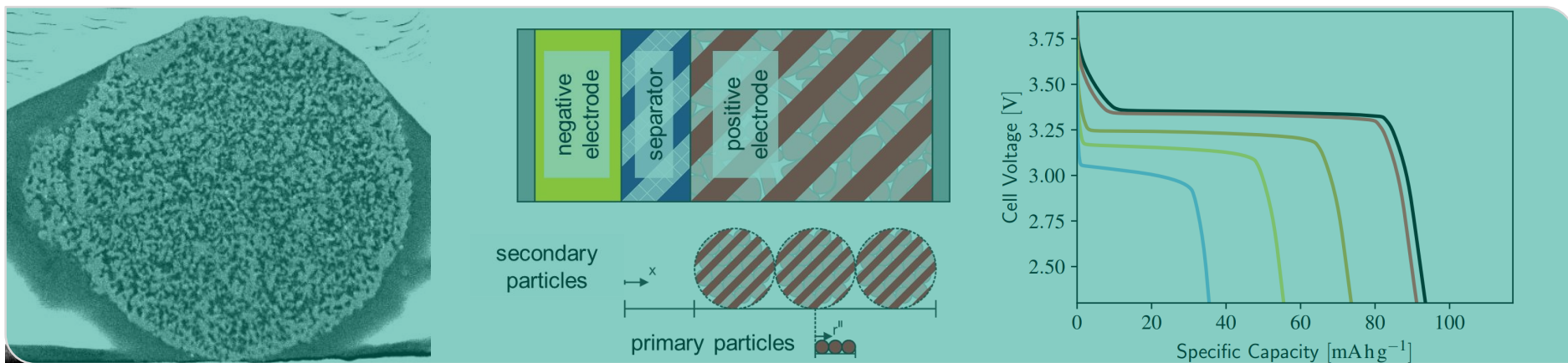


Combining Methods to Model the Performance of a Sodium-Ion Battery

J. Naumann, P. Maidl, T. Akcay, S. Daubner, A. Pamperin, M. Kamlah, M. Neumann



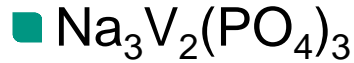
Novel Na-Ion Battery Materials

- sodium more abundant than lithium
- evaluate and improve novel electrode materials
- consider different scales
- establish workflow among simulation methods



POLiS

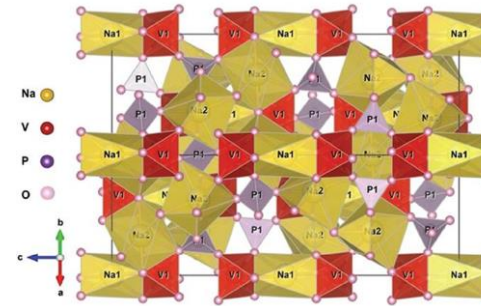
NVP



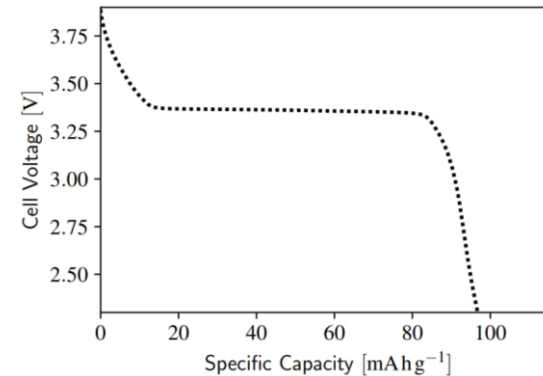
- 3D network for diffusion of Na ions^[1]

- voltage plateau

- low electronic conductivity^[2]



Front. Chem. **2020**, 8, 635



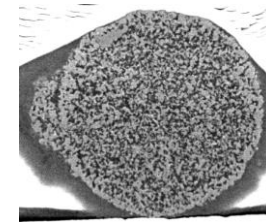
[1] *Adv. Funct. Mater.* **2022**, 30.34, 2001289

