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# THEORETICAL INSIGHTS INTO THE ELECTROCHEMICAL PROPERTIES OF IONIC LIQUID ELECTROLYTES IN LITHIUM-ION BATTERIES

Leila Maftoon-Azad

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# Theoretical Insights into the Electrochemical Properties of Ionic Liquid Electrolytes in Lithium-Ion Batteries

This book provides a concise overview of the use of ionic liquids as electrolytes in lithium-ion batteries (LIBs) from a theoretical and computational perspective. It focuses on computational studies to understand the behavior of lithium ions in different ionic liquids and to optimize the performance of ionic liquid-based electrolytes. The main features of the book are as follows:

- Provides a thorough understanding of the theoretical and computational aspects of using ionic liquids as electrolytes in LIBs, including the evaluation and reproducibility of the theoretical paths.
- Covers various computational methods such as density functional theory, molecular dynamics, and quantum mechanics that have been used to study the behavior of lithium ions in different solvents and to optimize the performance of ionic liquid-based electrolytes.
- Discusses recent advances such as new computational methods for predicting the properties of ionic liquid-based electrolytes, new strategies for improving the stability and conductivity of these electrolytes, and new approaches for understanding the kinetics and thermodynamics of redox reactions with ionic liquids.
- Suggests how theoretical insights can be translated into practical applications for improving performance and safety.

This monograph will be of interest to engineers working on LIB optimization.

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# Preface

In the name of God, the merciful, the compassionate.

Lithium-ion batteries (LIBs) have become ubiquitous in portable electronics, electric vehicles (EVs), and grid-scale energy storage systems due to their high energy density, long cycle life, and low self-discharge rate. While they have revolutionized technology and facilitated the widespread adoption of EVs and renewable energy sources, they are not without limitations. Safety concerns, limited energy density, and challenges related to the use of ionic liquid (IL) electrolytes have prompted the need for further research and development in this field.

In response to these limitations, researchers have turned to computational methods to gain a deeper understanding of the fundamental processes that govern the behavior of LIBs. This has led to significant advances in the field, enabling the accurate prediction of key properties and the identification of potential solutions to address existing challenges. However, the use of IL electrolytes in LIBs presents its own set of challenges, including safety concerns, high cost, and limited scalability.

To address these issues, researchers have explored various theoretical approaches, such as modifications to the chemical structure of ILs and their combinations with other materials. While these efforts have shown promise, there is a need to thoroughly evaluate the validity, data management, and reproducibility of the theoretical approaches used in these studies. By establishing a set of guidelines for validating, managing, and reproducing theoretical approaches, researchers can contribute to a more robust and reliable field of LIB research.

The potential of LIBs as an efficient energy storage system is undeniable, and ongoing research and enhancement strategies are essential to further improve their energy and power density. By addressing the current limitations and challenges, researchers can pave the way for the continued advancement and widespread adoption of LIBs in various energy storage and conversion applications. In this work, we provide an overview of the issues that have been associated with the use of ILs in LIBs. The safety concerns, high cost, and limited scalability of ILs have been identified as significant issues that need to be addressed in order to fully realize the potential of ILs in LIBs. To address these challenges, various theoretical approaches have been

explored in the literature, including modifications to the chemical structure of ILs and combinations with other materials.

Through a comprehensive review of the literature, we have identified several studies that have investigated the challenges associated with the use of ILs in LIBs. However, the validity, data management, and reproducibility of theoretical approaches used in these studies have not been thoroughly evaluated. To address these issues, we have conducted a review of the literature and identified several key factors that contribute to the validity, data management, and reproducibility of theoretical approaches. These factors include the use of appropriate models, the rigor of data collection and analysis, and the transparency of methodology and results.

To provide a framework for addressing these issues, we propose a set of guidelines for validating, managing, and reproducing theoretical approaches used in LIB research. These guidelines emphasize the importance of using appropriate models, conducting rigorous data collection and analysis, and ensuring transparency in methodology and results. By following these guidelines, researchers can improve the validity, data management, and reproducibility of theoretical approaches and contribute to a more robust and reliable field of LIB research.

In crafting this book, I have harnessed the power of artificial intelligence (AI) to explore diverse realms of knowledge. By leveraging AI-generated questions and refining the answers through extensive research in academic journals and books, I have delved into new frontiers. The process involved feeding the responses to another AI system and further enhancing and polishing them under human oversight and direction. While AI technology has been instrumental in shaping the content of this book, the final work is the result of careful curation and refinement under human leadership.

# Introduction 1

Lithium-ion batteries (LIBs) are widely used in portable electronics, electric vehicles (EVs), and grid-scale energy storage systems (1–4). This is attributed to their high energy density, long cycle life, and low self-discharge rate (5–10). They have revolutionized the way we use technology and have enabled the widespread adoption of EVs and renewable energy sources (11–14).

However, LIBs also have some limitations. One major limitation is their safety concerns, as they have a tendency to overheat and become unstable and can catch fire or explode if not handled properly (15–19). Another limitation is their limited energy density, which limits the range of EVs (20,21) and the amount of energy that can be stored in grid-scale energy storage systems (1,22,23). The driving range of EVs is a primary concern for customers and is determined by the energy density of the batteries. LIBs have high energy storage densities but fall short of gasoline. Next-generation batteries with energy densities beyond LIBs are needed to increase driving range effectively. New designs such as Li-sulfur, Li-air, or Mg-ion batteries have higher theoretical energy densities but suffer from safety or poor recyclability issues. Battery packs in EVs also include other components that reduce overall energy densities. Improving cell design and pack efficiency is critical to increasing the energy densities of EV batteries (20).

Ionic liquid (IL) electrolytes have been proposed as a potential solution to these limitations. ILs are salts liquid at or near room temperature and have unique properties that make them attractive as electrolytes in batteries. However, using ILs in lithium batteries also poses several challenges, including safety concerns, high cost, and limited scalability.

In this work, we provide an overview of the issues that have been associated with the use of ILs in LIBs. The safety concerns, high cost, and limited scalability of ILs have been identified as significant issues that need to be addressed in order to fully realize the potential of ILs in LIBs. To address these challenges, various theoretical approaches have been explored in the literature, including modifications to the chemical structure of ILs and combinations with other materials.

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This book aims to provide a comprehensive review of the theoretical approaches used in the study of LIBs that utilize ILs as electrolytes. Despite the growing interest in the use of ILs in LIBs, the validity, data management, and reproducibility of the theoretical approaches used in this field have not been thoroughly evaluated. To address this gap, this book identifies several key factors that contribute to the reliability and robustness of theoretical approaches in LIB research, including the use of appropriate models, rigorous data collection and analysis, and transparency in methodology and results. The book proposes a set of guidelines for validating, managing, and reproducing theoretical approaches used in LIB research, with an emphasis on the importance of using appropriate models, conducting rigorous data collection and analysis, and ensuring transparency in methodology and results. The book also provides a critical review of the literature on the use of ILs in LIBs, highlighting the challenges associated with ILs in terms of ion transfer, both in bulk and at the electrode interface. The book presents an overview of the computational methods used to study the case, including their evaluation and data management, with a focus on proper reproducibility.

# Ionic Liquids, Advantages and Limitations

# 2

Ionic liquids (ILs) have several properties and characteristics that make them suitable for use as electrolytes in lithium batteries.

One of the critical advantages of ILs is their high thermal stability. They have very low vapor pressure and do not evaporate easily, which makes them less prone to combustion or explosion than some other types of electrolytes. This fact is particularly important for high-energy-density batteries like lithium-ion batteries, which can generate much heat during charging and discharging.

ILs also have low flammability and toxicity, which makes them safer to handle and dispose of than some other types of electrolytes. They are also non-volatile, which means that they do not produce gas during cycling, reducing the risk of gas build up and potential rupture of the battery (24–29).

Another advantage of ILs is their wide electrochemical window. It means they can withstand a wide range of voltage potentials without breaking down or decomposing. This is important for lithium batteries because the voltage range in these batteries can be pretty high, and the electrolyte needs to withstand this without reacting or degrading. Thus, ILs can potentially increase the energy densities of lithium batteries (30–35).

Finally, ILs have a high degree of tunability. This implies that the characteristics of these materials can be customized to suit specific purposes. This allows for developing customized electrolytes with optimal properties for a particular battery design.

Overall, the combination of high thermal stability, low volatility, wide electrochemical window, and tunability make ILs a promising choice for electrolytes in lithium batteries. These properties and characteristics enable the development of safer, more efficient, and longer-lasting batteries.

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However, there are still challenges that need to be addressed, such as their high viscosity, low ionic conductivity, high cost, and limited availability compared to traditional electrolytes (36–41).

