Interpretable Tree-Based and Graph Neural Network Approaches for Novel Solid State Electrolyte Design

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All-solid-state batteries with Li metal anode can address the safety issues surrounding traditional Li-ion batteries as well as the demand for higher energy densities. However, the development of solid electrolytes simultaneously possessing high ionic conductivity and good chemical and electrochemical stabilities has proven to be a challenge. I will present our informatics approach to explore the Li compound space for promising solid electrolytes using high-throughput multi-property screening and interpretable machine learning. This is accomplished through the generation of a large database of battery-related materials properties of Li compounds. We use tree-based ensemble learning methods and graph neural network approaches to accurately learn relationships between crystal structures and corresponding thermodynamic and kinetic properties, with interpretability being a major focus. Our models give us the ability to enable rapid discovery and design of novel solid-state battery chemistries.