Artificial Intelligence/Machine Learning Advances in Screening Lithium-ion Battery Material Guide to Electrodes and Electrolytes

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This paper aims to demonstrate the advancements in utilizing artificial intelligence/machine learning (AI/ML) models to screen materials for lithium-ion batteries (LIBs). These advancements primarily focus on active electrodes and solid electrolytes, which are crucial for the next generation of LIBs. Consequently, extensive research and numerous papers have been published, showcasing various ML models used in LIB materials design and synthesis. The mathematical descriptors, which are key elements for ML models, vary depending on the target, including Fingerprints, SMILES, Potentials, Weighted Graph, Coulomb Matrix, Bag of Bonds/Fragments, and 3D Geometry [1]. Despite this, complete atomic representations of broad chemical spaces are still being researched, and developing a general model for all circumstances remains challenging. Therefore, a summary and guide of which model is suitable for each case of utilizing AI/ML methods is essential, and important in addressing the challenges of AI/ML accelerators in battery design. By integrating computational models with experimental data, AI/ML methods streamline the discovery process, predict material behavior, and facilitate the development of next-generation lithium-ion batteries. The potential impact of these technologies on sustainable energy storage solutions is significant, with promising breakthroughs in energy density, charging rates, and overall battery lifecycle management [2].

Keywords: Artificial Intelligence (AI), Machine Learning (ML), Lithium-ion batteries (LIBs), Electrode materials, Solid electrolyte, ML descriptors

References

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