A REVIEW OF QUANTUM MODELING AND SIMULATION APPROACHES FOR LITHIUM-ION BATTERIES

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ABSTRACT

Lithium-ion batteries (LIBs) are critical in modern energy storage systems, powering everything from portable electronics to electric vehicles. However, optimizing their performance and longevity remains a significant challenge. Quantum simulation has emerged as a promising tool to model the complex electrochemical processes within LIBs, offering insights into charging mechanisms and degradation pathways that classical methods struggle to capture. This paper presents a systematic literature review of quantum simulation techniques applied to LIBs, focusing on charging and degradation modeling. We analyze the current state-of-the-art, identify key techniques, and discuss the potential of quantum computing to revolutionize battery research. Our findings highlight the advantages of quantum simulations in capturing quantum mechanical and quantum chemistry effects which are critical for accurate battery modeling. Trends in the literature suggest a move toward algorithm optimization, integration with classical methods, and the development of quantum-inspired techniques.

Keywords: quantum simulation, battery materials, lithium-ion batteries, charging modeling.

1 INTRODUCTION

Lithium-ion batteries (LIBs) have become the foundation of modern energy storage due to their high energy density, long cycle life, and relatively low self-discharge rates. Despite their widespread adoption, challenges such as capacity fade, thermal instability, and charging inefficiencies persist. Traditional computational methods, including density functional theory (DFT) and molecular dynamics (MD), have provided valuable insights but are often limited by their computational cost and inability to fully capture quantum mechanical phenomena [1, 2].

Quantum simulation, using the principles of quantum mechanics, offers a novel approach to model the complicated processes within LIBs. By simulating the quantum states of electrons and ions, these methods can provide a more accurate representation of the electrochemical reactions occurring during charging and discharging cycles. This paper aims to systematically review the existing literature on quantum simulation of LIBs, with a particular focus on charging and degradation modeling.

Quantum computing exploits the principles of quantum mechanics to process information to solve problems that are too complex for classical computers [3]. Unlike classical bits, qubits possess the unique ability to represent numerous possible combinations of 0 and 1 at the same time. This simultaneous existence in multiple states is a phenomenon referred to as superposition. This property enables the processing of information in a parallel and exponentially expanded manner compared to classical computers [3]. In particular, quantum computing offers a promising approach for simulating complex systems and behaviors that are challenging for classical methods.

A quantum state is any possible state of a quantum mechanical system or quantum hardware. There are numerous examples of quantum mechanical two-level systems in nature that potentially could serve as qubits. The electronic states of an ion and the electron spin of an atom implanted in silicon serve as examples [4]. In quantum computing, we can generate pairs of qubits that are entangled, which means that changing the state of one of the qubits will instantly change the state of the other one. Qubits can have the value $|0\rangle$ and $|1\rangle$ or be in a state other than $|0\rangle$ or $|1\rangle$. A particular quantum state can be represented by a wave function $\psi(x)$ as follows:

$$\big|\psi\big\rangle = \alpha\big|0\big\rangle + \beta\big|1\big\rangle, \text{ where } \alpha, \beta \in \mathbf{C} \text{ and } \alpha^2 + \beta^2 = 1. \tag{1}$$

Quantum simulators play an important role in bridging the theoretical and practical aspects of quantum computing. Recent developments in quantum hardware, such as superconducting circuits and trapped ions, have facilitated the development of quantum simulators that mimic the behavior of quantum computers [5]. In this paper, we explore the advancements in quantum modeling and simulation techniques for LIBs addressing the limitations of classical computational methods in capturing quantum effects, non-linear charge dynamics, and material interactions. The key contributions of this work include a systematic review of the literature on quantum simulation of LIBs to especially identify the tools and techniques. The remainder of the paper is structured as follows: Section 2 provides an overview of the research methodology, Section 3 presents the results, Section 4 provides a discussion on the findings and Section 5 presents the conclusion and future research directions.

2 METHODS

We conducted a systematic review to identify the relevant studies on quantum simulation of LIBs in the literature [6]. We defined the research questions and objectives to identify the trends and classification of the studies as well as to understand what methods and tools have been used in these studies. All queries were executed in January 2025; and rerun to include papers until 2 February 2025. We did not put any date restrictions, so the searches included all years. We mainly excluded the gray literature in this survey; however, we included a few important developments and advances in the field in the Introduction section.