[2] *Rare Met.* **2022**, 41.1, 115–124

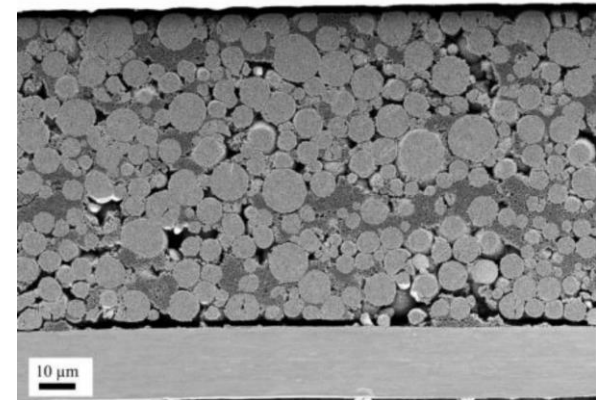
NVP/C Electrodes

- porous NVP carbon composite (NVP/C)
- boost electronic conductivity
- short paths for solid-state diffusion
- capacity close to theoretical value^[3]

[3] *ChemElectroChem* **2024**, 11.3, e202300401

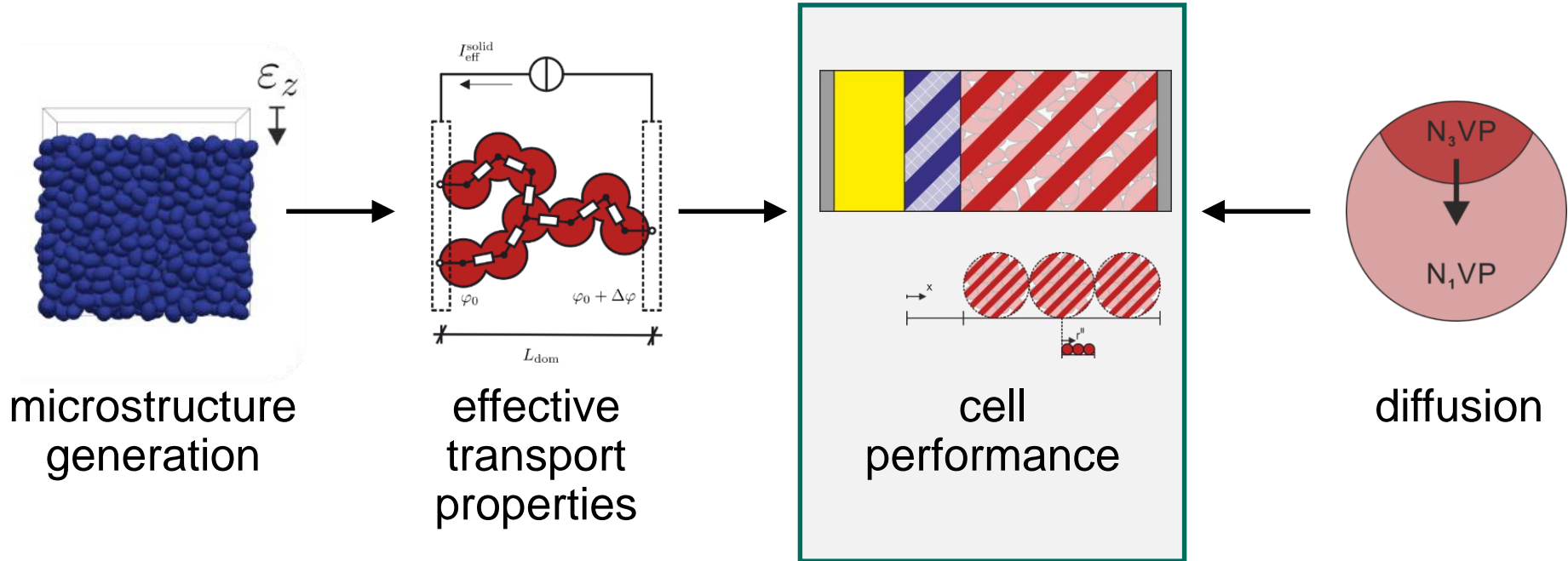


Batteries Supercaps **2024**, 7.4, e202300409



REM image by Luca Schneider

Combining Methods

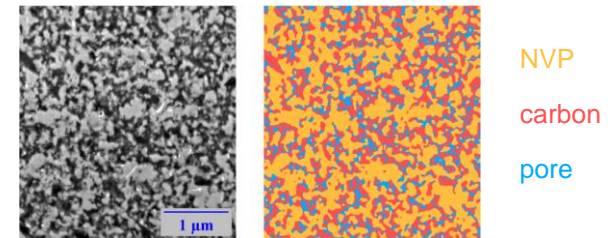
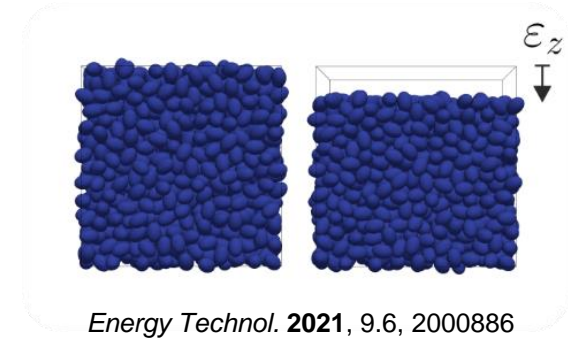


Microstructure Generation