ILs can have a relatively high viscosity, which can limit their ionic conductivity and diffusion rates in the battery. This can lead to performance issues such as low power density and poor cycling stability (42–45).

ILs can be relatively expensive to produce, making them less competitive with other types of electrolytes in terms of cost. The primary reason for this is the utilization of various chemical substances during the synthesis procedure, coupled with advanced purification methods (46–49).

While ILs are generally stable over a wide range of voltages and temperatures, some types may be less stable under certain conditions. For example, some ILs can decompose or react with the lithium electrode at high potentials or temperatures, reducing battery performance or posing safety risks (50).

ILs may have limited solubility for some types of lithium salts, which can affect their ionic conductivity and overall battery performance (51,52).

Integrating ILs into existing battery designs may be challenging due to their unique properties and requirements. This may require modifications to the battery design or the development of new manufacturing processes (53–58).

Addressing these challenges will require continued research and development to optimize the properties of ILs as electrolytes for lithium batteries. This may involve the development of new types of ILs with lower viscosity, higher solubility, and improved stability, as well as the optimization of battery design and manufacturing processes to integrate ILs more effectively. Additionally, cost-reduction efforts will be necessary to make ILs more competitive with other electrolytes. Despite these challenges, the potential benefits of IL electrolytes, such as improved safety, higher energy density, and longer cycle life, make them an area of active research and development in the field of advanced battery technologies (59).

# STRATEGIES FOR OVERCOMING LIMITATIONS OF IL ELECTROLYTES

There are several ways to address the limitations of IL electrolytes.

## Viscosity

To overcome the issue of high viscosity, researchers are exploring ways to modify the structure of ILs or add small amounts of other solvents to reduce

their viscosity. For example, researchers are exploring the utilization of functionalized ILs or the addition of small amounts of co-solvents to improve the ionic conductivity and reduce the viscosity of the electrolytes.

## *Modifying the Structure of Ionic Liquids to Reduce Viscosity*

Modifying the structure of ILs is one way to reduce their viscosity. One approach is to introduce structural features that disrupt the packing of ions and reduce the strength of interionic interactions. This can be achieved by varying the size, shape, and, or functional groups of the ions that make up the IL. For example, introducing alkyl chains of different lengths or branching patterns can increase the distance between the ions and reduce the strength of interionic interactions, leading to lower viscosities.

Another approach is introducing functional groups that can weaken the interionic interactions and reduce viscosity.

Tansel (60) focused on the importance of thermodynamic and physical characteristics in the permeation of ions during membrane separation. Specifically, the hydrated radius, hydration-free energy, and viscous effects were studied concerning how they impact ion transport through a membrane. The authors suggested that a deeper understanding of these factors can help to optimize membrane separation processes and improve the efficiency of ion transport.

Izgorodina et al. (61) explored the role of dispersion forces in predicting the thermodynamic and transport properties of common ILs. The authors suggested that dispersion forces, a type of intermolecular force, play a crucial role in determining the ILs properties, including viscosity, density, and thermal conductivity. The authors use an assembly of experimental measurements and molecular simulations to investigate the influence of dispersion forces on these properties. They concluded that accurate modeling of dispersion forces is essential for predicting the ILs characteristics and designing new ILs with tailored properties.

Dean et al. (62) discussed the importance of structural analysis in understanding the behavior of low-melting organic salts, particularly in the context of ILs. The authors reviewed various techniques that can be used to study the structure of these materials, including X-ray crystallography and NMR spectroscopy. They also discussed the importance of understanding the structural properties of ILs, such as their intermolecular interactions and the organization of their constituent ions, in relation to their unique physical and chemical properties.

Sanchora et al. (63) highlighted the importance of considering the effects of the alkyl chain length and water content on the properties of ILs. Using

a combination of experimental and computational techniques, the authors explored how changes in the alkyl chain length and water content affect the 1-alkyl-3-methylimidazolium chloride IL's physical and chemical properties, such as its ion pairing energy and hydrogen bonding which impact density, viscosity, and surface tension.

Molecular dynamic simulations provide valuable insights into the reason behind the lower viscosity observed when alkoxy chains are incorporated instead of alkyl chains. These simulations suggest that the reduced viscosity result from the alkoxy chains being less efficient in assembling and interacting with each other, leading to minimal aggregation. Experimental findings support this, showing that the presence of alkoxy chains reduces intermolecular correlations and cation-anion electrostatic interactions, resulting in faster dynamics compared to alkyl counterparts. Raman-induced Kerr spectroscopy studies demonstrate that including ether-substituted groups weakens interionic interactions due to their larger volume. However, their flexibility allows for faster reorientation and stronger interionic interactions. Moreover, certain imidazolium and pyridinium cations produce stable complexes with polyethylene glycol (PEG) chains through ion-dipole interactions. Consequently, ILs containing long and flexible alkoxy chains are expected to exhibit diminished Coulombic interactions between the cation and anion species (64–69).

Fumino et al. (70) utilized far infrared and terahertz spectroscopy to study the interactions in Coulomb fluids. The results indicated that the overall interaction between cations and anions in ILs is a delicate balance between Coulomb forces, hydrogen bonding, and dispersion forces. In the case of protic ILs, the low-frequency spectra showed distinct vibrational modes that revealed the presence of medium to strong hydrogen bonds between the cations and anions. The researchers also employed isotopic substitution to isolate frequency shifts related to interaction strength and reduced masses.

The study further investigated how these interactions impact the physical properties of ILs, such as their melting point, viscosity, and enthalpy of vaporization.

Hayyan et al. (71) conducted a study to synthesize Deep Eutectic Solvents (DESs) by combining triethylene glycol (TEG) with five different phosphonium and ammonium salts. They examined the physical properties of these synthesized DESs at different temperatures ranging from 25°C to 80°C. Fourier transform infrared spectroscopy (FTIR) was also used to analyze the functional groups present in the DESs. The physical properties of deep eutectic solvents (DES) were significantly influenced by blending either ammonium or phosphonium salts with triethylene glycol (TEG) as the hydrogen bond donor (HBD). These properties include freezing point, viscosity, electrical conductivity, and density. The study demonstrated that the physical properties of DESs can be tailored by selecting appropriate HBDs and salts.

Briefly, modifying the structure of ILs to reduce their viscosity involves balancing the competing effects of interionic interactions and structural features that can disrupt these interactions. By carefully designing the structure of ILs, it is possible to achieve the desired balance and create ILs with lower viscosities for specific applications.

## *Co-solvent Addition*

The choice of co-solvent depends on the specific application and performance requirements, as well as the compatibility of the co-solvent with the IL and the electrode materials. It is essential to carefully select co-solvents to ensure that they do not adversely affect the stability and safety of the battery. In addition, the amount and type of co-solvent added should be optimized to balance the trade-off between viscosity reduction and ionic conductivity improvement. Some co-solvents that are appropriate to be added to ILs to reduce viscosity are introduced below:

- *Organic Solvents*: Organic solvents such as acetonitrile, propylene carbonate, and dimethyl carbonate can be added to ILs to reduce their viscosity and improve their ionic conductivity. These solvents can also improve the solubility of lithium salts in ILs, which can further improve their electrochemical performance (72–78).
- *Water*: Adding small amounts of water to ILs can reduce their viscosity and improve their ionic conductivity (79–83). Water can also improve the solubility of lithium salts in ILs and promote the formation of stable solid electrolyte interphase (SEI) layers on electrode surfaces (84).
- *Ionic Liquids*: Mixing two or more ILs with different molecular structures and properties can result in a decrease in viscosity and an increase in ionic conductivity (85–88). This is because the different ILs can interact with each other to form a more fluid and mobile mixture.

  For instance, in the mixing of PAN/BAN and [C2MIM][BF4] ILs, the [C2MIM] cations integrate into protic networks, while the [BF4] anions occupy previously vacant regions near protic cation tails. This subtle microstructural adjustment results in complex variations in the transport properties of the ions. Similarly, for EAN–[C2MIM][BF4] mixtures, a novel conductivity curve exhibits pronounced deviations from the simple ideal mixing rule, with three different regions defined by a local maximum and a global minimum at intermediate concentrations. These regions are defined by the onset of the formation of EAN HB networks and the

virtual disappearance of aprotic IL structures, where long-range ordering for [C2MIM][BF4] breaks down (89).

- *Surfactants*: Surfactants can be added to ILs to reduce their surface tension and improve their wetting properties (90). This can improve the contact between the electrolyte and electrode surfaces, improving battery performance. Contact angle testing and electrolyte absorption are commonly used to measure wettability, with a lower contact angle indicating better wettability.