In this study, relevance to quantum simulation is handled broadly to cover more papers. For example, studies that address key atomic scale processes (such as cathode behavior or molecular design) during charging or discharging, even if they do not simulate an entire charging cycle explicitly, are also included.

2.1 Data Repositories and Keywords

We selected three databases as ACM Digital library, Scopus and IEEE Xplore. In the first step, we had 261 results from these three databases. Additionally, we cross checked the results with Google Scholar based on only title search, due to its limited search filters and large volume of results. Although there were 24 papers in Google Scholar list, eventually we only included one paper from this search in the screening round as most of the papers were either irrelevant or already included in the list.

We defined the keywords and search strings to cover the studies about quantum modeling and simulation of LIBs, specifically for charging process or degradation. We also established the inclusion/exclusion criteria to filter the relevant studies. The selected keywords were "quantum" AND ("simulation" OR "model") AND battery. Some of the databases automatically included the alternative search terms as "modeling", "modelling", "simulate", "simulating", "batteries", etc. or allowed using wildcards (*). If not included, we performed the searches manually. We mainly searched the keywords in the title, abstract, or author keywords to limit the number of results and retrieve the most relevant papers.

2.2 Review Process

We executed the search strategy in selected online databases to find the papers based on title, abstract and keyword search. We used the export feature of the databases to retrieve and collect the results with papers' metadata including title, publication year, abstracts, keywords, etc. Then we merged the raw data from the four databases where 285 papers were identified (n=285). After the identification step, 123 duplicates and 8 non-paper entries such as conference proceedings information are removed too (n=154).

Figure 1 shows the steps in the review process and number of papers after each round. During the eligibility step, we removed the irrelevant papers based on title and abstract screening if papers are related to quantum batteries or not in the context of quantum simulation of lithium-ion batteries (e.g. papers about planning of battery energy storage systems) (n=78). Inclusion criteria are as follows: (a) Papers are related to quantum simulation, (b) Papers focus on Li-ion battery simulation, and (c) Papers are not related to quantum batteries.