- virtual reconstruction
 - electrode and porous particle

- discrete element method^[7]
 - basis for resistor network method

- alternative: digital image reconstruction^[6]



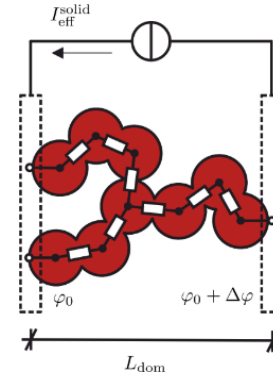
Batteries Supercaps **2024**, 7.4, e202300409

[6] *Batteries Supercaps* **2024**, 7.4, e202300409

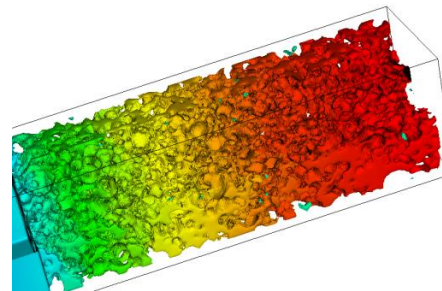
[7] *Energy Technol.* **2022**, 9.6, 2000886

Effective Transport Properties

- effect of microstructure on transport
 - sodium ions and electrons
- resistor network method^[5]
- alternative: steady state flow



