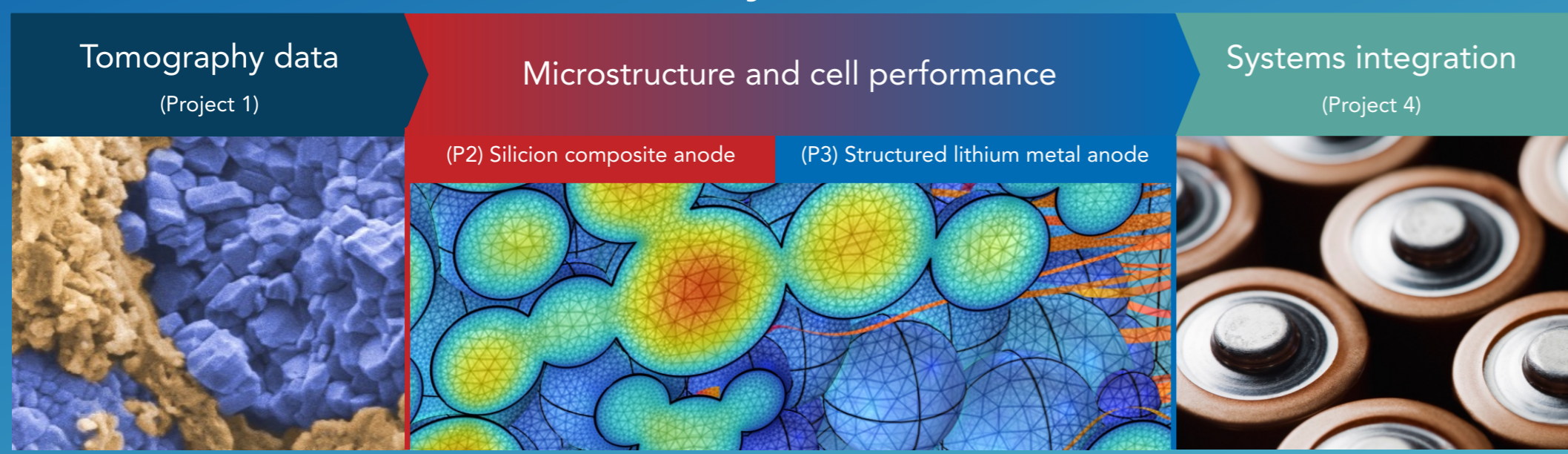


Segmentation and Augmentation of Scanning Electron Microscopy Data by Deep Learning Methods

Segmentierung und Augmentierung von Rasterelektronenmikroskopie-Daten mittels Deep Learning-Methoden

