

APS Scientific Computation Seminar Series

Speaker: Yijin Liu
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Title: Data-guided, Multi-scale, and High-dimensional Understanding of the Battery Degradation

Date: Monday, July 18, 2022

Time: 1:00 p.m. (Central Time)

Location: <https://argonne.zoomgov.com/j/1615356746>
Meeting ID: 161 535 6746
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Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract: Lithium-ion battery (LIB) is featured by structural and chemical complexities across a broad range of length and time scales. The studies of battery operation, degradation, and failure mechanisms require a thorough and systematic investigation from the structural, chemical, mechanical, and dynamic perspectives. Understanding and interpreting the big data generated by state-of-the-art experimentation in this research field need to leverage the novel computing developments [1-7]. In this talk, I will review my group's research activities in this field over the past few years. I will discuss the macro-to-nano hierarchy of a lithium battery cell. We utilize a suite of state-of-the-art X-ray techniques and develop data mining methods to harvest valuable information from the big data. We look into the morphological and structural defects and their electrochemical consequences from the electrode-level down to the atomic-scale. We demonstrate the effectiveness of our approach for understanding the detrimental effects, which, in turn, informs the next-generation battery material design. Finally, I will provide my perspective for the future developments in this field.

References:

- (1) J. Li, Y. Liu* et al., Science (2022) DOI: 10.1126/science.abm8962.
- (2) S. Tan, Y. Liu* et al., Nature Energy (2022) DOI: 10.1038/s41560-022-01020-x.
- (3) T. Fu, Y. Liu* et al., Advanced Functional Materials (2022) 2203070.
- (4) J. Li, Y. Liu* et al., Energy Storage Materials 45 (2022) 647-655.
- (5) Z. Jiang, Y. Liu* et al., Nature Communications 11 (2020) 2310.
- (6) G. Qian, Y. Liu* et al., ACS Energy Letters 6 (2021) 687-693.
- (7) Y. Mao, Y. Liu* et al., Advanced Functional Materials (2019) 1900247.