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# Impact of Inter-Particle Interactions on Electrochemical Performance of Lithium-Ion Battery Electrodes

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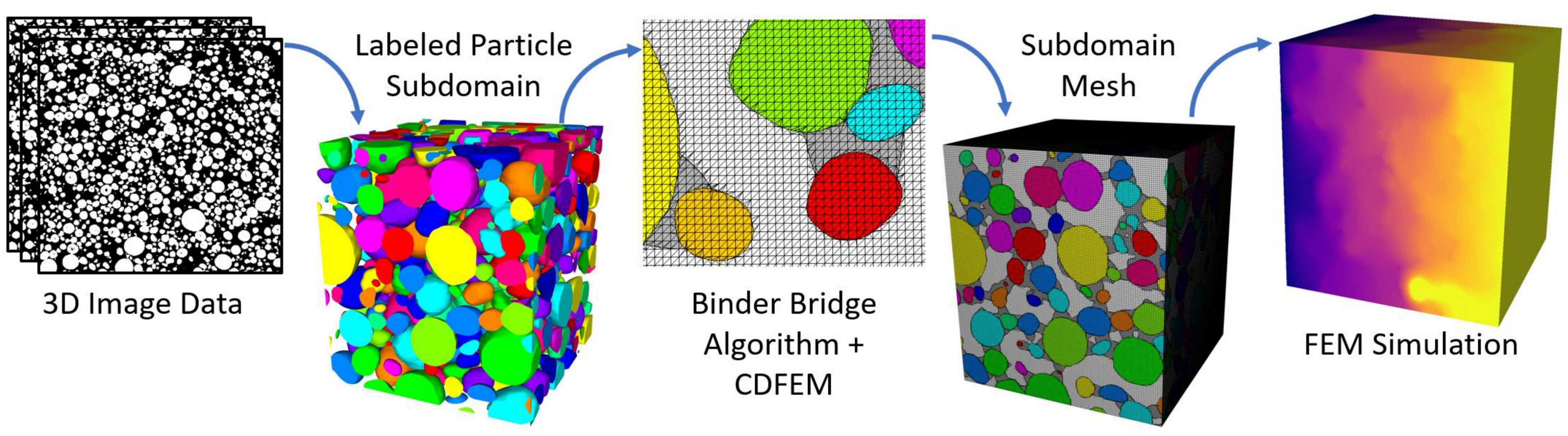
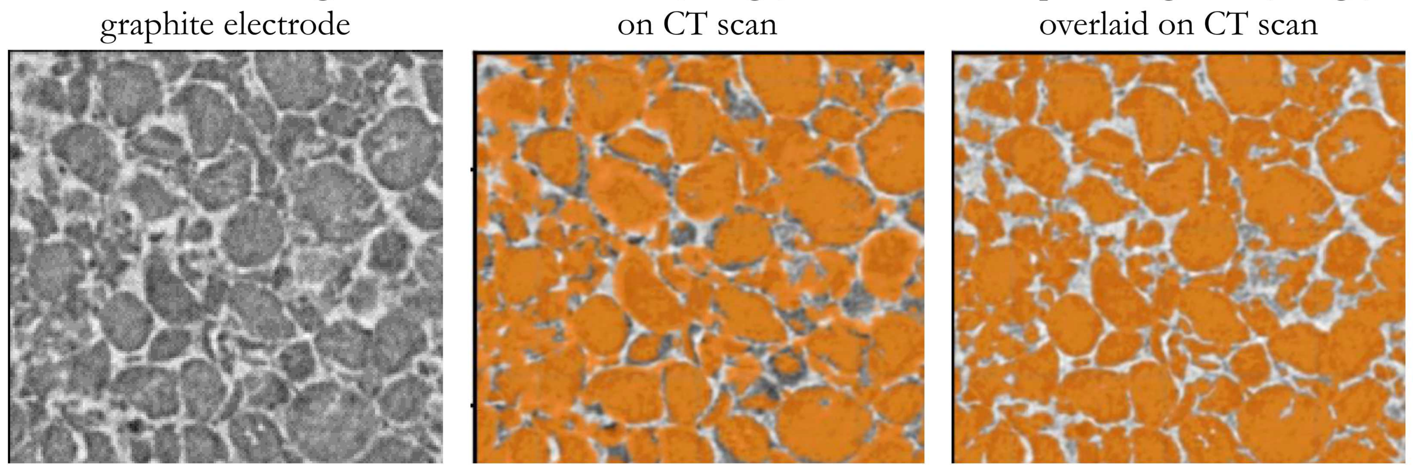
## 3D Image-to-Simulation Workflow[1, 2]