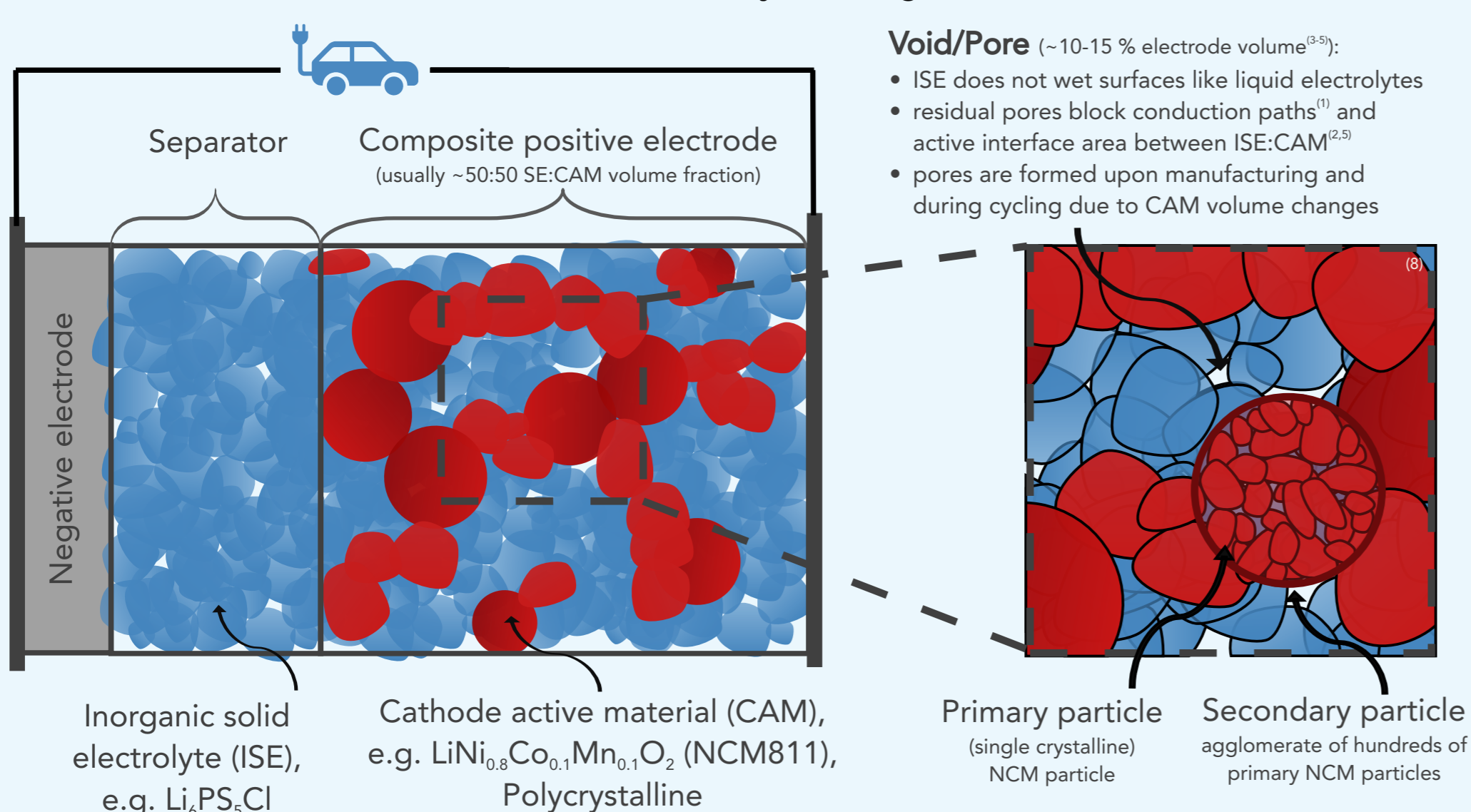
Anja Bielefeld*, Alexander Weiß, René Rekers, Safoura Vaez, Moritz Pawlowsky
Center for Materials Research, Justus Liebig University Giessen

The Way (Forward)



Microstructure(s) in Solid-State Batteries

Solid-state battery cell design



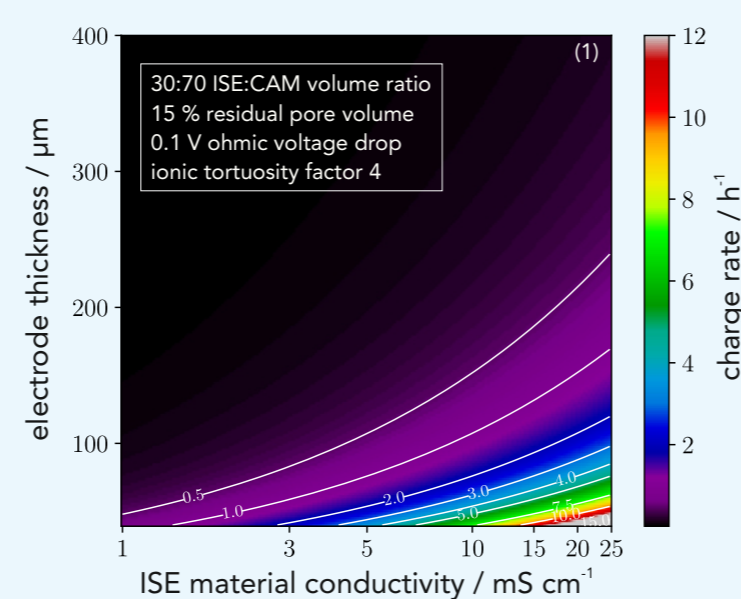
Microstructure counts even more in solid-state batteries. Why?

By contrast with conventional cells, **solid-state batteries feature (micro-)porosities**. These result from the particle-morphology of the ISE and its non-wetting behavior.

