Accelerating Simulations of Kinetic Processes in Energy Materials with Machine Learning and Data Science

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Many energy storage and conversion devices rely on complex chemical and transport processes that tend to occur at buried materials interfaces that are often difficult to probe experimentally. Computational simulations of these processes can help elucidate interface behavior, but the associated structural and compositional complexity is difficult to address with conventional approaches. Likewise difficult is addressing the wide ranges of length and time scales involved, which span from atomic to microscale and beyond. Recently, machine learning and data science techniques have emerged as important companions to direct simulations to bridge scales and address needed complexities in ways that are inaccessible to human intuition. I will provide a few key examples of how we are using machine learning and data science methods within our LLNL LEAF Center to accelerate and interpret multiscale simulations of kinetic processes in materials relevant for energy storage and production. First, I will illustrate how we integrate machine learning-trained molecular simulations, microstructure analysis, and feature extraction from mesoscale simulations to understand multiscale factors that govern ion transport in solid-state batteries and hydrogen storage materials. I will highlight how the data science approaches have elucidated previously unknown relationships between composition and microstructure in determining performance of these devices. Next, I will show how materials training data from molecular simulations are being implemented in surrogate models and integrated into larger-scale kinetic evolution models to directly simulate changes in the surface oxide composition of metals in electrochemical operating environments. These models reveal emergent phenomena at much longer time scales compared to molecular dynamics, with implications for understanding durability of components in operating energy conversion devices.

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