Advances in Na-Ion Battery Cathode Materials: Comparison of DFT and Machine Learning Approaches

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Abstract

Over the past decades, energy storage technologies have advanced significantly, driven by the increasing demand for efficient and sustainable energy solutions. Challenges related to the lithium supply chain, costs, and safety issues have led to the investigation of alternative battery chemistries. As a result, research into replacing widely used lithium batteries with sodium-ion batteries has garnered growing interest. In this study, we present a research on diverse cathode material compositions for Na-ion batteries, utilizing first-principles calculations within the AiiDA framework. We employed crystal graph convolutional neural networks, demonstrating the capability of these machine learning algorithms to predict the formation energy of hypothetical materials, as determined by density functional theory, and subsequently estimate their redox potential. This innovative materials discovery approach is significantly faster compared to traditional physics-based computational methods.