Pore properties are barely known and **depend on the materials**, the **manufacturing method**⁽¹⁾, the **particle size(s)** and **distributions**^(1,2,4,5), the **particle morphologies**⁽⁶⁾ and the **electrode composition**^(1,3).

In composite electrodes (NCM, silicon, graphite, ...) there are three strategies to **assure sufficient ionic conductivity**⁽¹⁾:

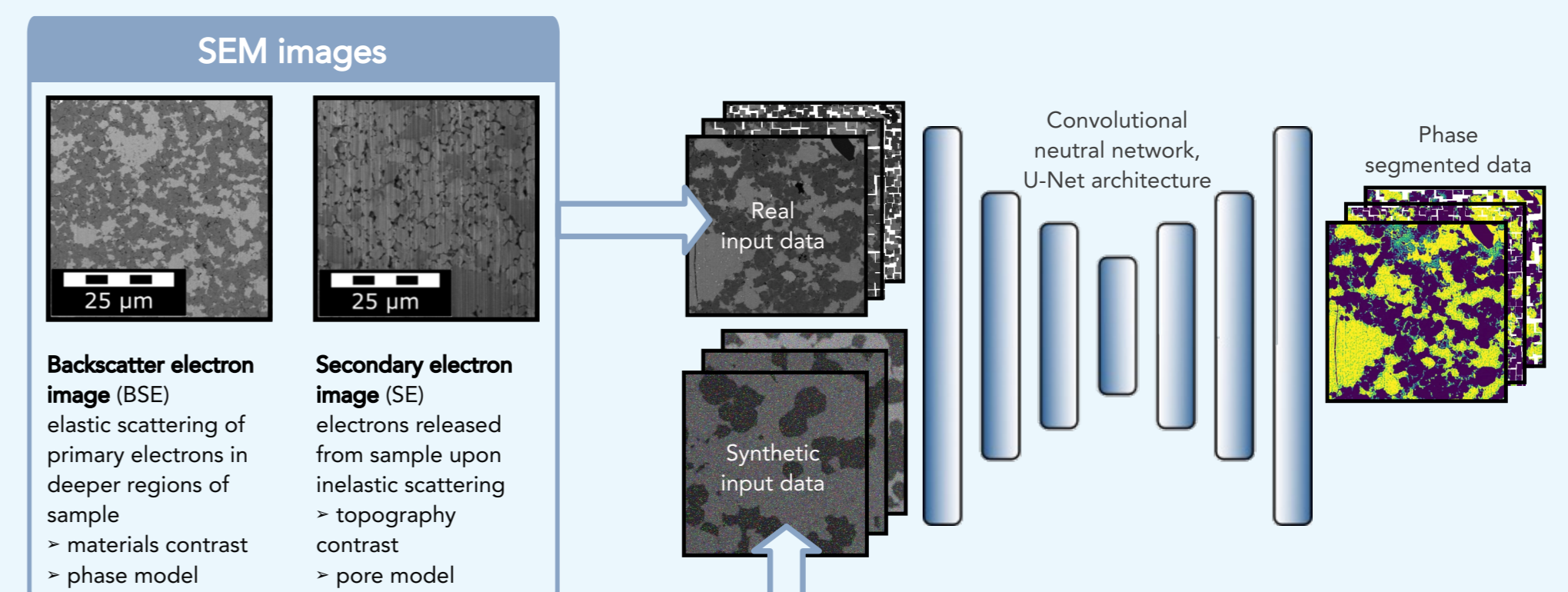
- high catholyte conductivity (> 10 mS cm⁻¹, see figure)
- elevated ISE volume fraction
- optimized microstructure



