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臺灣大學應用力學研究所

演　講　公　告

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主 講 人：游輝嘉(Hui-Chia Yu) 助理教授

Department of Chemical Engineering and Materials Science, Michigan State University

Department of Computational Mathematics, Science and Engineering, Michigan State University

講　　題： High-throughput, high-performance microstructure electrochemical simulation enabled electrode architecture design

摘　　要： 如附件

主 持 人： 陳志鴻副教授

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地　　點： 臺灣大學應用力學研究所 400 會議室

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High-throughput, high-performance microstructure electrochemical simulation enabled electrode architecture design.

Hui-Chia Yu
Department of Chemical Engineering and Materials Science, Michigan State University
Department of Computational Mathematics, Science and Engineering, Michigan State University

While the battery research community has been actively searching for high-performance electrode materials, the importance of electrode architecture is often overlooked. Specifically at high-rate cycling, the electrochemical processes occur at far-from-equilibrium conditions. This essentially means a battery's operational performance is indeed dictated by electrode microstructures. However, due to the dual layers of complexity of multiphysics-coupling and microstructural geometries, computational studies at microstructure level are poorly embraced. In this talk, we will first introduce an image-based numerical method that allows a facile implementation for electrochemical simulations of multiphysics processes in explicitly considered electrode complex microstructures. We will use literature thermodynamic and kinetic data in the simulations to unravel the complicated interactions between graphite and hard carbon particles, and how that affects the cycling behavior of the hybrid anodes. Next, thanks to the capability of rapidly implementing direct voxel-based simulations, we will demonstrate a high-throughput framework of high fidelity detailed, autonomous microstructures electrochemical simulations that allows to screen optimal secondary structure, e.g., tunnels, for high-rate charge of thick electrodes. As we are open sourcing this simulation framework, we believe this tool is greatly useful for battery developers and materials scientists.

Bio

Hui-Chia Yu joined MSU in 2017. He is jointly appointed in the Department of Computational Mathematics, Science and Engineering and the Department of Chemical Engineering and Materials Science. His expertise is simulating moving boundary problems, such as phase transformation and crack propagation, using the phase-field method or level set method. He also developed the smoothed boundary method for complex microstructure simulations, and applies the method to study various materials phenomena, such as electrochemical process in porous electrodes, solid and fluid mechanics, sintering process, and diamond growth.