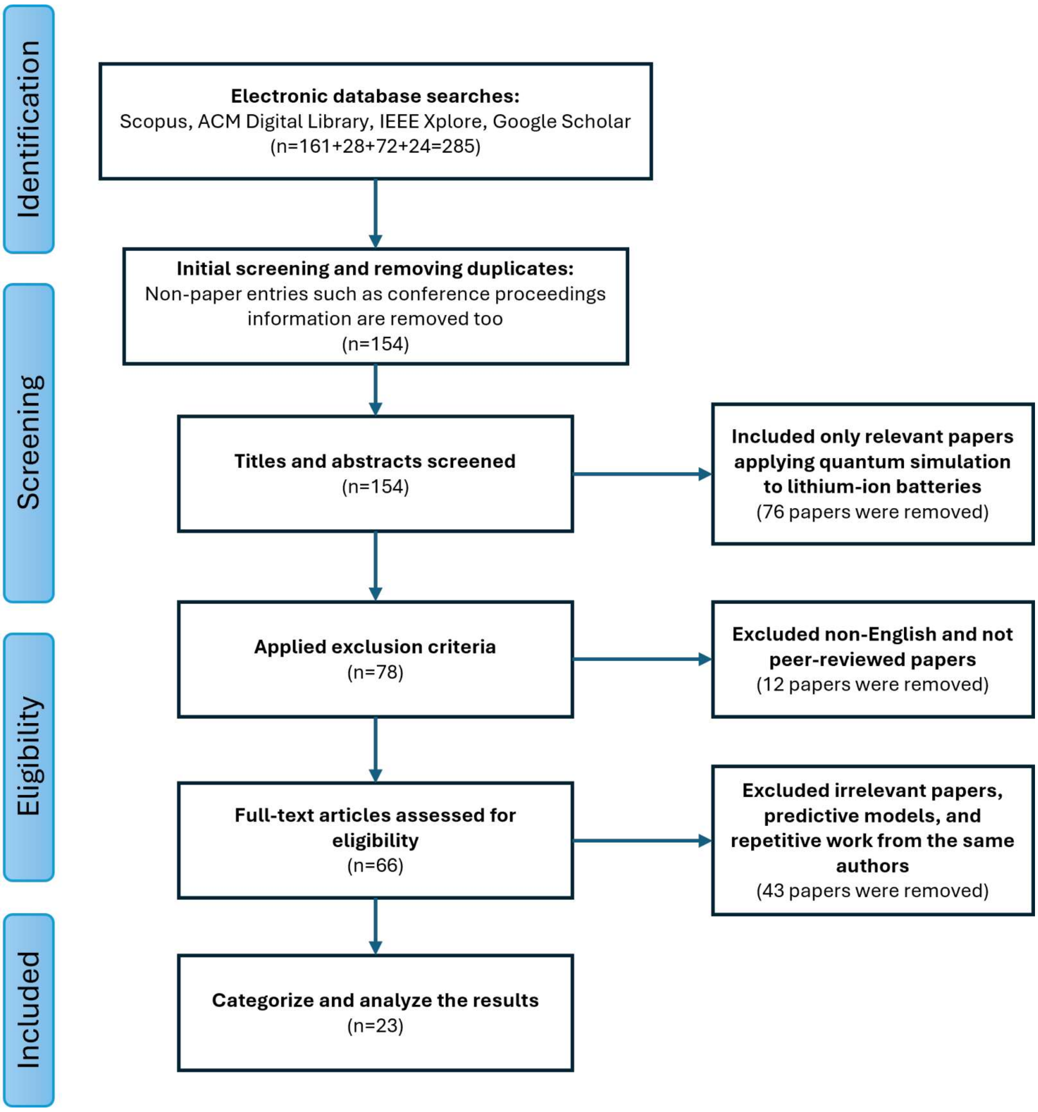

Figure 1: Steps in the review process.

After that, we applied the exclusion criteria to remove unpublished work or pre-prints as well as papers that are not written in English. So, 8 papers were removed because they were either not peer-reviewed papers or not written in English (n=66). Exclusion criteria are as follows: (a) Not peer-reviewed papers, pre-prints, theses or unpublished work, and (b) Papers that are not written in English.

Finally, we assessed the full-text articles on the remaining papers to refine the selection. 43 papers were removed after detailed analysis to exclude irrelevant papers (e.g. papers focusing on prediction models rather than simulation) or repetitive work from the same authors, and we completed the review map and analyzed the results (n=23). Table 1 presents the list of the final selected papers whereas there were 23 papers (20 journal and 3 conference papers). Quantum techniques are explained in the next section.

Table 1: List of the papers included in the review

Paper Ref	Year	Source (where it is published)	Quantum Techniques
[7]	1997	Journal of the Electrochemical Society	First principles quantum chemistry
[8]	2011	CMES - Computer Modeling in Engineering and Sciences	Hybrid, DFT
[9]	2011	Journal of Physical Chemistry B	Quantum mechanics, AIMD
[10]	2014	Int. Conference on Information Technology and Electrical Engineering	QNN
[11]	2016	Physical Chemistry Chemical Physics	Quantum chemical simulation, ANN
[12]	2017	ChemSusChem	First-principles, DFT
[13]	2019	Nature Communications	DFT, MD simulations
[14]	2020	Energy Proceedings	Machine learning, QPSO
[15]	2021	Journal of Chemical Physics	First principles quantum mechanics, DFT
[16]	2021	Journal of Physical Chemistry Letters	Hybrid, quantum mechanics-based reaction dynamics, AIMD
[17]	2022	Applied Soft Computing	Machine learning, quantum assimilation
[18]	2022	Journal of Energy Storage	QPSO
[19]	2022	Physical Review A	Quantum computing
[20]	2023	Applied Soft Computing	Machine learning, quantum fuzzy neural network
[21]	2023	IEEE Green Technologies Conference	Machine learning, quantum computing, QNN
[22]	2023	Journal of Power Sources	Hybrid, DFT
[23]	2023	Quantum	Quantum computing and simulation
[24]	2024	Energy Reports	Quantum computing, variational quantum algorithm
[25]	2024	IEEE Int. Conference on Quantum Computing and Engineering	Quantum computing
[26]	2024	Ionics	Hybrid, QPSO
[27]	2024	Ionics	QPSO
[28]	2024	Scientific Reports	Reactive step MD
[29]	2025	Canadian Journal of Chemical Engineering	First principles quantum chemistry

We systematically extracted the following information from the selected papers: publication details (title, authors, year, source title, publisher, document type, etc.), simulation techniques, software tools, battery chemistry, research focus and main contributions.

