Beyond lithium: Enhancing material development by artificial intelligence

Dr. Jesús I. Medina Santos[1], Prof. Valeria Nicolosi[1]
[1]Trinity College Dublin, College Green, D02 W9K7, Dublin, Ireland

medinasj@tcd.ie

Lithium-ion batteries are integral components in a wide range of devices, from mobile phones to electric vehicles. However, the growing demand for these batteries prompts the need to explore viable alternatives. Among these options, sodium-based batteries have attracted considerable interest due to the more abundant global supply of sodium [1]. Since their operating principles closely resemble those of lithium-based batteries, certain materials currently used in lithium systems could potentially be repurposed for sodium-based applications.

However, materials such as graphite demonstrate that not every lithium-compatible material is equally suitable for sodium [2]. Identifying lithium-based materials that can be successfully adapted to sodium systems presents a significant challenge, especially given the extensive volume of lithium battery research. In this context, artificial intelligence (AI) stands out as a powerful tool for extracting and analyzing the wealth of information contained in scientific literature.

Previous studies have leveraged natural language processing (NLP) techniques to extract and classify material properties from scholarly documents [3]. While NLP can efficiently consolidate textual data, the resulting information often requires further interpretation. To address this, machine learning (ML) methods have been employed to handle complex, high-dimensional data in fields like genomics, environmental science, and materials research. In the energy sector, for instance, deep learning models trained on lithium-based materials have been used to predict average voltages in sodium batteries [4].

Our approach integrates these advanced AI techniques into a comprehensive workflow (**Figure 1**). First, we utilize a large language model to extract relevant information from the literature. Next, we apply ML algorithms to classify lithium-based materials according to their potential suitability for sodium batteries. Finally, we plan to characterize their physical and electrochemical properties, providing a pipeline that seamlessly bridges data extraction, analysis, and materials development.

References

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Figures

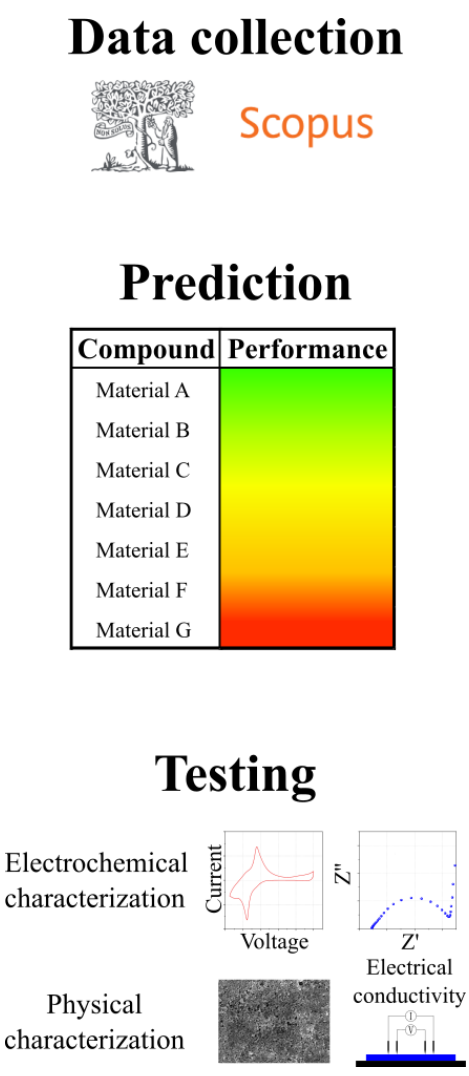

Figure 1. Workflow for material development.