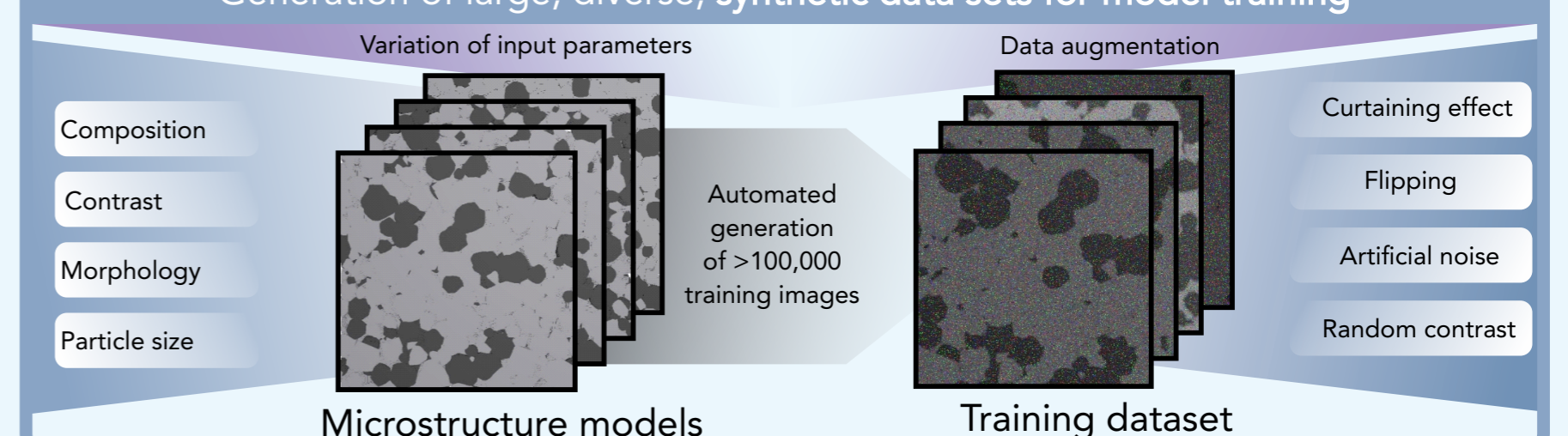
Imaging and Tomography

- basis for microstructure modeling and simulation
- FIB-SEM 2D cross sections and 3D tomographies
- deep learning-based methods for segmentation of 2D images and 3D reconstruction of 2D data
- microstructure evolution and chemo-mechanics upon cycling and aging

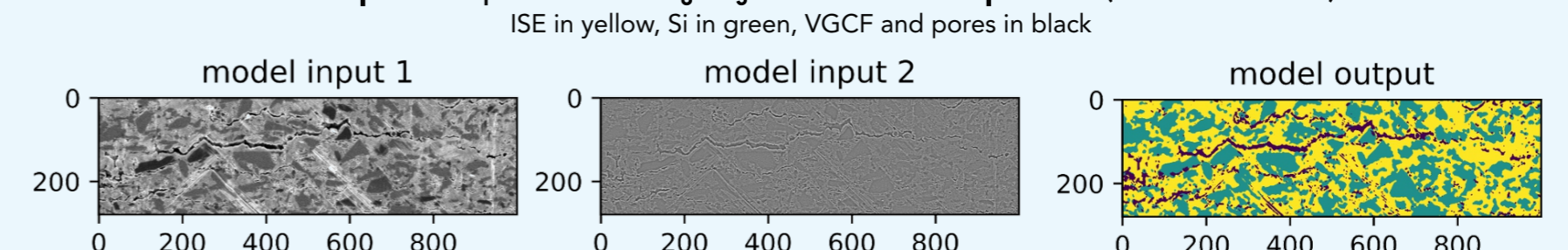
Semantic segmentation of ISE, CAM and pore phases combining SE and BSE images



Generation of large, diverse, synthetic data sets for model training



Example output for $\text{Si}:\text{Li}_6\text{PS}_5\text{Cl}:\text{VGCF}$ -composite (50:47:3 wt%)