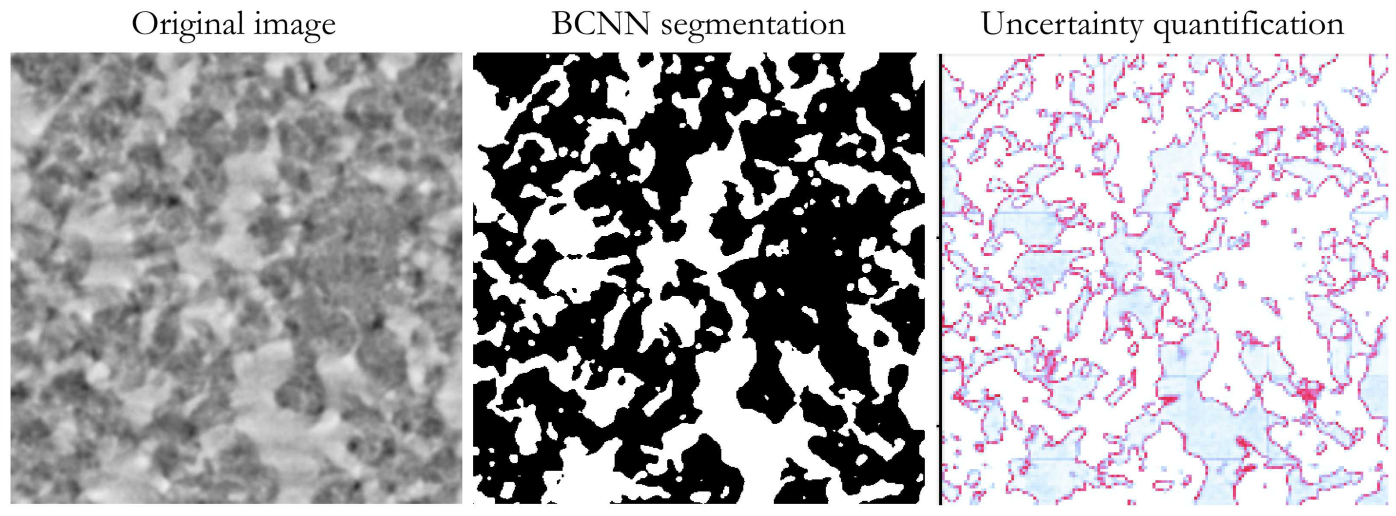

## Deep Neural Networks for Segmentation and Geometric Uncertainty[3]

Slice from CT image of graphite electrode | Human label (orange) overlaid on CT scan | Deep learning label (orange) overlaid on CT scan