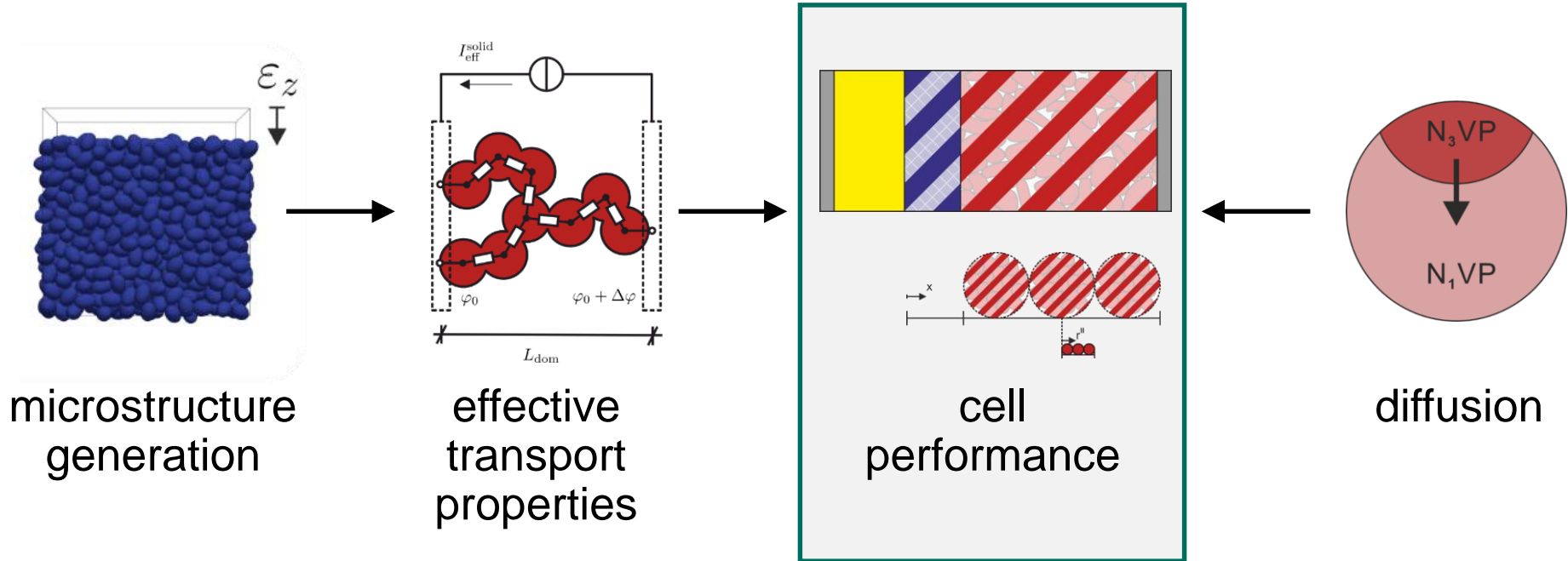
Powder Technol. **2021**, 378, 659-666



J. Power Sources **2016**, 334, 191-201

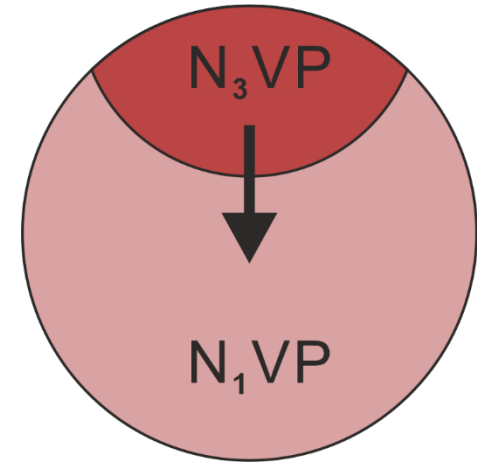
[5] *Powder Technol.* **2021**, 378, 659-666

Combining Methods



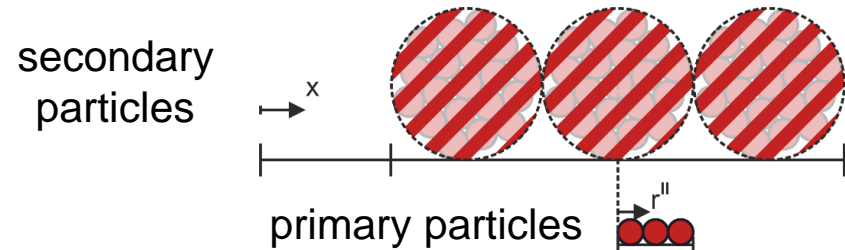
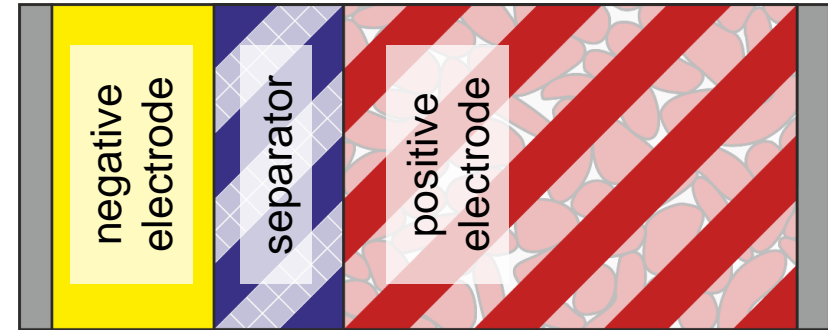
Diffusion of Sodium in Host Material