## Co-solvent Considerations

When selecting co-solvents for ILs, there are several safety concerns that need to be considered. Some of these concerns include:

- *Volatility*: Some co-solvents can be highly volatile, which can increase the risk of flammability and explosion (91–93). When selecting co-solvents, it is crucial to choose ones that have low volatility and are stable under the conditions of battery operation.
- *Toxicity*: When selecting co-solvents, it is essential to choose ones that are non-toxic and have a low environmental impact (94,95). To assess the environmental impact of co-solvents, it is essential to consider their life cycle, from manufacturing to disposal, through a life-cycle assessment (LCA). However, this data is often tailored to specific applications and is not always available. In practice, it is more realistic to assess solvents on key properties for which data is available, such as hazard labels, physical properties, or biobased feedstock percentage.
- *Compatibility*: When selecting co-solvents, it is vital to ensure that they are compatible with the chosen electrode materials and other components of the battery (96,97). This can be achieved by considering the co-solvent's impact on the battery's ionic conductivity, electrode compatibility, and overall safety during the selection process. Novel cosolvent mixtures have been developed for cutting-edge uses like rapid charging or suitability with lithium-metal electrodes. These mixtures were created using similar design strategies, considering the compatibility of the cosolvent with the battery's electrode materials and other components (98).
- *Stability*: Some co-solvents may not be stable under the conditions of battery operation, leading to degradation and reduced battery performance. It is important to consider the battery's operating

conditions, such as temperature, pressure, and the presence of other chemicals. The co-solvent should also not react with the electrolyte or other battery components, as this could cause degradation and reduced performance. When selecting co-solvents, it is important to choose ones that are stable under the conditions of battery operation.

- *Cost*: Some co-solvents such as fluorinated ones may be more expensive than others, which can increase the overall cost of battery production (99). When selecting co-solvents, it is important to balance the cost with the desired performance and safety requirements.

To address these concerns, it is important to carefully evaluate the properties of co-solvents and their potential impact on battery performance and safety. This can be done through experimental and computational methods, such as electrochemical measurements, spectroscopy, and molecular simulations.

In addition, it is essential to follow best practices for handling and disposing of co-solvents to minimize their impact on human health and the environment. This includes using appropriate personal protective equipment, ensuring proper ventilation, and properly storing and disposing of co-solvents according to local regulations (100).

## Cost Limitations

To address the cost issue, researchers are investigating alternative methods of IL synthesis that are more cost-effective. For example, some researchers are exploring the use of renewable or waste materials as starting materials for IL production or recovery (101–103) or lithium battery waste (104). Additionally, the use of ILs in high-value applications, such as aerospace and defence may help to justify their higher cost (105–108).

There are primarily two main methods for the preparation of ILs: metathesis of a halide salt with a desired anion and acid-base neutralization reactions. These methods typically require the use of molecular solvents, which can be expensive and contribute to the overall cost of IL production (109). However, recent research has focused on developing novel methods of synthesis that replace molecular solvents with ILs themselves, which can be more cost-effective. Although ILs are typically considered expensive compared to traditional solvents, their ease of recycling makes them a favorable option for various applications. Researchers are exploring techniques such as membrane separation, extraction, and distillation to recover ILs. These

methods have the potential to lower the overall cost of IL production and enhance their sustainability (110).

## Stability

To improve the stability of ILs, researchers are exploring new types of ILs that are more stable under high potentials or temperatures. These new ILs are designed to have higher thermal stability, lower polarization, and lower loss of active material at elevated temperatures. The anions in ILs have a significant influence on their tribological properties, with hydrophobic anions such as BF4 and PF6 may cause corrosion of steel under humid conditions. However, other hydrophobic anions such as bis(fluorosulfonyl)imide (FSI) anion are less corrosive and exhibit good tribological properties (111). Additionally, the use of additives or coatings on the electrode or separator (112–116) can help to minimize the interaction between the IL and other materials in the battery.

## Solubility

To address the issue of limited solubility, researchers are exploring using different types of lithium salts or modifying the structure of the IL to improve its solubility. For example, some researchers are exploring the use of functionalized ILs or the addition of small amounts of co-solvents to improve the solubility of the electrolytes, which has been discussed in the viscosity section.

## Toxicity

To address the issue of toxicity, researchers are exploring the use of ILs with lower toxicity or modifying the structure of the IL to reduce its toxicity. By changing the chemical compositions of the cations and anions, like utilizing non-aromatic compounds, pairing them with particular anions, and adjusting the length and hydrophobicity of the side chains, it is possible to reduce toxicity levels in ILs, rendering them safer for diverse uses. For example, cholinium-based ILs are recognized as the least toxic, while enhancing the hydrophobicity and length of the side chains can elevate toxicity. Hence, the careful selection of cations and anions and the modification of their characteristics are vital in creating less toxic ILs. Additionally, proper handling and disposal protocols can help to minimize the risk of exposure to toxic ILs (117–122).

## Integration

To address the issue of integration, researchers are exploring the use of new battery designs or modification of existing designs to better accommodate the unique properties of IL electrolytes. This may involve the development of new manufacturing processes or the use of specialized equipment to handle and store the electrolytes (123–127). The integration of IL electrolytes in battery systems requires careful consideration of the electrolyte selection, design, and manufacturing processes. The use of simulation solutions, additives or coatings, and the development of new manufacturing processes or specialized equipment can help optimize battery design and engineering, making them more stable, safer, and cost-effective. Simulation solutions for all physics (chemical, electrical, mechanical, thermal) and scales (from material to cell, module, pack, full vehicle integration) are also being developed to optimize battery design and engineering.

Overall, addressing the limitations of IL electrolytes will require continued further research and innovation to enhance their functionality and performance for specific battery applications. This may involve a combination of modifying the structure of the IL, developing new synthesis methods, and optimizing battery designs and manufacturing processes.

### *Some New Battery Designs that can Better Accommodate the Unique Properties of Ionic Liquid Electrolytes*

There are several new battery designs that can better accommodate the unique properties of IL electrolytes. Some examples include the following:

- *Solid-State Batteries*: Solid-state batteries use a solid electrolyte instead of a liquid electrolyte, which can improve safety, stability, and energy density, Figure 1. IL electrolytes can be used as solid electrolytes or as additives to improve the properties of the solid electrolyte. For example, ILs can improve ionic conductivity and reduce the interfacial resistance between the solid electrolyte and the electrodes (128–135).
- *Flow Batteries*: Flow batteries use a liquid electrolyte stored in external tanks and circulated through the battery during operation. IL electrolytes can be used as the electrolyte in flow batteries, which can improve energy density and reduce the risk of leakage or combustion (136–143).