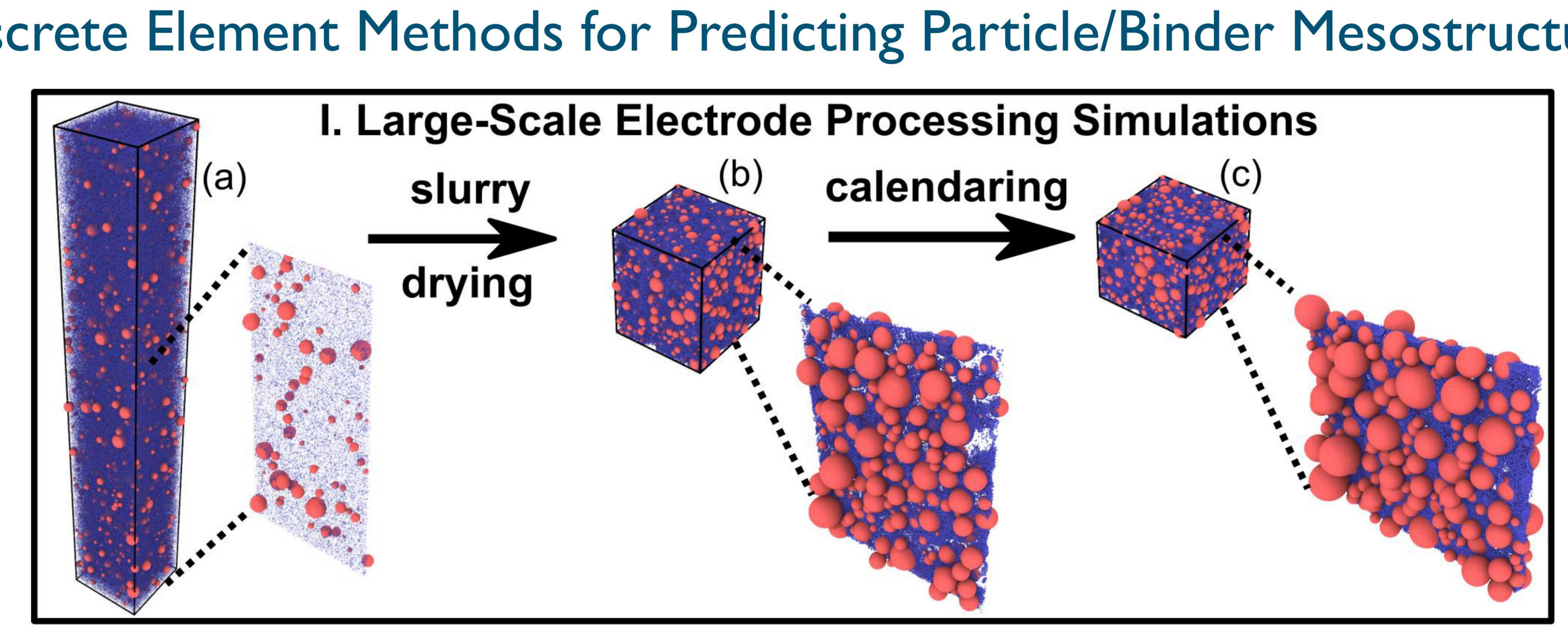
Deep neural networks segment images to high accuracy, higher than human labels in some cases.

Original image | BCNN segmentation | Uncertainty quantification

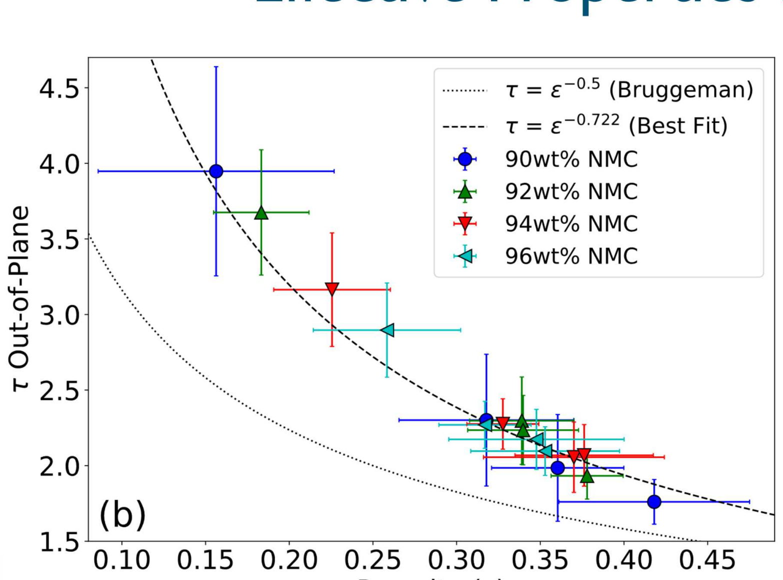


Bayesian convolutional neural networks (BCNNs) provide interpretable geometric uncertainty for physics propagation.