3 RESULTS

Quantum computing offers unique capabilities for battery simulation, ranging from fundamental material design to optimization and predictive maintenance. While some methods are already being tested on near-term quantum hardware, full-scale implementation of these techniques requires fault-tolerant quantum computers [30]. Although quantum computing has shown significant theoretical and experimental progress, current quantum hardware is in the early stages of development, with noisy intermediate-scale quantum (NISQ) computing technology being the most common. There is an increasing number of publications in the last decade, and recent papers use quantum computing techniques and machine learning approaches. Figure 2 shows the number of publications per year in the last decade.

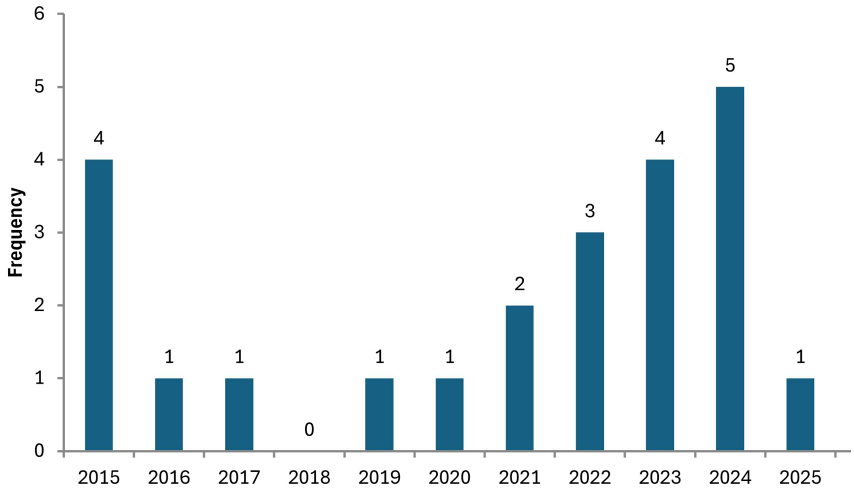

Figure 2: Number of publications in the last decade.

3.1 Techniques Used in Quantum Simulation of Li-ion Batteries

The literature review indicates a growing interest in applying quantum simulation techniques to model the complex electrochemical processes within LIBs [23]. A key trend identified in the literature is the increasing focus on hybrid quantum-classical approaches, which aim to balance computational cost and accuracy by using quantum methods for critical components of the simulation while relying on classical techniques for large-scale modeling [22]. Algorithmic advancements, such as error mitigation techniques and circuit optimization for quantum simulations, are also gaining attraction, addressing current limitations in quantum hardware. Additionally, several studies suggest that quantum computing has the potential to enhance machine learning models for battery health prediction for more efficient battery management systems [17, 20].

The literature on quantum simulation of LIBs relies on a diverse range of datasets, encompassing both experimental and computational data [31]. Some recent works incorporate machine learning-assisted quantum simulations, where large-scale battery aging datasets help train quantum-enhanced predictive models. NASA's battery datasets are highly used in the literature [32]. While existing datasets provide a solid foundation for quantum modeling, the limited availability of high-fidelity quantum-computed battery datasets remains a challenge, highlighting the need for further benchmarking and standardization in the field.

Various computational techniques have been employed to model the complex electrochemical processes in LIBs. These approaches can be broadly categorized into traditional computational methods, which rely on classical physics and quantum chemistry approximations, and quantum computing methods, which use quantum mechanical principles on quantum hardware to achieve higher accuracy and efficiency in battery simulations. Figure 3 shows the most commonly used techniques that are explained in the following sections.