- NVP experiences phase separation
- concentration-dependent diffusion coefficient
- phase-field method



Cell Model^[4]

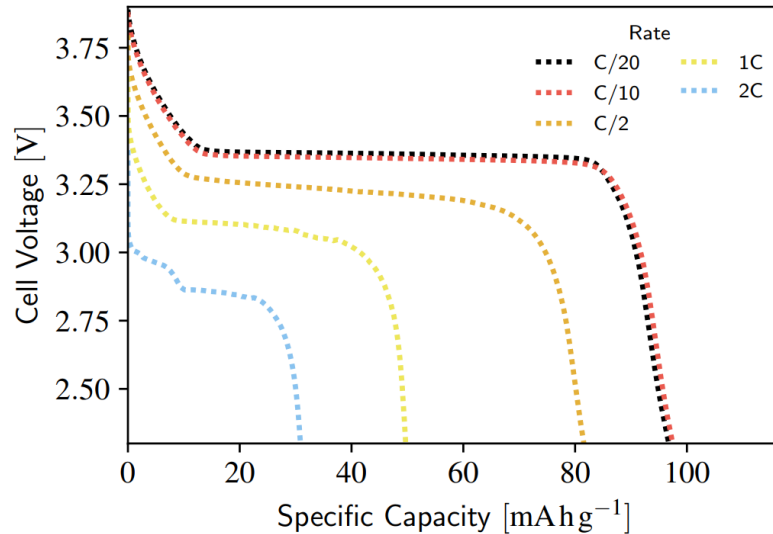
- transport of sodium ions & electronic transport
- insertion reaction
- diffusion of sodium in host material



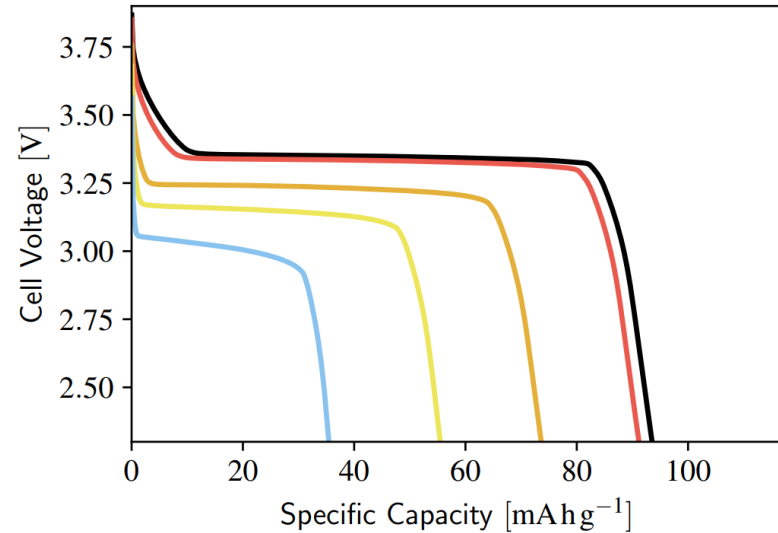
[4] *Energy Technol.* **2021**, 9.6, 2000910