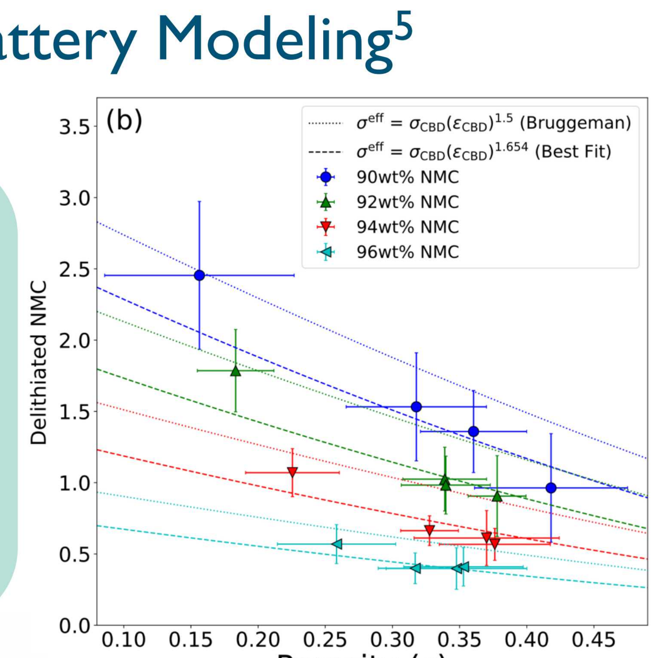
## Discrete Element Methods for Predicting Particle/Binder Mesostructure[4]




## Effective Properties for Macroscale Battery Modeling[5]




Effective transport properties simulated using image-based and DEM mesostructures to improve P2D models.