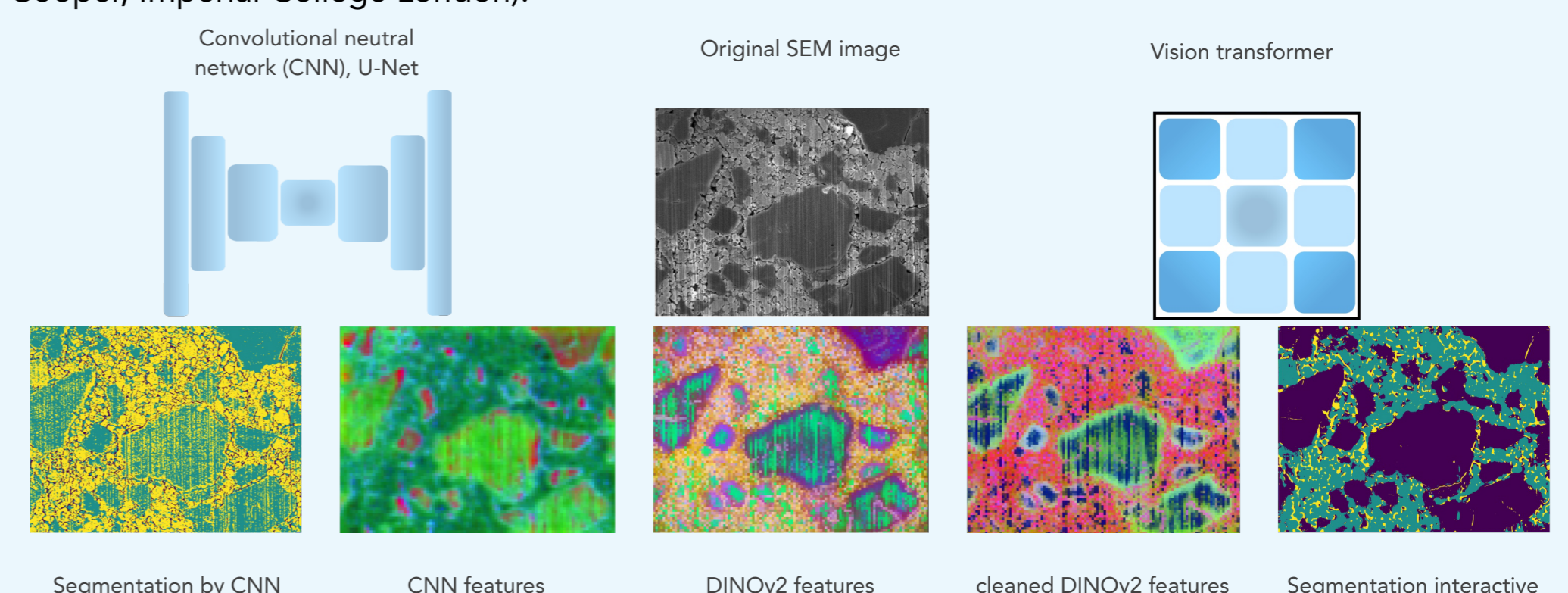
Interactive Image Segmentation

- interactive segmentation⁽⁸⁾ based on the "Weka Segmentation Framework"⁽⁹⁾
- self-supervised pretrained vision transformer (ViT) to extract semantic features
- ViT features have low spatial resolution, so feature upsampling strategy required for segmentation⁽⁸⁾
- learned features, combined with sparse user-provided labels, train a Random Forest classifier to segment entire image (and tomography subsequently)



Challenges for segmentation of SEM data

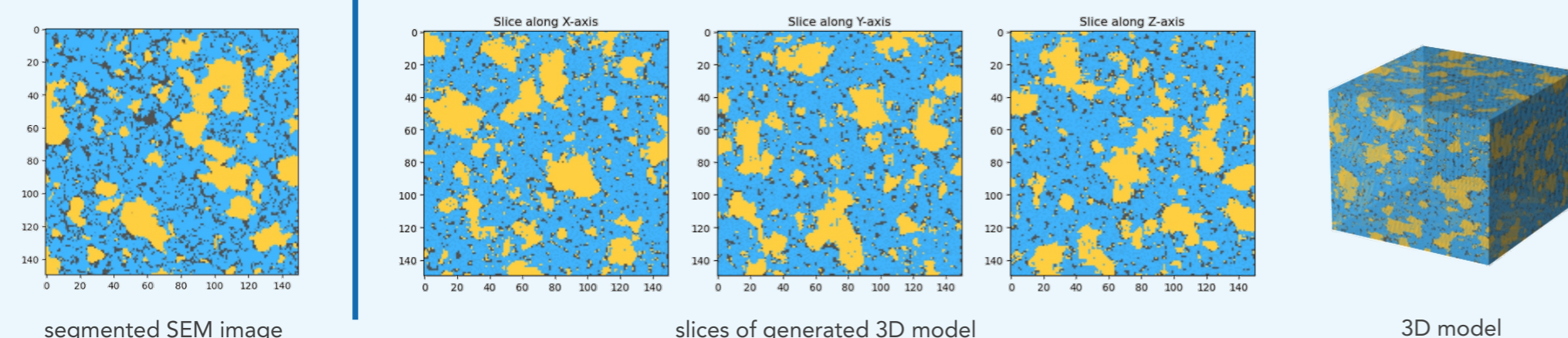
Inhomogeneous feature representation, as ViTs are optimized for natural images and learn gradients that emphasize edges and central objects, but SEM images are typically homogeneous⁽⁸⁾. Therefore, positional bias must be removed (work in progress, in cooperation with group from Sam Cooper, Imperial College London).