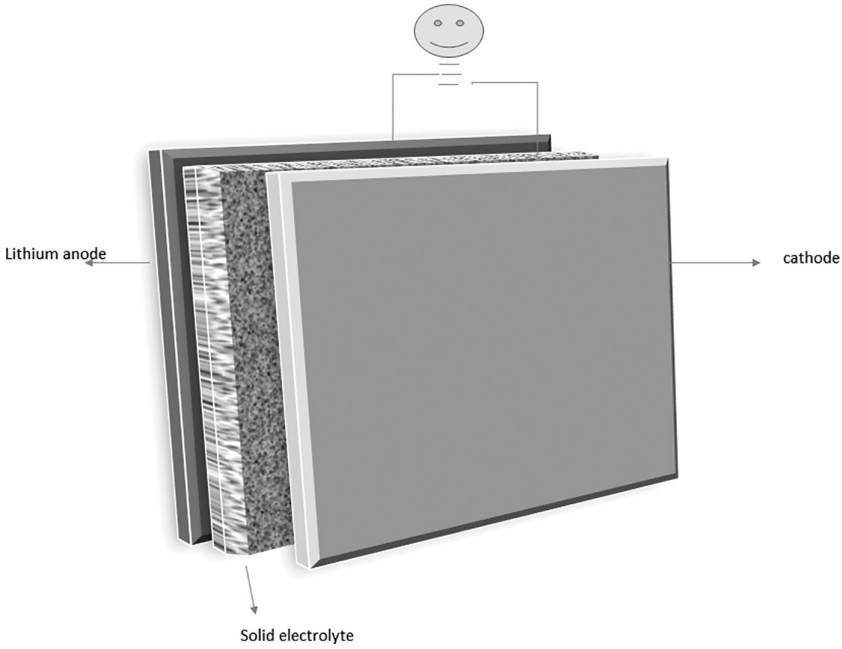


**FIGURE 1** Schematics for a solid state battery.

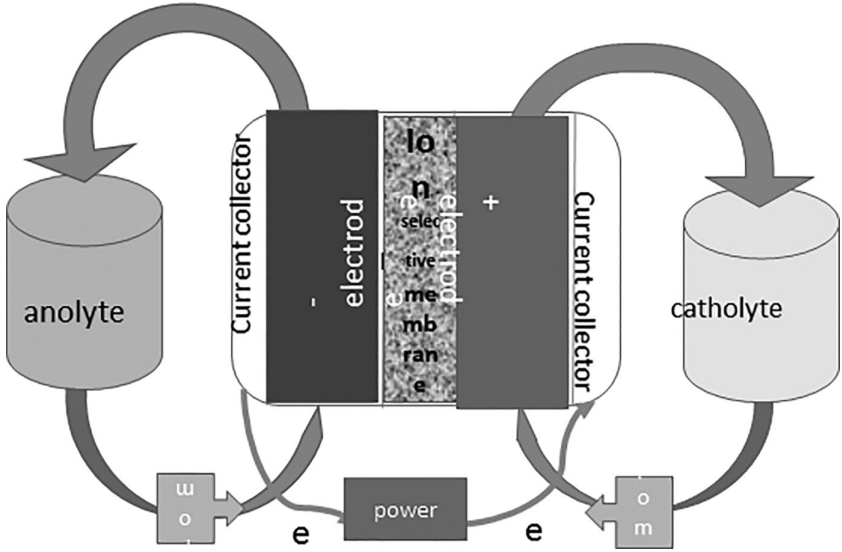


**FIGURE 2** Schematics for a typical flow battery.

- *Lithium-Sulfur Batteries*: Lithium-sulfur batteries use a sulfur cathode and a lithium anode, which can provide high energy density and low cost. However, sulfur cathodes typically have poor stability and low conductivity (144–146). IL electrolytes can be used as additives to improve the stability and conductivity of the sulfur cathode, leading to better battery performance (147–153).
- *Three-Dimensional Batteries*: Three-dimensional (3D) batteries use a porous electrode structure that allows for better electrolyte penetration and ion transport (154–157). IL electrolytes can be used in 3D batteries to improve the transport properties of the electrolyte and reduce the concentration polarization at the electrode/electrolyte interface, leading to better battery performance (158,159).
- *Electrolyte-Filled Batteries*: Electrolyte-filled batteries use a porous electrolyte-filled structure instead of a traditional separator. This structure allows for better ion transport and reduces the risk of short circuits or dendrite formation (160–165). IL electrolytes can be used in electrolyte-filled batteries to improve their stability and reduce the risk of leakage or combustion (166–170).

Overall, these new battery designs can better accommodate the unique properties of IL electrolytes and improve their performance in terms of energy density, safety, and stability. However, developing these new battery designs will require significant research and development to optimize their properties and performance. Additionally, the high cost of IL electrolytes may be a limiting factor in some of these designs, and further cost-reduction efforts will be necessary to make them more competitive with other types of electrolytes.

# Ion Transport, Electrode-Electrolyte Interface

# 3

The ion transport mechanism in ionic liquid electrolytes differs from traditional organic solvent-based electrolytes. In ionic liquids, ions can move through the bulk liquid or along the surface of the electrode, depending on the specific properties of the electrolyte and the electrode. This can impact the battery's performance, as different ion transport mechanisms may have different rates of ion transfer and different levels of resistance.

The impact of these properties on the performance of the lithium battery can vary depending on the specific application and battery design. For example, in high-power applications, such as electric vehicles, high ionic conductivity and fast ion transport are important for achieving high power output. However, in high-energy-density applications, such as stationary energy storage, the stability of the electrolyte is more important, as the battery must be able to operate reliably over many cycles without degradation.

The viscosity of the ionic liquid electrolyte can impact the rate of ion transport and diffusion in the battery. Higher viscosity can lead to slower ion transport, resulting in lower power output and reduced cycling stability. To address this issue, researchers are exploring ways to modify the structure of the ionic liquid or add small amounts of co-solvents to reduce the viscosity of the electrolyte.

The ion transport mechanisms in ionic liquid electrolytes can also affect the battery's performance. For example, if the ion transport occurs predominantly through the surface of the electrode, the battery may experience higher resistance and lower capacity.

The electrode-ionic liquid interface is an essential component of the lithium battery, as it governs the transfer of ions between the electrode and the electrolyte. Here are a few ways that researchers are working to optimize the electrode-ionic liquid interface to improve ion transport and reduce resistance:


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A. *Surface Modification*: One approach to optimizing the electrode-ionic liquid interface is to modify the surface of the electrode to improve its wettability and reduce the interfacial resistance (171–173). For example, researchers have experimented with applying a thin layer of metal oxide or a conductive polymer coating to the surface of the electrode to improve its interaction with the electrolyte (174–176). Researchers have also used ionic liquid as a wetting agent for the interface between solid-state electrolytes and electrodes to enhance interfacial wetting and improve battery performance. The optimization of the ionic liquid content in the interface has been crucial for achieving high performance in solid-state batteries (177).
B. *Nanostructuring*: Another approach is to modify the surface of the electrode at the nanoscale. Nanostructuring can increase the surface area of the electrode and improve its interaction with the electrolyte (178–183). Several materials are considered promising for nanostructured electrodes in lithium-ion batteries. These materials possess unique properties that make them attractive for electrode applications, such as high surface area, high conductivity, and good stability. Here are a few examples:
    a *Carbon Nanotubes (CNTs)*: CNTs are one-dimensional structures made of carbon atoms arranged in a cylindrical shape. They have a high surface area and excellent electrical conductivity, making them attractive for use as electrode materials in lithium-ion batteries. In addition, CNTs have good mechanical strength and flexibility, which can improve the electrode's durability (184–186).
    b *Graphene*: It is a two-dimensional material made of a single layer of carbon atoms arranged in a hexagonal lattice. It has a high surface area, excellent electrical conductivity, and good mechanical properties, making it attractive for use as an electrode material in lithium-ion batteries. Graphene can also be easily functionalized with other materials to improve its performance (187).
    c *Metal Oxides*: Metal oxides, such as titanium dioxide (TiO2) and iron oxide (Fe2O3), have attracted attention as potential electrode materials due to their high stability and low toxicity (188,189). Metal oxides can also have a high theoretical capacity, which can further improve the energy density of the battery (190–192). However, their low electrical conductivity can limit their performance as electrode materials (193–195).

d *Metal Sulfides*: Metal sulfides, such as molybdenum disulfide ($MoS_2$) and cobalt sulfide (CoS), have also been studied as potential electrode materials in lithium-ion batteries (196–200). Metal sulfides have a high theoretical capacity and good electrochemical stability, making them attractive for use in high-performance batteries (201,202). However, their low electrical conductivity can limit their performance, and more research is needed to improve their conductivity.

e *Silicon*: It is a promising material for use as an electrode material in lithium-ion batteries due to its high theoretical capacity and abundance (203,204). However, silicon electrodes can suffer from significant volume changes during cycling, which can lead to mechanical degradation and reduced performance. Researchers are exploring ways to mitigate this issue by using nanostructured silicon electrodes, which can improve the mechanical stability of the electrode (205,206).

The smaller size and nanostructured design of these silicon electrodes can help accommodate the volume changes better and prevent cracking, pulverization, and loss of electrical contact that can occur in larger silicon electrodes (207).

However, the commercialization of these delicate nanostructured silicon electrodes is still challenging due to issues like poor first-cycle coulombic efficiency (208) and higher manufacturing costs compared to larger silicon particles.

C. *Electrolyte Additives*: Adding electrolyte additives can also improve the electrode-ionic liquid interface (209–213). For example, researchers have added small amounts of lithium salts or other additives to the electrolyte to improve the wetting of the electrode surface and reduce the interfacial resistance (210). Tuning the reaction time and/or electrolyte composition (e.g., using different lithium salts like LiFSI, LiPF6, and LiAsF6) can lead to diverse surface morphologies on the lithium metal electrode, which can impact the wettability and interfacial resistance (214,215).

D. *Interface Modelling*: Finally, researchers are using computational methods to model and optimize the electrode-ionic liquid interface at the molecular level (216–222). These models can provide insights into the specific interactions between the electrode and the electrolyte, allowing for the design of more effective electrode materials and electrolytes. While computational modelling is a powerful tool for optimizing the electrode-ionic liquid interface in lithium-ion batteries, it has some limitations. Here are a few examples:

a. *Complexity*: The electrode-ionic liquid interface is a complex system with many interacting components, including the electrode material, the ionic liquid electrolyte, and the interface between them. Modeling this system accurately requires a high level of computational complexity and can be computationally expensive, especially for large-scale systems.
b. *Accuracy*: The accuracy of computational models for the electrode-ionic liquid interface depends on the accuracy of the input parameters and assumptions used. For example, the properties of the ionic liquid electrolyte, such as its viscosity and dielectric constant, can vary depending on the specific formulation and conditions, and accurate modelling of these properties can be challenging (223).
c. *Validation*: Validation of computational models for the electrode-ionic liquid interface can be complex, as experimental measurements of the interface are often limited and can be affected by surface roughness, impurities, and sample preparation. As a result, it can be challenging to validate the accuracy of computational models and to ensure that they are representative of the real-world system (224).
d. *Limitations of Current Models*: Current computational models for the electrode-ionic liquid interface often rely on simplifying assumptions and approximations, such as treating the ionic liquid as a continuum medium and ignoring the effects of solvent molecules and other small ions. These approximations can limit the accuracy and applicability of the models, and more advanced models that incorporate more detailed information about the ionic liquid electrolyte are needed (225,226).
e. *Scaling*: Finally, computational modelling is often limited by scalability, as simulating larger systems requires higher computational resources. This can limit the ability of researchers to model the electrode-ionic liquid interface in complex systems, such as in multi-layered electrodes or systems with multiple interfaces (227). Despite these limitations, computational modelling remains an important tool for optimizing the electrode-ionic liquid interface in lithium-ion batteries.