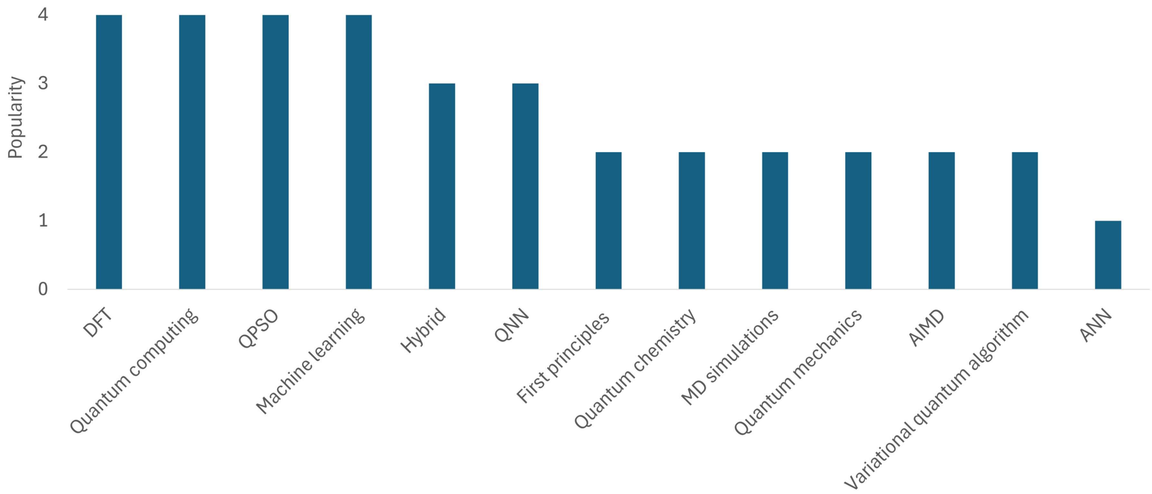

Figure 3: Most commonly used techniques in the selected studies.

3.1.1 Traditional computational methods

Traditional computational methods have been widely applied in the literature. However, they face limitations when dealing with the quantum effects and non-linear processes involved in battery operation [19]. DFT is a quantum mechanical modeling technique used to investigate the electronic structure of atoms, molecules, and solids. This method considerably simplifies the computational challenge by treating electron density as the primary variable while still delivering reliable accuracy for a broad spectrum of systems. DFT has become an essential tool in physics, chemistry, and materials science due to its balance between computational efficiency and precision [33]. MD is a simulation approach used to investigate the temporal evolution of atomic and molecular systems. By applying the principles of classical mechanics, MD computes the trajectories of individual particles within a system [28]. This method enables researchers to explore the structural, thermodynamic, and dynamic properties of materials, bio molecules, and other complex systems by observing how particles interact and move over time.

First principles or ab initio quantum chemistry methods encompass a set of computational techniques that solve the electronic Schrödinger equation based solely on fundamental physical principles, without recourse to empirical data [29]. The term "ab initio" (Latin for "from first principles") highlights the fact that these methods rely exclusively on universal physical constants, along with the precise positions and number of electrons in the system. This approach allows for the detailed modeling of chemical reaction mechanisms, kinetics, and thermodynamics directly from quantum mechanics.

Ab initio Molecular Dynamics (AIMD) simulations involve quantum mechanical calculations of atoms and molecules' dynamics [28]. AIMD is employed to simulate battery systems at the atomic level, particularly useful for studying ionic conductivity, electrode reactions, and degradation due to ion migration or phase transitions within materials under operational conditions.

Quantum Mechanics/Molecular Mechanics (QM/MM) is a hybrid computational method used to simulate complex systems by combining the accuracy of quantum mechanics (QM) with the efficiency of molecular mechanics (MM) [22]. In QM/MM, the system is divided into two regions: a QM region, where electronic structure calculations (e.g., using DFT) are performed to model processes involving bond breaking/formation, charge transfer, or other quantum effects; and an MM region, where classical force fields are used to describe the remaining part of the system, such as the surrounding solvent or protein environment.

Other hybrid techniques also exist that apply other approaches. For example, Liu et al. use Monte Carlo Simulated Annealing to optimize the ReaxFF force field parameters [16]. Quantum Monte Carlo (QMC) is a stochastic quantum simulation technique used for highly accurate energy calculations and correlation effects in battery materials.

