Chapter 9
Machine Learning–Driven Optimization of Battery Materials via Quantum Computing

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ABSTRACT

This research explores the possible synergy between machine learning algorithms and quantum computers to advance the progress of battery materials. To streamline the investigation of materials suitable for high-performance batteries, we introduce a novel framework that employs optimization approaches guided by machine learning. This comprehensive collection of properties for Mg-ion and Li-ion battery electrode materials allows machine learning algorithms to accurately forecast their voltage, capacity, and energy density. This advancement is anticipated to expedite the exploration of more effective materials for energy storage. The results showed a strong relationship between energy density and capacity, but no such relationship was found between average voltage and the aforesaid factors. Implementing this technique in high-throughput systems has the potential to greatly expedite breakthroughs in computational materials research.

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INTRODUCTION

Leung, K 2012, Christo Ananth 2015 This research, focusing on Machine Learning (ML), is mostly concerned with batteries. To be more specific, a new method has been developed to forecast the electrochemical properties of specific electrode materials, such as their potential, capacity, and energy density. The introduction will give an overview of the research's context and settings. This chapter describes the thesis' reasoning, scope, and structural structure. The motivation for this research derives from the desire to build batteries with more capacity, lower costs, and longer lifespans. The batteries will be used for both mobile and fixed applications.

P.S. Ranjit 2012 The topic of battery research has recently received a lot of attention and resources, with an increasing trend towards the use of 3-D printed batteries. Batteries are quite complex. Although extensive research has been undertaken on electrochemical cells, the search for batteries with ever-expanding property boundaries will continue indefinitely. There is a greater need for superior batteries today than in the past. For example, the number of electric vehicles in use has nearly doubled in the last year, reaching more than 5.1 million. Our goal is to achieve a 30% growth in electric vehicle (EV) sales by 2030, excluding two-wheelers. This is because this industry accounts for more than 25% of all worldwide greenhouse gas emissions. The predicted yearly sales of electric vehicles (EVs) will exceed 43 million, with a global supply of more than 250 million EVs. The expanding need for battery technology is driven by the market's desire for higher capacity and energy density batteries, as well as the growing number of electric vehicles.

DeGroat, 2024 Voltage, energy density, specific energy or capacity, flammability, operational temperature range, shelf life or self-discharge, cost, and global consumer distribution are among the most important cell features. These qualities are primarily determined by the composition of the batteries. Because of the complexity of the chemical processes involved, it is critical to develop predictive modeling methods to improve compositions and performance. The approaches presented in this publication can forecast the physical stability, energy density, specific energy, and voltage of possible electrode materials.

G. Ceder 2006 Currently, molecular dynamics (MD) simulations, machine learning, and density functional theory (DFT) are critical tools for progressing theoretical parts of battery research. Over the last two decades, computational materials science has generated a large amount of data, including both theoretical and research information. The advancement of DFT (Density Functional Theory) and MD (Molecular Dynamics) simulations, together with increased computing capacity, are critical factors leading to the phenomena. By cooperating with large programs such as the Materials Genome Initiative, these technologies, along with high-throughput (HT) techniques, have created and made large volumes of data available. Molecular dynamics (MD) simulation is ideal for studying the atomic-level properties of solid-state materials, whereas density functional theory (DFT) is an important modeling tool in materials research.

P. Johnson 2017 The traditional and research methodologies for improving battery technology include costly and time-consuming synthesis activities. Due to the costs associated with mass production, many applications are typically limited to using only a single type of material. As a result, a material change is called revolutionary due to its unusual nature. The long-term viability of a technology is inextricably linked to the quality of the first materials used for its development. Emerging developments in specialized technologies frequently need the development of innovative materials with relevant properties for those technologies. Choosing appropriate materials is a difficult task due to the relevance of issues such as compatibility and toxicity.