Construction of 3D Models from 2D Data

Transfer learning with pre-trained VGG19-model

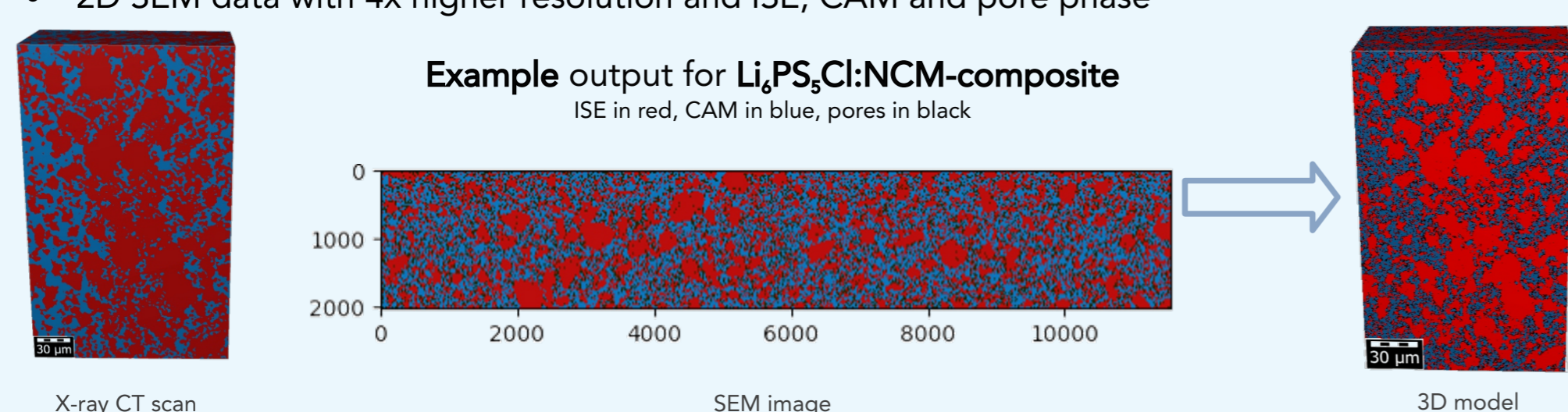
- features are extracted from 2D SEM image and random 3D model
- feature comparison by loss function followed by update for 3D model



Example output for $\text{Li}_3\text{PS}_4\text{-}0.5\text{LiI}:\text{Ni}_{0.83}\text{Co}_{0.11}\text{Mn}_{0.06}\text{O}_2$ -composite (70:30 wt% with 21% residual porosity)
ISE in yellow, CAM in blue, pores in black

Super-resolution⁽⁷⁾ from 2D SEM images and 3D X-ray sub- μ -computer tomography (CT) in cooperation with group from Sam Cooper, Imperial College London

- large 3D CT data set with poor resolution and no pore phase combined with
- 2D SEM data with 4x higher resolution and ISE, CAM and pore phase



References and Abbreviations

References

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4. Jiang, W. et al. *Adv. Energy Mater.* **2022**, *12*, 2103473.
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Abbreviations

- 2D, 3D: two-dimensional, three-dimensional
- BSE: Backscatter electron image
- CAM: Active material at positive electrode
- FIB: Focused ion beam
- ISE: Inorganic solid electrolyte
- SE: Secondary electron image
- SEM: Scanning electron microscopy
- VGCF: Vapor grown carbon fiber
- ViT: Vision transformer

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