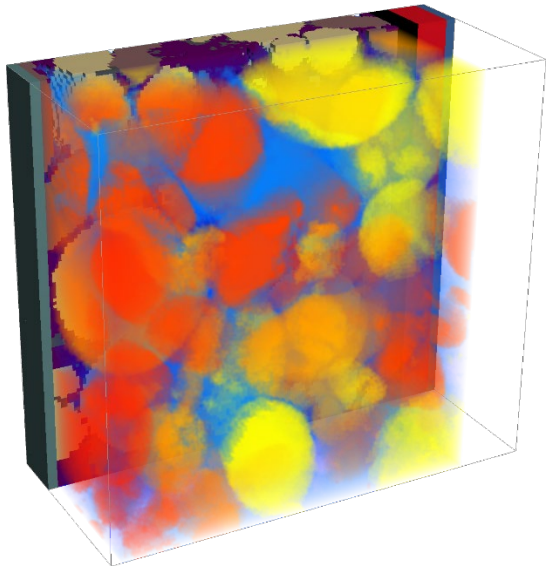
- Lower concentration means better battery?



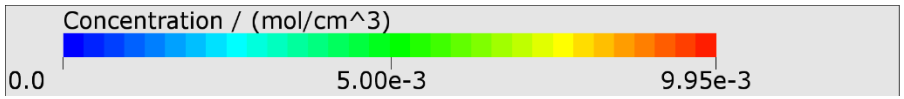
11% Binder+Carbon



15% Binder+Carbon



18% Binder+Carbon



min: 0.0
max: 9.95e-3

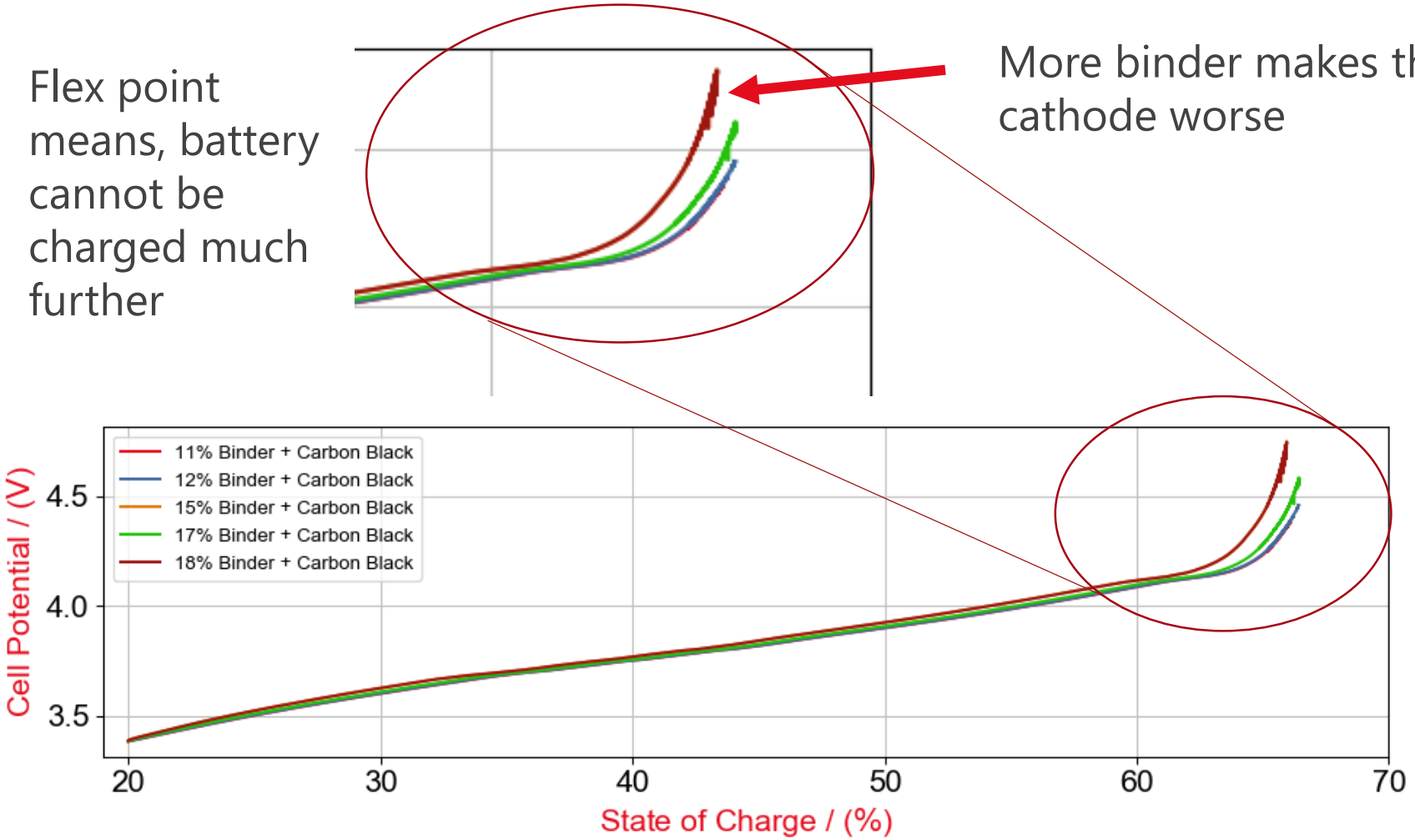
MATH 2 MARKET

Charge curves for different amount of Binder + Carbon Black

GeoDict

- Flex point means, battery cannot be charged much further

