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Molecular Simulation-Driven Digital Twin Optimization for Synchrotron Radiation Characterization of Solid-State Batteries

Thursday 29 August 2024 18:00 (15 minutes)

All-solid-state lithium-sulfur batteries are hailed as one of the most promising candidates in the realm of battery materials, boasting higher energy density, lower extraction costs, enhanced safety, and improved cycling performance. While synchrotron radiation-based characterization techniques offer insights into the elemental distribution, bonding situations, and local coordination environments of all-solid-state lithium-sulfur batteries, capturing dynamic molecular functional motion remains a critical challenge. This project introduces a novel digital twin methodology to explore the molecular mechanisms governing discharge processes and the dynamic evolution of interfaces across multiple spatiotemporal scales in all-solid-state lithium-sulfur batteries using synchrotron radiation characterization systems. Initially, a potential function is trained for the all-solid-state lithium-sulfur battery system based on deep potential methods, facilitating the construction of an efficient, multiscale molecular simulation digital space conducive to real-time interaction. Additionally, a physical space dedicated to synchrotron radiation characterization experiments for all-solid-state lithium-sulfur batteries is successfully established. Furthermore, a real-time interactive integration of the molecular simulation digital space and the synchrotron radiation characterization physical space is achieved, forming a digital twin system platform, which enables microscopic characterization of multi-stage discharge reactions in all-solid-state lithium-sulfur batteries. Finally, it offers novel insights into the research paradigm of synchrotron radiation characterization for all-solid-state lithium-sulfur batteries.

I plan to submit also conference proceedings

Yes

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