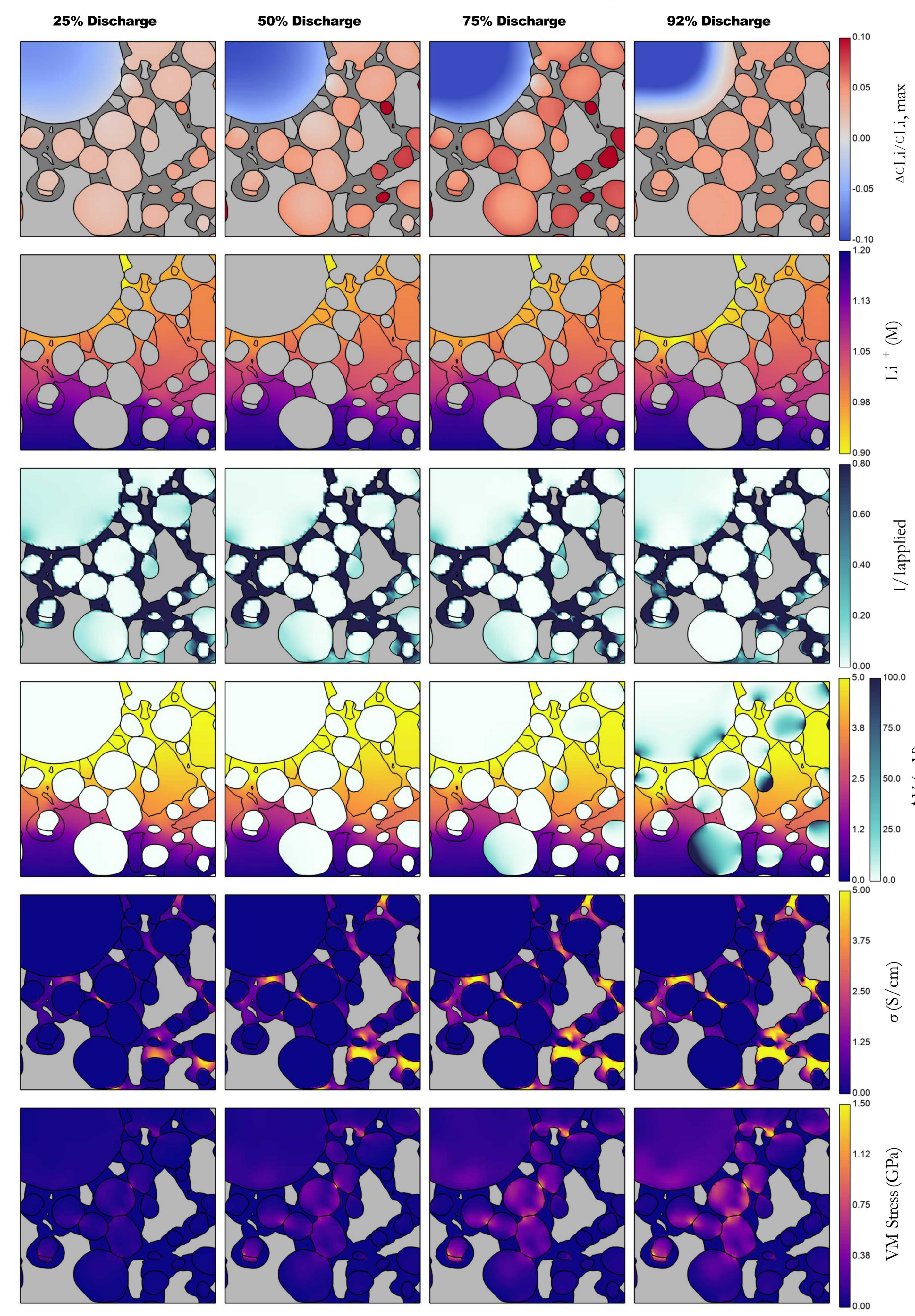


## Abstract

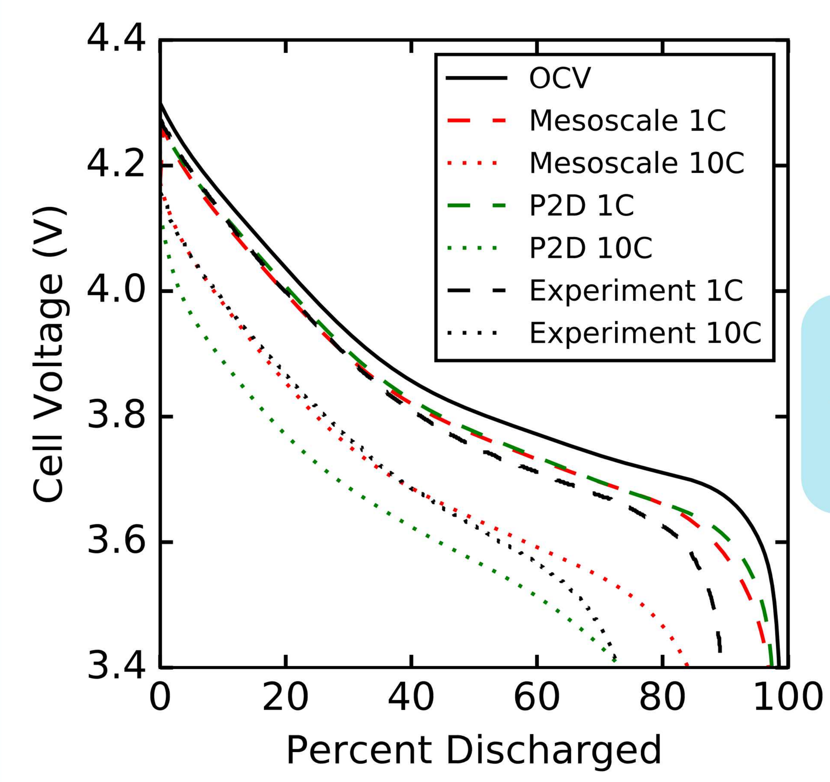
While lithium-ion battery electrodes are manufactured in large-scale, high-speed, roll-to-roll manufacturing processes, it is the morphology of the particle and conductive binder structures greatly affect macroscale properties and can vary significantly as a function of manufacturing conditions. To explore the process-structure-property relationship, we employ mesoscale finite element simulations of the three-phase particle-conductive binder-electrolyte composite of a NMC battery cathode. Particle and conductive binder domain mesostructures are derived from both x-ray computed tomography imaging and simulated using discrete element methods. The Conformal Decomposition Finite Element Method is applied to create conformal three-phase finite element meshes of these mesostructures.

In this poster, we explore the how simulated mesostructures can be used to approximate as-manufactured geometries, while providing additional insights into how electrode slurry chemistry and processing conditions affect the mesostructure. We focus on examining how particle-to-particle interactions affect electrochemical discharge performance. Additionally, the mechanical impacts of calendaring and lithiation-induced swelling are explored in the context of external mechanical loads.


