

The 136th GREEN Seminar



Data-Driven Electrolyte Discovery and Lifetime Prediction for Lithium Batteries

Chair: Dr. Shoichi MATSUDA(GREEN)

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Advanced lithium batteries require electrolytes that enable efficient ion transport, stable interfaces, and long cycle life. In this talk, I will present our data-driven approaches to electrolyte discovery and battery lifetime prediction. We first established physics-informed molecular descriptors that capture key solvation, coordination, and compatibility requirements for liquid electrolytes. By integrating these descriptors with DFT calculations and uncertainty-aware machine learning, we screened large chemical spaces and experimentally identified new electrolyte components. We are now extending this framework through a self-driving laboratory that autonomously formulates, evaluates, and learns from electrolyte candidates.

In parallel, we develop machine-learning models that predict long-term battery performance from early-cycle electrochemical data. By identifying degradation signatures before substantial capacity loss occurs, these models shorten the time required to assess electrolyte formulations. Integrating molecular screening, autonomous experimentation, and early lifetime prediction provides a closed-loop strategy for accelerating electrolyte development for lithium batteries.

Venue: Auditorium, 1F, NanoGREEN/WPI-MANA Bldg.,
Namiki-site

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