By combining computational modelling with experimental measurements and other analytical techniques, researchers can gain a better understanding of the complex interactions at the interface and develop more effective strategies for improving the performance and stability of lithium-ion batteries (228–232).

# 4 Theoretical and Experimental Investigation of Ionic Liquids in Lithium Ion Batteries

The behavior of IL electrolytes in lithium batteries has been extensively studied using theoretical models that take into account the thermodynamics and kinetics of the electrochemical reactions. These models play a crucial role in understanding the complex electrochemical processes occurring within batteries and are essential for predicting and optimizing battery performance.

- *Poisson-Nernst-Planck (PNP) Equation*: One theoretical model used to describe the behavior of IL electrolytes is the PNP equation, which is a partial differential equation that describes the transport of ions in an electrolyte solution. The PNP equation takes into account the electrostatic interactions between ions, the concentration gradients of the ions, and the external electric field. The PNP equation can be solved using numerical methods, such as finite difference or finite element methods, to obtain the spatial distribution of ions in the electrolyte (233).
- *Molecular Dynamics (MD) Simulation*: Another theoretical model used to study the behavior of IL electrolytes in lithium batteries is MD simulation. MD is a computational method that simulates the movement of atoms and molecules over a period of


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time, using classical mechanics. In MD simulation, the interactions between atoms and molecules are described by a potential energy function, which can be parameterized using experimental data or quantum mechanical calculations. MD simulation can be used to study the structure and dynamics of IL electrolytes, as well as the interactions between IL electrolytes and electrode surfaces (234–239).

As a case study, a key challenge in the utilization of polymerized ionic liquids (polyILs) as electrolytes in energy storage devices is the observed reduction in anion diffusivities compared to their parent ionic liquids (ILs). This disparity in ion transport behavior between the two systems has prompted the need for a deeper understanding of the underlying mechanisms governing ion transport in these materials. In the following case study, we explore a comparative analysis of ion transport in ILs and polyILs, leveraging the insights gained from molecular dynamics simulations. By exploring the distinct ion transport mechanisms in these materials, we aim to provide valuable guidance for the design and optimization of polyIL electrolytes with enhanced performance in advanced energy storage applications. The findings from this case study offer a comprehensive understanding of the factors influencing ion diffusion in ILs and polyILs, shedding light on the challenges and opportunities associated with the utilization of polyILs in next-generation energy storage technologies (240).

## Case Study 1: Comparative Analysis of Ion Transport in ILs and PolyILs

### SYNOPSIS

This case study investigates the comparative assessment of ion transport dynamics in conventional ILs and polyILs. The investigation centers on unraveling the fundamental mechanisms governing ion movement in these distinct systems, shedding light on the obstacles and potentials associated with incorporating polyILs into energy storage and electrochemical devices.

### OBJECTIVE

The primary aim of this research is to compare and analyze ion transport mechanisms in ILs and polyILs through the lens of molecular dynamics simulations. By scrutinizing the factors influencing ion diffusion in these materials, the study seeks to offer insights that can shape the design and

enhancement of polyIL electrolytes for superior performance in energy storage applications.

## METHODOLOGY

- Utilized molecular dynamics simulations to explore ion transport in ILs and polyILs.
- Examined ion transport mechanisms in ILs, with a focus on ion association dynamics and structural relaxation.
- Explored the distinctive aspects of ion transport in polyILs, particularly emphasizing the impact of polymer chain dynamics and anion diffusion within cationic polymer cages.

## FINDINGS

- Revealed that in ILs, ion transport is intricately linked to ion association dynamics and structural relaxation, affecting the rate of ion diffusion.
- Uncovered that in polyILs, anion diffusion is predominantly governed by anions hopping between cationic polymer cages, with the "trap time" dictating the pace of anion transport.
- Emphasized the influence of factors like free volume fraction, polymer chain oscillations, and chain translation speed on ion diffusivities in polyILs across different temperatures.

## CONCLUSION

The comparative exploration of ion transport in ILs and polyILs yields valuable insights into the distinct mechanisms dictating ion diffusion in these materials. By discerning the variations in ion transport behavior, researchers can refine the design of polyIL electrolytes for enhanced performance in energy storage and electrochemical devices.

## KEY INSIGHTS

- Molecular dynamics simulations serve as a potent tool for investigating ion transport mechanisms in ILs and polyILs.
- The unique characteristics of polyILs, including polymer chain dynamics and cationic polymer cages, significantly impact ion diffusion behavior.
- Lessons from this study can steer the development of advanced polyIL electrolytes with improved ion transport properties for cutting-edge energy storage applications.
- Insights from this study can guide the development of advanced polyIL electrolytes with enhanced ion transport properties for next-generation energy storage applications.

This case study underscores the importance of understanding and comparing ion transport in traditional ILs and emerging polyILs, providing valuable insights for the design and optimization of polyIL electrolytes in advanced energy storage systems.

- *Density Functional Theory (DFT)*: DFT is a quantum mechanical method that can calculate the electronic structure and energetics of molecules and materials. DFT can be used to study the adsorption of ions and molecules on electrode surfaces, as well as the formation and decomposition of solid electrolyte interphase (SEI) layers (241–245). In this section, we delve into the realm of computational analysis to unlock the potential of alicyclic ILs as electrolytes in lithium metal batteries. The study presented here aims to uncover the intricate electrochemical stability, charge transfer moments, and ion interactions within these ILs, paving the way for optimized performance in battery applications (246–248).

As we navigate through the methodology employed to dissect the properties of alicyclic ILs, we uncover key findings that shed light on their suitability as electrolytes for lithium metal batteries. By understanding the complex interplay between anions, cations, lithium ions, and ion pairs within these IL electrolytes, we gain valuable insights into enhancing battery performance and longevity.

Join us on this journey as we leverage computational modeling to unravel the behavior and potential of alicyclic ILs in lithium metal battery electrolytes.

## Case Study 2. Computational Analysis of Alicyclic ILs in Lithium Metal Battery Electrolytes

### OVERVIEW

This case study delves into the computational exploration of alicyclic ILs as electrolytes in lithium metal batteries. The research focuses on understanding the electrochemical stability windows, charge transfer moments, and ion interactions within these ILs to enhance their performance in battery applications.

### OBJECTIVE

The primary objective of the study is to investigate the electrochemical stability, bulk properties, and ion interactions of alicyclic ILs to optimize their utilization as electrolytes in lithium metal batteries. By employing computational approaches, the aim is to enhance the efficiency and reliability of these ILs in battery systems.

## METHODOLOGY

- Utilized computational modeling to analyze the electrochemical stability windows of alicyclic ILs as lithium metal battery electrolytes.
- Investigated how the ionic structure of alicyclic ILs influences their bulk properties and charge transfer moments.
- Explored the interactions between anions, cations, lithium ions, and ion pairs within alicyclic IL electrolytes for lithium metal batteries.

## FINDINGS

- Identified the electrochemical stability windows of alicyclic ILs, providing insights into their suitability as electrolytes for lithium metal batteries.
- Analyzed the charge transfer moments of alicyclic ILs to understand their charge distribution and transfer behavior in battery systems.
- Investigated the complex interactions between anions, cations, lithium ions, and ion pairs within alicyclic IL electrolytes, shedding light on their impact on battery performance, see Figure 3.

