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ABSTRACT:

High-Throughput Style Screening for Desired Electrode Microstructures

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This work presents a simulation framework for high-throughput screening of desirable microstructures. As motivation, we present a brief study of battery microstructural architecture optimization. Realistic 3D microstructures are reconstructed from voxel data. The voxel data can be easily modified, enabling rapid manipulation and making high-throughput investigation possible. The microstructure-level simulations are made computationally feasible by using the Smoothed Boundary Method to embed complicated microstructures in the computational domain. Additionally, our efforts toward an open-source microscale battery simulation software, titled BESFEM, are previewed.