Cell Performance

experiment

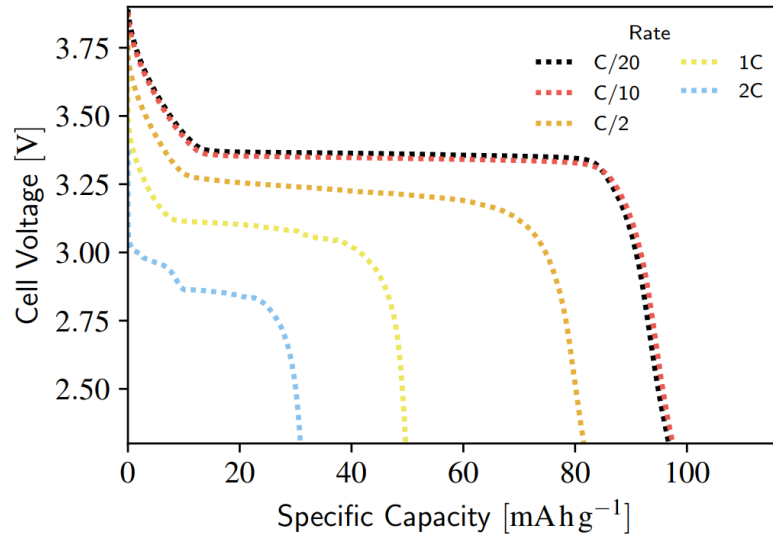


model

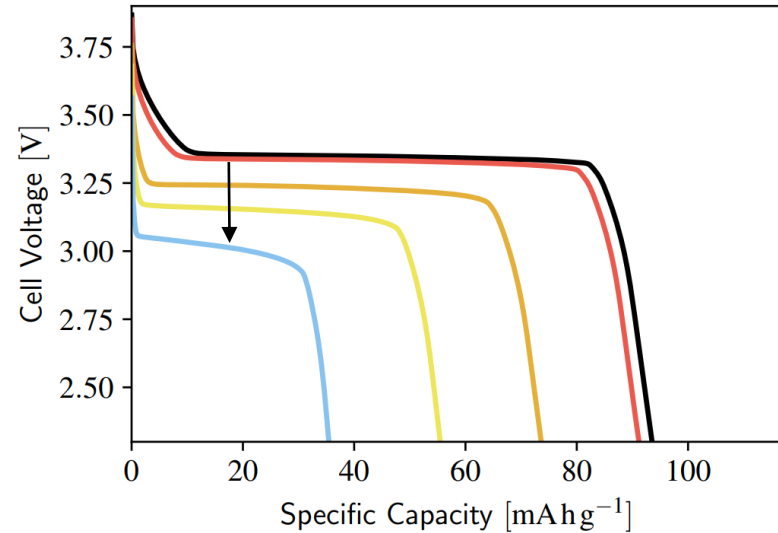


Cell Performance

experiment



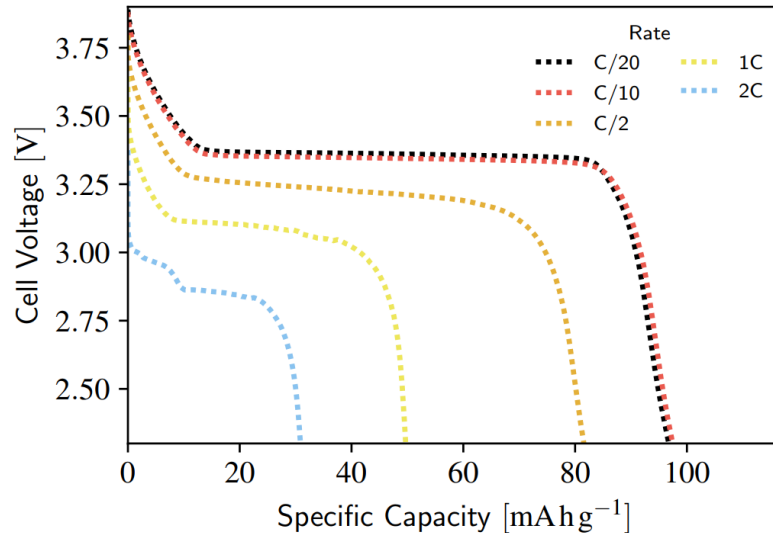
model



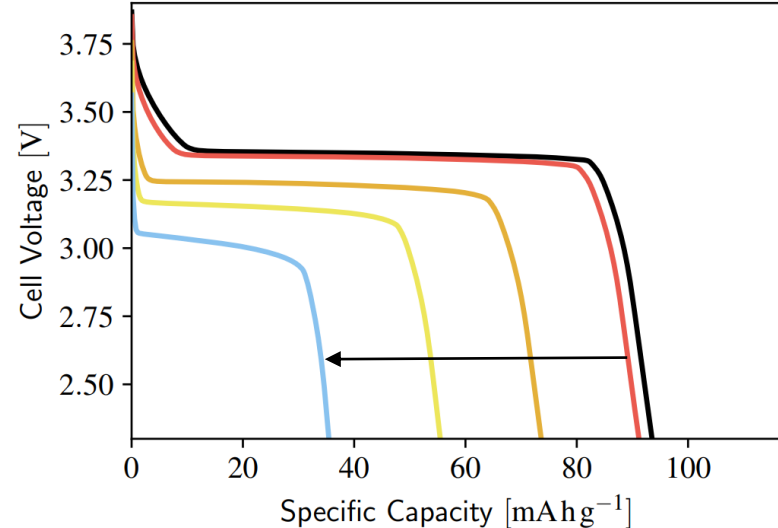
■ significant contact resistance lowers voltage

Cell Performance

experiment



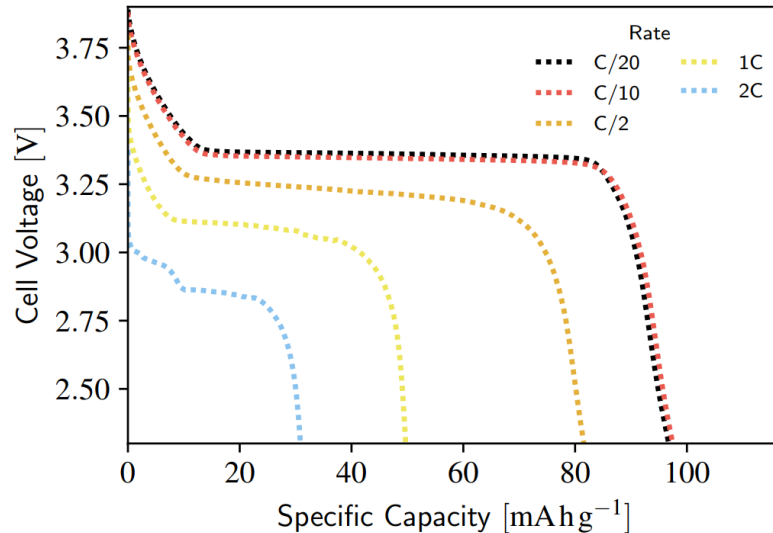
model



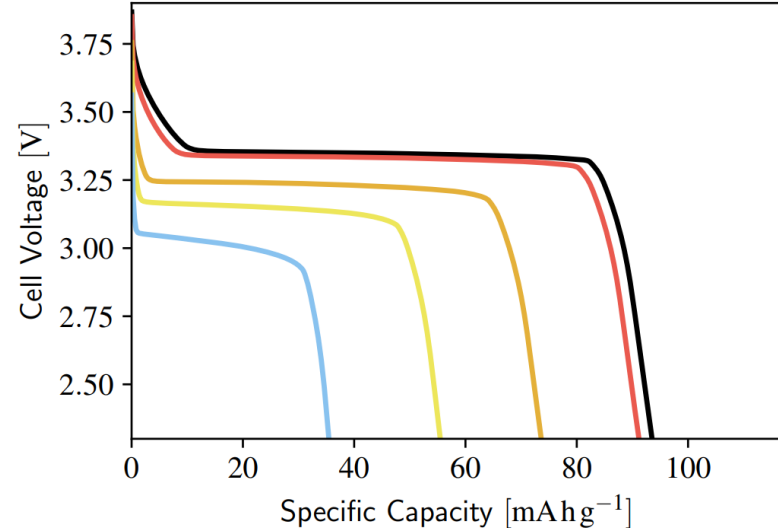
- significant contact resistance lowers voltage
- solid state diffusion limits rate performance

Cell Performance

experiment



model



- significant contact resistance lowers voltage
- solid state diffusion limits rate performance

OPTIMIZATION
POTENTIAL

Summary and Outlook

- combine methods to model cell behavior
- understand effects on different scales
- improvement of electrode structure and composition