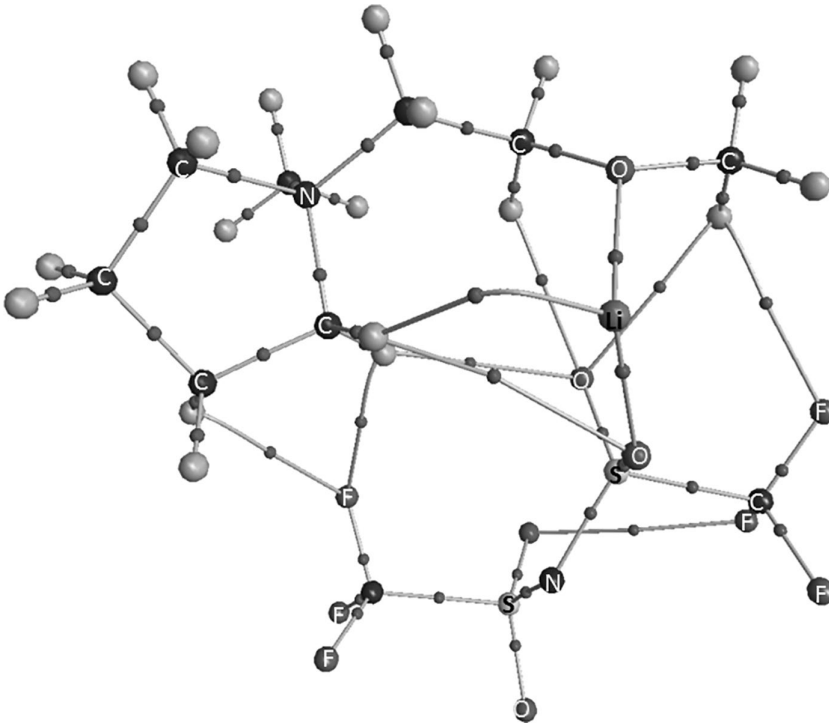


**FIGURE 3** AIM picture for RmAzp+NTf2+Li. The symbols for every atom except hydrogen are indicated on the corresponding atom.

## CONCLUSION

The computational analysis of alicyclic ILs in lithium metal battery electrolytes offers valuable insights into their electrochemical behavior, bulk properties, and ion interactions. By understanding these aspects, researchers can tailor the design and composition of alicyclic ILs to enhance their functionality and stability in lithium battery applications.

## KEY TAKEAWAYS

Computational modeling provides a powerful tool for studying the electrochemical behavior of alicyclic ILs in lithium metal batteries. Understanding the charge transfer moments and ion interactions within these ILs is crucial for optimizing their performance. Insights from this study can guide the development of advanced electrolytes for more efficient and reliable lithium metal battery systems.

This case study highlights the significance of computational analysis in elucidating the behavior and properties of alicyclic ILs as electrolytes in lithium metal batteries, paving the way for enhanced battery performance and longevity.

- *Monte Carlo (MC) Simulation*: This is a statistical method that can be used to simulate the behavior of a system with many interacting particles. MC simulation can be used to study the thermodynamics and kinetics of ion transport and reactions in IL electrolytes (249–252).
- *Continuum Models*: These models can be used to describe the transport of ions and electrons in the electrolyte and electrode materials. Continuum models are based on the laws of conservation of mass, momentum, and energy. They can be used to describe the behavior of a system at a larger scale than molecular simulations (253–257).
- *Hybrid Models*: These models combine multiple computational approaches, such as MD and continuum models, to capture both the detailed molecular interactions at the interface and the macroscopic behavior of the electrode-IL system. Hybrid models can provide a more complete understanding of the interface by incorporating both electronic and ionic interactions, as well as the effects of external factors, such as temperature and pressure (258).

Experimental techniques, such as electrochemical measurements, spectroscopy, and microscopy, have been used to study the behavior of IL electrolytes in lithium batteries.

- *Electrochemical Measurements*: Measurements such as cyclic voltammetry and electrochemical impedance spectroscopy can be used to measure the electrochemical properties of the electrolyte

and electrode materials, including their capacitance, resistance, and diffusion coefficient. Cyclic voltammetry (CV) is a valuable electrochemical method utilized in battery research to assess the electrochemical characteristics of materials used in batteries. It involves analyzing the current response of a redox active solution to a linear potential sweep, providing insights into redox processes, energy levels, and electronic-transfer kinetics. By sweeping the electrode potential linearly over time and measuring the resulting current flow in an electrochemical cell, CV yields essential electrochemical data about the material being studied. This technique is widely applied in diverse fields like analytical chemistry, materials science, and electrochemistry for both research purposes and practical applications, offering crucial information on electroactive species behavior, electrochemical kinetics, diffusion coefficients, concentration analysis, and electrode surface properties.

Electrochemical impedance spectroscopy (EIS) is a technique used to measure the impedance of a system as a function of the AC potentials frequency. It is a powerful method that provides insights into the behavior of complex electrochemical systems by isolating and distinguishing the influence of various physical and chemical phenomena. EIS is widely employed in diverse fields, including batteries, catalysis, corrosion processes, semiconductor interfaces, and ion diffusion across membranes. EIS measures the resulting current response as a sine wave superimposed on the DC current, providing valuable information about the system's impedance as a function of frequency. EIS is used in electrochemical measurements to characterize the behavior of electrochemical systems, study electrode kinetics, analyze mass transport phenomena, and evaluate the performance of protective coatings against corrosion1. It is a versatile technique that allows researchers to rapidly characterize electrochemical systems, study processes from high to low frequencies, and optimize system behavior at different operating points, such as different states of charge in batteries. Overall, EIS is a valuable tool in electrochemical measurements, providing detailed insights into the electrochemical behavior of systems, enabling the characterization of various electrochemical processes, and offering opportunities for system optimization and performance enhancement in a wide range of applications. Some other electrochemical techniques used to measure the electrochemical properties of electrolyte and electrode materials include: chronoamperometry, chronopotentiometry, potentiostatic intermittent titration technique (PITT), and linear sweep voltammetry.

- *Spectroscopy Techniques*: Techniques such as infrared and Raman spectroscopy can be used to study the chemical structure and composition of the electrolyte and electrode materials. Spectroelectrochemistry (SEC) combines electrochemistry and spectroscopy techniques to offer enhanced insights compared to using them separately. It enables real-time characterization of electrogenerated species. Among the four spectroscopy techniques with high potential in SEC, IR-SEC, and Raman-SEC are highlighted for their ability to analyze the chemical structure and composition of electrolyte and electrode materials. NMR-SEC is also recognized as a valuable method for understanding electrochemical systems.
- *Microscopy Techniques*: Microscopy techniques, including scanning electron microscopy (SEM) and transmission electron microscopy (TEM), are valuable tools used to visualize the morphology and structure of electrode materials and solid electrolyte interphase (SEI) layers. These techniques provide high-resolution imaging capabilities that allow researchers to examine the surface morphology, structure, and composition of electrode materials at the micro- and nano-scale levels. SEM is particularly useful for studying the surface topography and elemental composition of materials, while TEM provides detailed insights into the internal structure and composition of materials at the atomic level. By utilizing SEM and TEM, researchers can gain a comprehensive understanding of the physical characteristics and properties of electrode materials and SEI layers, aiding in the development and optimization of advanced energy storage devices (259).

In summary, studying the behavior of IL electrolytes in lithium batteries is a complex and interdisciplinary field. By combining theoretical models, computational methods, and experimental techniques, researchers can gain a comprehensive understanding of the behavior of IL electrolytes in lithium batteries. This can lead to the design of new IL electrolytes with improved performance, such as higher conductivity, stability, and safety, as well as the optimization of electrode materials and system designs to maximize battery performance and lifetime.

# Validation, Management, and Reproducibility

# 5

## HOW TO VALIDATE THE ACCURACY OF COMPUTATIONAL MODELS FOR THE ELECTRODE IONIC LIQUID INTERFACE?

Validating the accuracy of computational models for the electrode-ionic liquid interface is an important step in ensuring that the models represent the real-world system. Here are a few ways that researchers can validate the accuracy of computational models:

- *Comparison with Experimental Measurements*: Researchers validate computational models by comparing their predictions with experimental measurements of the electrode-ionic liquid interface using techniques like X-ray photoelectron spectroscopy (XPS), infrared spectroscopy (IR), or scanning tunneling microscopy (STM). This comparison helps assess the accuracy of the computational model and pinpoint areas for enhancement based on the agreement with experimental data (260–263).
- *Sensitivity analysis*: This is a method utilized to evaluate how sensitive a model is to changes in input parameters and assumptions. By adjusting these parameters and observing the resulting impact on the model's predictions, researchers can determine which parameters significantly influence the model's accuracy and may require further refinement or detailed characterization (264,265).
- *Consistency with Known Physical Principles*: Another way to validate a computational model is to ensure that it is consistent


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with known physical principles (266,267). For example, the model should conserve energy and momentum, and it should satisfy fundamental laws such as the laws of thermodynamics (268). By verifying that the computational model upholds these physical constraints and principles, researchers can increase confidence in the model's accuracy and reliability. This type of validation complements the comparison to experimental data, as it ensures the model is not only predictive, but also grounded in the underlying physical reality. Validating a computational model against physical principles is an important step in the overall validation process, as it helps identify potential flaws or inconsistencies in the model formulation, prior to comparing it to empirical observations.