## NMC Electrochemical-Mechanical Discharge at the Mesoscale[6]

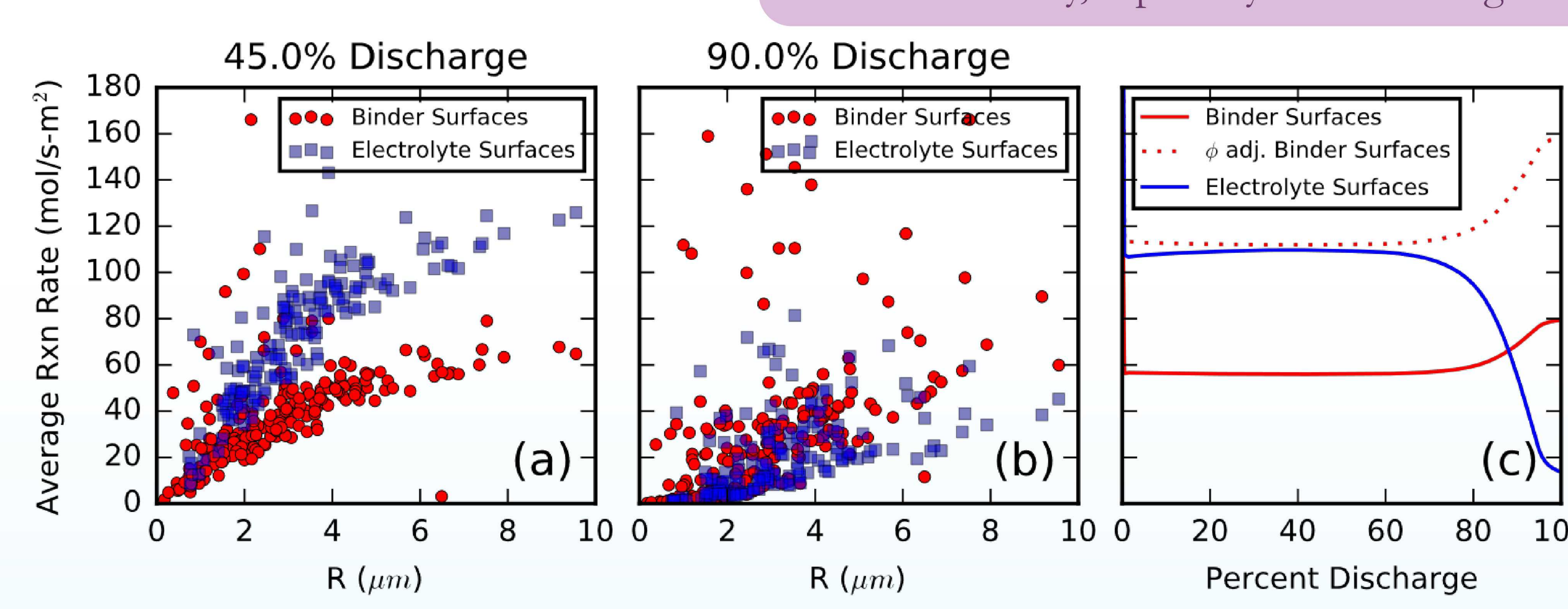



Simulating multi-physics discharge at 5C highlights the complex interplay between transport, mechanics, and chemistry.




Mesoscale simulations agree well with experimental measurement and outperform P2D models.

Reactions are *promoted* at particle surfaces under porous binder because of its high electrical conductivity, especially near discharge.





## Publications

(1) S. A. Roberts et al., "A verified conformal decomposition finite element …," J. Comp. Phys. (2018) doi: 10.1016/j.jcp.2018.08.022
(2) B. L. Trembacki et al., "Mesoscale Analysis of Conductive Binder …," J. Electrochem. Soc. (2018) doi:10.1149/2.0981813jes
(3) C. Norris et al., "Structural Uncertainty Analysis on Graphite Electrodes Using Convolutional Neural Networks," in preparation
(4) I. Srivastava et al., "Controlling Binder Adhesion to Impact Electrode Mesostructure …," under review doi: 10.1149/osf.io/ehdq6
(5) B. L. Trembacki et al., "Mesoscale Effects of Composition …," J. Electrochem. En. Conv. Stor. (2020) doi: 10.1115/1.4045973
(6) M. E. Ferraro et al., "Electrode Mesoscale as a Collection of …," J. Electrochem. Soc. (2020) doi: 10.1149/1945-7111/ab632b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