3.1.2 Quantum computing methods

Recent progress in quantum computing has encouraged the development of quantum simulation techniques that hold promise for overcoming these limitations. While these quantum-based approaches are still in the research phase, they hold great promise for advancing battery technology by providing deep insights into material behavior that traditional classical models cannot fully capture.

Quantum computing and machine learning methods are being investigated for their potential to accelerate the discovery of new materials and predict charge-transfer processes in batteries, especially for advanced energy storage technologies like quantum batteries. Most commonly used techniques in quantum computing based studies are as follows:

- *Variational Quantum Eigensolver (VQE)* is a hybrid quantum-classical algorithm that controls quantum circuits to approximate the ground state of a Hamiltonian. It has been used to study the electronic properties of cathode materials, offering insights into charge transfer mechanisms [25, 34].
- *Quantum Phase Estimation (QPE)* is a quantum algorithm that can precisely determine the eigenvalues of a Hamiltonian. While computationally demanding, it has shown promise in simulating the quantum dynamics of lithium ions during charging cycles [23, 19].
- *Quantum Neural Networks (QNN)* and other quantum-inspired machine learning models are also commonly used in the recent years [10, 21, 20]. QNN models are inspired by the structure of Artificial Neural Networks (ANN), adapting concepts like neurons, layers, and activation functions into the quantum domain. Although, these methods utilize ideas from quantum computing, they may not directly simulate the charging process at the quantum level. Most of the machine learning based studies present predictive models or data-driven monitoring systems.
- *Quantum Particle Swarm Optimization (QPSO)* is a quantum-inspired optimization algorithm used for battery parameter estimation, charge optimization, and machine learning models for battery health monitoring. Each particle updates its position based on the global best solution and quantum potential well [18, 26, 27].
- *Quantum Annealing* is a quantum optimization technique used for battery design, scheduling, and energy storage management [21, 34]. It encodes an optimization problem into a quantum system that evolves toward the lowest energy state.

3.2 Charging and Degradation Modeling

Quantum simulations have provided new perspectives on the charging mechanisms of LIBs. For example, quantum simulations have revealed the importance of electron correlation in determining the charge distribution within cathode materials. This has implications for the design of high-capacity cathodes with improved charging efficiency. Additionally, quantum simulations have captured the quantum mechanical nature of lithium-ion diffusion, highlighting the role of quantum tunneling in ion mobility [34, 25, 35]. This has led to the development of more accurate models of ion transport within the electrolyte.

Degradation in LIBs is a complex process influenced by factors such as solid-electrolyte interphase (SEI) formation, lithium plating, and mechanical stress [28]. Quantum simulations have provided insights into the formation and growth of the SEI layer, which is critical for battery longevity.

3.3 Simulation Software and Tools

Quantum simulations of battery systems, including their charging behavior and degradation mechanisms, are a rapidly evolving field. These simulations aim to model the atomic and electronic structure of materials at a fundamental level, offering insights that can complement classical battery modeling. Some tools and software platforms that are commonly used for quantum simulations in battery research include:

- *Quantum ESPRESSO* is an open-source suite for quantum simulations of materials based on DFT [25, 23]. It is widely used for electronic structure calculations, which are essential for understanding the properties of battery materials at the quantum level [36].
- *VASP (Vienna Ab-initio Simulation Package)* is a quantum simulation tool that performs ab-initio calculations based on DFT [8]. It is used to model the electronic properties of materials, allowing for deep insights into the atomistic mechanisms of battery operation and degradation.
- *Gaussian* is a computational quantum chemistry software that provides quantum mechanical simulations for a wide range of molecular systems [13]. It is primarily used to calculate electronic structures and reaction pathways.
- *Q-Chem* is a computational quantum chemistry software suite that uses quantum mechanical methods to simulate electronic structure, reaction dynamics, and other properties of materials [2].

Quantum computing platforms like IBM Qiskit [37] or Google Cirq [38] also offer hybrid quantum-classical approaches for simulating complex chemical reactions and materials properties, though the application to battery research is still emerging [21, 24, 35].