- *Comparison with Other Models*: Researchers may also validate their computational models by comparing them with other models validated in the literature (269). By comparing the predictions of different models, researchers can identify areas of agreement and disagreement and gain insights into the limitations and uncertainties of the models. This may be achieved by comparing their predictions, analyzing the consistency in outcomes, and assessing the alignment or discrepancies in results.

  Researchers compare the outputs of different computational models to determine where they agree or disagree in their predictions. They evaluate the consistency in predictions across various models, with consistent results indicating agreement and inconsistencies highlighting disagreements. Researchers also analyze the alignment or discrepancies in results concerning specific parameters or assumptions to identify factors contributing to agreement or disagreement between the models.
- *Reproducibility*: Another critical aspect of validating computational models is reproducibility. The model should be well-documented and the code should be made available to other researchers, so that others can reproduce the results and validate the model independently (270–272).
- *Benchmarking*: Finally, researchers may validate their computational models by benchmarking them against known or reference systems (273). For example, researchers may use standard test cases or reference systems to validate the accuracy of their models. By benchmarking the model against a known system, researchers can assess the accuracy and reliability of the model and identify areas for improvement.

A common benchmarking system for validating computational models of the electrode-ionic liquid interface is the graphite-electrolyte interface. The graphite electrode is a widely used electrode material in lithium-ion batteries, and its interface with the electrolyte has been extensively studied experimentally and computationally (37,228,239,274,275). These studies have demonstrated the importance of accurately modeling the interactions between the graphite electrode and the electrolyte, including the effects of surface roughness, solvent molecules, and charge transfer processes. They have also highlighted the limitations and uncertainties of the models and identified areas for improvement.

Experimental measurements of the graphite-electrolyte interface can be obtained using techniques such as X-ray photoelectron spectroscopy (XPS), infrared spectroscopy (IR), and scanning tunneling microscopy (STM). These measurements can be used to validate the accuracy of computational models, by comparing the model predictions with the experimental data.

Computational models of the graphite-electrolyte interface typically involve molecular dynamics simulations, in which the atomic interactions and dynamics are simulated over a while. The accuracy of the model can be assessed by comparing the simulation results with experimental measurements, as well as with other computational models that have been validated in the literature. Sensitivity analysis can also be used to identify which parameters are most critical to the accuracy of the model, and which may need to be refined or better characterized.

The graphite-electrolyte interface provides a well-defined system for benchmarking computational models and has been used in numerous studies for this purpose (276–278).

In conclusion, validating the accuracy of computational models for the electrode-ionic liquid interface involves a comprehensive approach. This includes integrating experimental measurements, sensitivity analysis, adherence to physical principles, comparison with existing models, ensuring reproducibility, and benchmarking. By employing these diverse strategies, researchers can enhance their confidence in the precision and dependability of their models. This, in turn, enables the development of more efficient strategies for enhancing the performance and stability of lithium-ion batteries.

# SOME COMMON CHALLENGES RESEARCHERS FACE WHEN VALIDATING COMPUTATIONAL MODELS

Validating computational models can be challenging, and researchers may face several common challenges. Here are a few examples:

- *Limited Experimental Data*: The main challenge in validating computational models is the scarcity of experimental data for comparison, particularly in the context of the electrode-ionic liquid interface. Obtaining experimental measurements for this interface is often challenging, expensive, and prone to errors and uncertainties. Consequently, researchers may have to work with a restricted amount of experimental data for validation, which can hinder the thorough assessment of the model's accuracy and reliability.
- *Variability of Experimental Data*: Even when experimental data is available, it can be subject to variability and uncertainty. For example, measurements of the electrode-ionic liquid interface can be affected by factors such as surface roughness, impurities, and sample preparation, which can lead to variability in the data. This can make it challenging to validate the accuracy of the model and to identify the sources of error and uncertainty.
- *Complexity of the System*: The electrode-ionic liquid interface is a complex system with many interacting components, including the electrode material, the ionic liquid electrolyte, and the interface between them. Modeling this system accurately requires a high level of computational complexity, and may require simplifying assumptions and approximations that can limit the accuracy of the model.
- *Limitations of the Model*: Computational models for the electrode-ionic liquid interface often rely on simplifications and approximations, potentially overlooking crucial phenomena and interactions at the interface. These models may omit factors like solvent molecules, small ions, or charge transfer mechanisms, impacting their accuracy and relevance. Researchers must carefully consider the model's constraints and the assumptions underlying it to interpret results accurately.
- *Computational Resources*: Validating computational models can be computationally intensive and may require significant computational

resources, especially for large-scale systems or for models that incorporate multiple levels of detail and complexity. This can make it challenging for researchers to run and validate the model within a reasonable time frame or with available computational resources.

- *Model Transferability*: Another challenge in validating computational models is their transferability to other systems or conditions. Models that are validated for a specific system or set of conditions may not be applicable for other systems or under different conditions, which can limit their utility. Researchers need to carefully assess the transferability of the model and its assumptions when applying it to new systems or conditions.

Validating computational models for the electrode-ionic liquid interface requires careful consideration of the limitations and challenges involved, as well as the strengths and weaknesses of the model and the available experimental data. By addressing these challenges and refining the models over time, researchers can develop more accurate and reliable models that can guide the development of new materials and devices for lithium-ion batteries.

## TECHNIQUES FOR MANAGING AND ANALYZING LARGE AMOUNTS OF DATA GENERATED BY SIMULATIONS

Managing and analyzing large amounts of data generated by simulations is a common challenge in computational modeling. Here are a few techniques that can help researchers manage and analyze the data efficiently:

- *Parallel Processing*: This is a technique used to distribute the computational workload across multiple processors or nodes (279,280). By running simulations in parallel, researchers can reduce the time required to generate the data and increase the efficiency of the simulations. Parallel processing can be implemented using specialized software and hardware, such as graphical processing units (GPUs) and high-performance computing (HPC) clusters.

  GPUs are designed with parallel processing architecture, allowing them to handle resource-intensive tasks efficiently. They consist of multiple cores that can perform extensive calculations simultaneously, making them well-suited for tasks like ML model

training, data mining operations, and high-resolution graphics rendering. GPUs can integrate multiple units to enhance processing potential, consume less memory, and execute tasks faster due to their parallel processing nature.

HPC clusters leverage both CPUs and GPUs to perform diverse operations simultaneously. While CPUs handle serial processing for various applications and the operating system within the cluster, GPUs excel at parallel processing for massive external workloads like ML model training and data mining. HPC clusters can be designed without GPUs, but including GPUs significantly boosts the system's performance. CPUs are essential for running an HPC system, and GPUs further enhance the processing power, especially for resource-intensive tasks.

- *Data Compression*: This is a technique used to reduce the size of the data generated by the simulations without losing important information (281,282).

  Data compression is the process of encoding information using fewer bits than the original representation. This technique, also known as source coding or bit-rate reduction, aims to reduce the size of data without losing its essential content.

  There are two main types of data compression:

  Lossless Compression: This method reduces bits by eliminating statistical redundancy without losing any information. The original data can be perfectly reconstructed from the compressed form.

  Lossy Compression: This approach removes unnecessary or less important information, resulting in a smaller file size but with some loss of data accuracy or detail.

  For example, researchers may use lossless compression techniques, such as gzip or bzip2, to compress data files without losing any information (283–286). Alternatively, researchers may use lossy compression techniques, such as JPEG or MP3, to reduce the size of data files while sacrificing some level of accuracy or detail (287,288).

  The device that performs the data compression is referred to as an encoder, while the one that reverses the process (decompression) is known as a decoder.

- *Data Visualization*: This is a technique used to represent the data generated by the simulations in a visual format that is easy to interpret and analyze (289,290). For example, researchers may use plots, graphs, or 3D visualizations to represent the data and identify patterns and trends Figure 4. Data visualization can be implemented

using specialized software tools, such as MATLAB, Python, or ParaView.

The choice of data visualization technique depends on factors such as the type of data, the research question, and the target audience. Principles of effective data visualization, such as clarity, conciseness, and appropriate use of color and scale, should be considered when creating visualizations.

- *Machine Learning*: This is a technique used to analyze large amounts of data and identify patterns and trends automatically (291,292). For example, researchers may use clustering or regression algorithms to analyze the data generated by the simulations and identify correlations between variables or features (224,232,293–295). Machine learning can be implemented using specialized software tools, such as scikit-learn (296) or TensorFlow.

  The choice of machine learning technique depends on the type of data, the research question, and the desired insights.