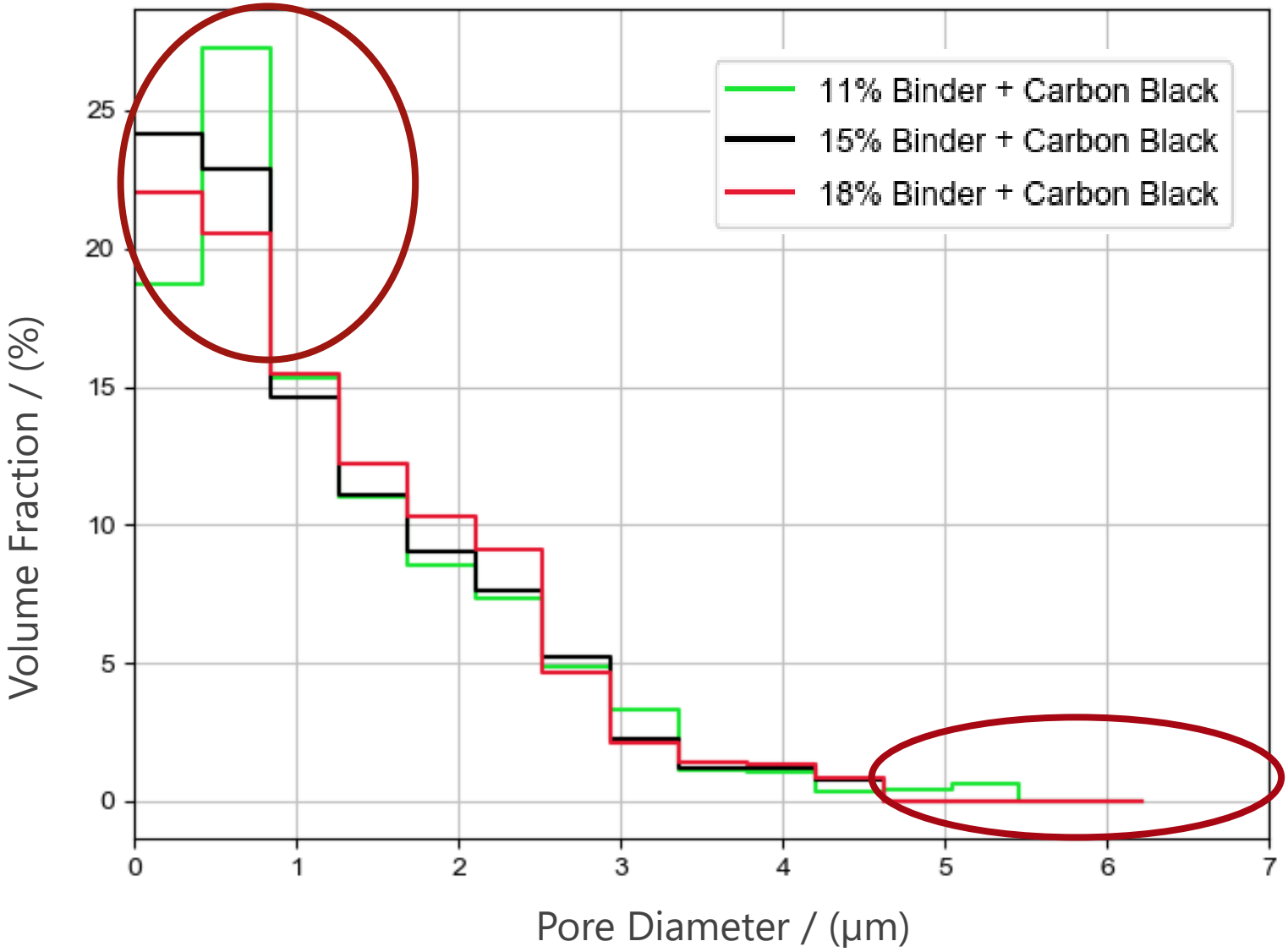
More binder makes the cathode worse



MATH 2 MARKET

Pore Size Distribution

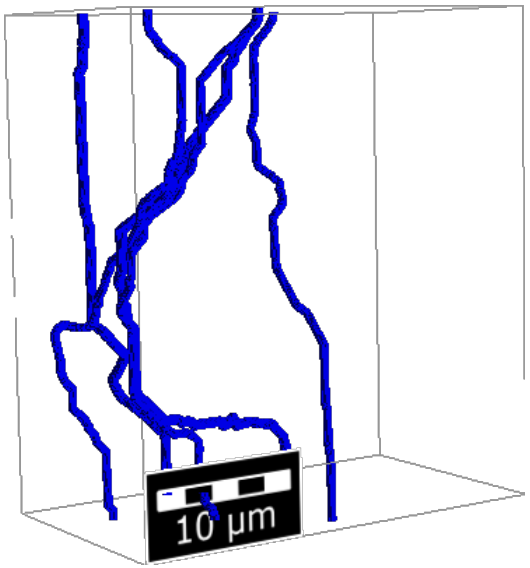
GeoDict



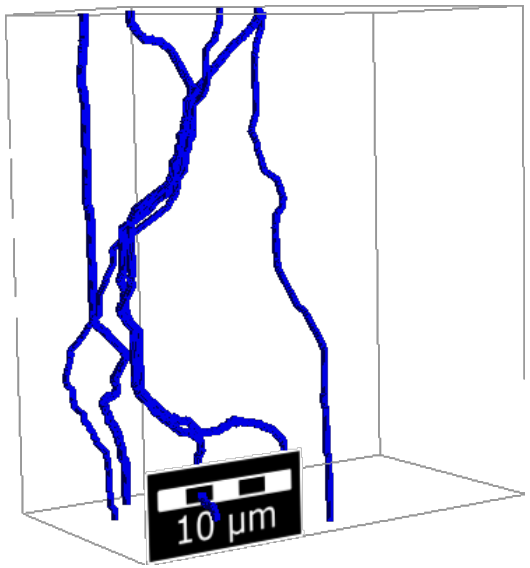
MATH 2 MARKET

Widest Through Paths

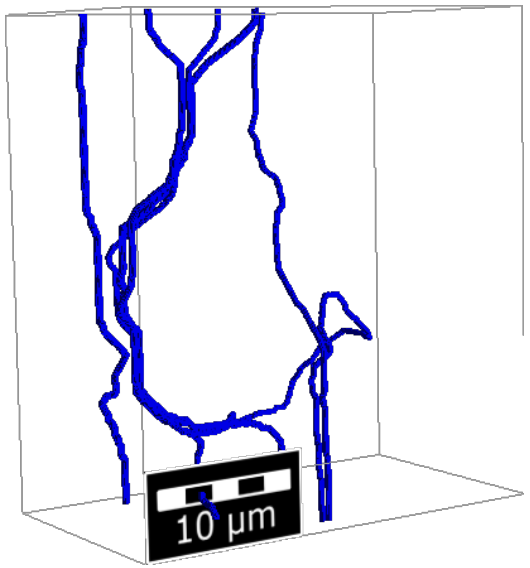
GeoDict



11% Binder+Carbon



15% Binder+Carbon



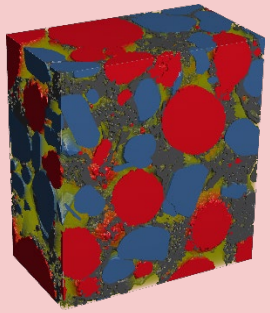
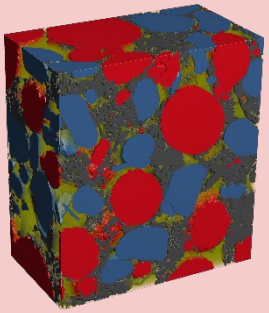
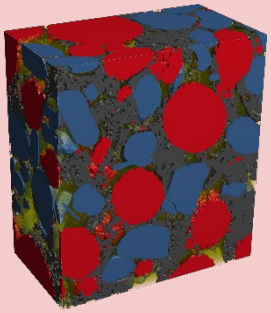
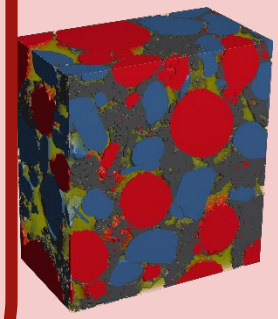
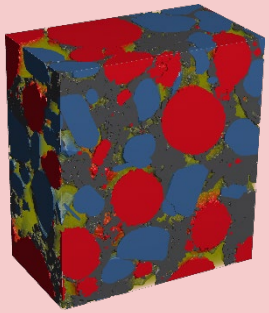
18% Binder+Carbon

- The widest through paths get thinner with more binder + carbon black
- For 18% binder the paths change shape and get longer

MATH 2 MARKET

Conclusion

GeoDict

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

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Thank You!

GeoDict