These quantum simulation tools are primarily used for studying the atomic and electronic level properties of battery materials, helping researchers understand fundamental phenomena such as ion transport, charge/discharge cycles, electrochemical reactions, and degradation mechanisms like phase changes. Additionally, several software tools and platforms are commonly used for the hybrid simulation of charging behavior, degradation, and performance of batteries. Some of the widely used ones include:

- *MATLAB*, particularly when combined with Simulink, provides a comprehensive environment for modeling and simulating battery systems. With tools like the Battery Pack Model Builder or Simscape Battery toolbox, users can model battery dynamics, including charging/discharging cycles and degradation mechanisms [18, 20, 27].
- *COMSOL Multiphysics* is a multiphysics simulation software that offers modules for battery modeling. It allows for the simulation of electrochemical processes, thermal management, and mechanical stress, making it suitable for studying charging, degradation, and related phenomena [2].
- *ANSYS* provides several tools for battery modeling, including capabilities for simulating electrochemical, thermal, and mechanical aspects of batteries. Its software suite is used to assess battery performance and degradation due to factors such as temperature and charge cycles [2].

- *PyBaMM (Python Battery Mathematical Modeling)* is an open-source framework for simulating battery systems. It enables efficient simulations of battery performance and aging, accelerating battery design and innovation [2, 39].

There are also other modeling techniques and tools for classical simulation of batteries but these are not covered in this study [2, 32].

4 DISCUSSION

The reviewed literature reveals both promising advancements and persistent challenges. On the one hand, quantum computing based simulation methods have shown potential for delivering higher accuracy in electronic structure calculations and for handling complex, non-linear interactions within battery systems. The polynomial scaling of quantum algorithms, compared with the exponential scaling observed in some classical methods, represents a significant advantage.

However, these advantages come with substantial challenges. Many studies emphasize the high computational cost and resource requirements (e.g., large numbers of logical qubits and extensive gate operations) that currently limit the practical implementation of these quantum simulations. Error mitigation and fault-tolerance remain critical challenges. In addition, integration of quantum simulation outputs with classical battery management systems is an area that requires further research.

Trends in the literature indicate a growing focus on hybrid quantum-classical methods, which appear to offer a balanced approach in the near term. There is also increasing interest in algorithm optimization and the development of quantum-inspired techniques that can bridge the gap until fully scalable quantum computers become available.

Despite the comprehensive scope of this survey, several limitations should be acknowledged. First, the study relies on publicly available research papers, which may introduce publication bias, as certain findings or proprietary developments in quantum battery simulations may not be disclosed. Papers not published in peer-reviewed venues (e.g. conferences or journals) are not included in the review. So, abstracts, theses, and pre-prints are removed from the list. Only papers written in English are included in the final list. We checked Springer database as well, but we could only apply title-based search due to the limitations of the search filters. There were 10 results which were not related to our research questions, or the results were too generic, so this database was excluded in this review. Hence, while efforts have been made to include a wide range of quantum computing techniques, the rapidly evolving nature of the field means that emerging algorithms and hardware advancements may not be fully captured.

Additionally, the comparison of quantum and classical methods is constrained by variability in computational resources and hardware limitations, as many quantum algorithms remain in theoretical or early experimental stages. Finally, practical applications of quantum simulations for battery research are still limited by the noise and error rates of current quantum hardware, making direct experimental validation challenging.

5 CONCLUSION

Quantum simulation represents a transformative approach to modeling LIBs, offering unprecedented insights into charging and degradation processes. Despite the promise of quantum simulation, several challenges remain including scalability and experimental validation. While challenges remain, the potential of quantum computing to revolutionize battery research is undeniable. Hybrid quantum-classical approaches, combining the strengths of both paradigms, may offer a practical path forward. As quantum hardware and algorithms continue to advance, we anticipate significant progress in the development of next-generation LIBs with enhanced performance and longevity.

While quantum simulation techniques show great potential, hardware limitations, scalability challenges, and algorithmic inefficiencies remain significant barriers to widespread adoption. Future studies could address these limitations by incorporating real-time benchmarking of quantum methods, allowing for direct comparisons with classical approaches in terms of accuracy and computational efficiency. Additionally, the development of hybrid quantum-classical frameworks will be crucial for making quantum simulations more practical.

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