  Effective use of machine learning requires careful data preprocessing, model selection, and validation to ensure the reliability and accuracy of the results.

  Some advantages of using machine learning over traditional methods of data analysis include:

  In summary, machine learning excels at uncovering intricate patterns and relationships in data that traditional statistical methods may overlook. Its scalability allows for efficient processing of large datasets, making it ideal for big data analysis. Machine learning models can adjust to data changes, ensuring ongoing accuracy. By minimizing human biases, machine learning delivers more objective predictions. It automates decision-making, enhancing speed and reducing manual intervention. With the ability to analyze diverse data sources, machine learning enhances forecasting and decision-making accuracy. Its flexibility and adaptability across various domains make it a versatile tool for a wide range of applications.

  The limitation of machine learning is its dependence on the quality and quantity of data. Insufficient or biased data can lead to inaccurate results, impacting the effectiveness and reliability of machine learning algorithms.

- *Data Management Software*: This is a tool used to organize, store, and retrieve large amounts of data generated by simulations (297). For example, researchers may use specialized software tools, such as MongoDB (298) or Cassandra (299), to manage and query large datasets efficiently and effectively. Data management software can

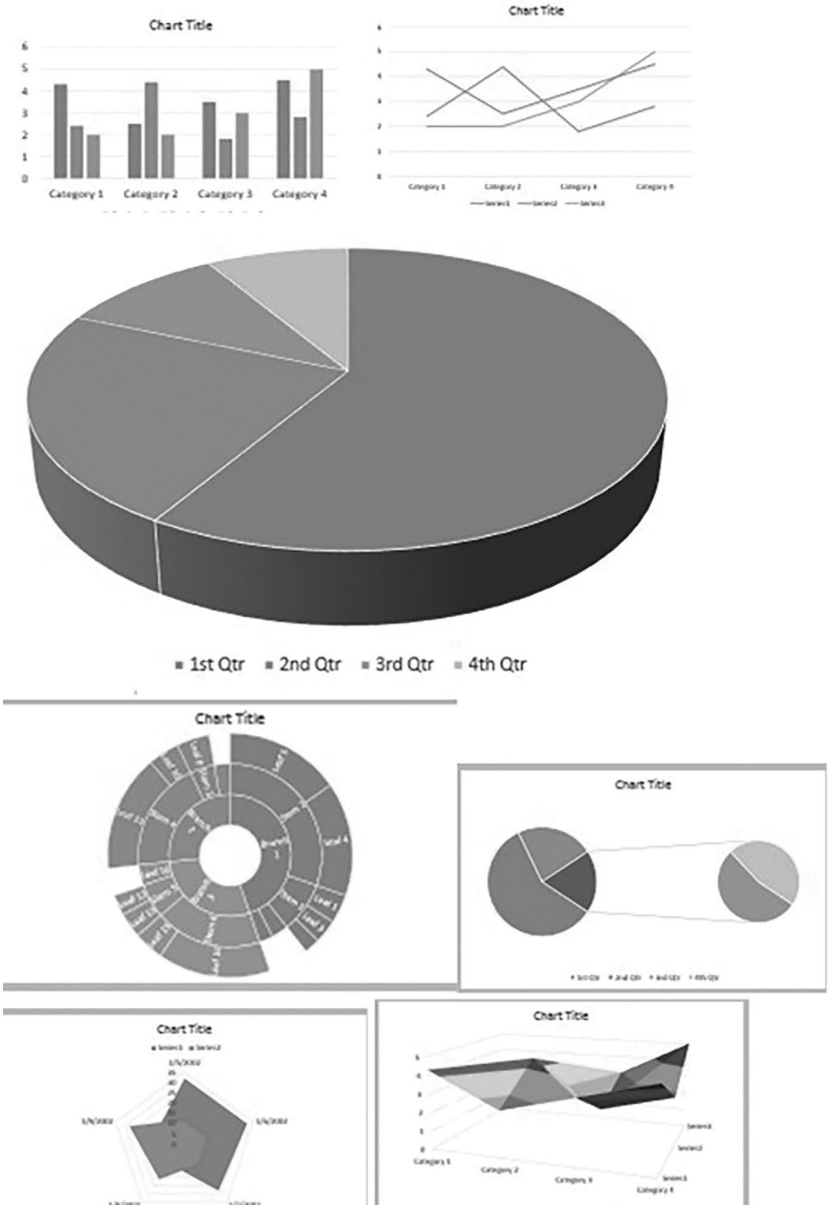


**FIGURE 4** Some types of charts for data visualization.

also be used to automate routine tasks, such as data backup and archiving (300).

In contemporary enterprises, data management software is essential. For the purpose of managing, organizing, and storing enormous volumes of data, data management services offer an organized framework. Databases are the foundation of everything from keeping track of inventory to maintaining customer data. Data management software effectively stores large amounts of data, arranging it into rows, tables, and columns. This structured organization facilitates efficient data retrieval, allowing users to quickly obtain specific information through the use of queries. The software also enables data manipulation, empowering users to add, edit, or remove data, ensuring the accuracy and currency of the database. To safeguard sensitive information, data management services employ security features such as encryption, authorization, and authentication, preventing breaches or unwanted access. Additionally, these tools offer robust data recovery and backup capabilities, routinely backing up data to ensure the continuation and integrity of the information, even in the event of system failures.

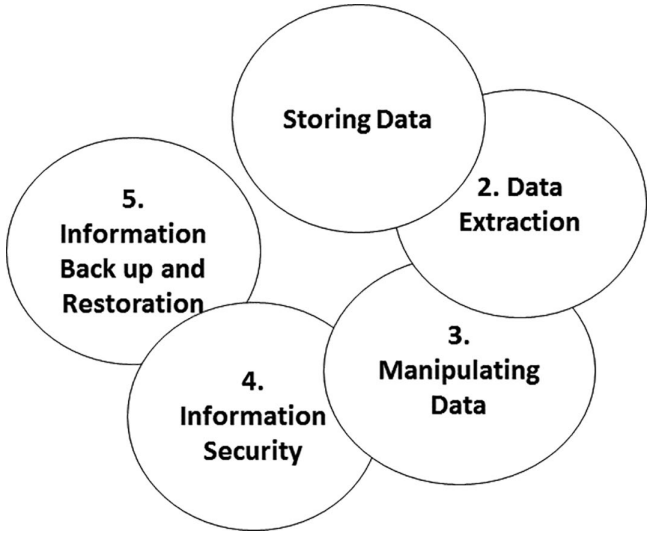


**FIGURE 5** Five essential functions in data management.

By addressing these core database management functions, data management software plays a crucial role in supporting businesses, enabling them to effectively leverage their data to drive informed decision-making and foster innovation (301).

- *Collaborative Platforms*: Collaborative platforms are online tools that allow researchers to share and analyze data collaboratively (302). For example, platforms such as GitHub or GitLab can be used to share code and data between researchers (300,303). While platforms such as Jupyter Notebooks or Google Colab can be used to run and analyze simulations in a collaborative environment (304,305).

## HOW TO IMPROVE THE REPRODUCIBILITY OF COMPUTATIONAL MODELS

Improving the reproducibility of computational models is an important goal for researchers, as it enables other researchers to validate and build upon their work, and ensures that the results are reliable and accurate. Here are a few strategies that can help improve the reproducibility of computational models:

- *Documenting the Methodology*: Researchers should document the methodology used to develop and validate the computational model, including the software tools, input parameters, and simulation protocols. This documentation should be detailed and transparent, and should be made available to other researchers through published papers, technical reports, or online repositories.
- *Version Control*: Version control is a technique used to track changes to the code and data used in the computational model, and to ensure that the results can be reproduced precisely. Researchers should use version control tools, such as Git or SVN, to track changes to the code and data, and to document the history of the model development (306).
- *Sharing the Code*: Sharing the code used to develop the computational model is an important step in improving reproducibility, as it allows other researchers to reproduce the results and build upon the work. Researchers should make their code available in online

repositories, such as GitHub or GitLab, and should ensure that the code is well-documented and easy to use.

- *Providing Input Data and Results*: This strategy used in the computational model is another important step in improving reproducibility. Researchers should make their input data and results available in online repositories, such as Figshare or Zenodo, and should ensure that the data is well-organized and annotated (307). This will enable other researchers to reproduce the results and build upon the work.
- *Using Open-Source Software*: Using open-source software tools can also help improve the reproducibility of computational models, as it allows other researchers to use and modify the software without restrictions. Researchers should use open-source software tools and should ensure that they use well-established and widely-used libraries and frameworks.
- *Conducting Sensitivity Analysis*: This is an important step in improving the reproducibility of computational models, as it enables researchers to identify the input parameters that are most critical to the accuracy of the model (308,309). Sensitivity analysis should be conducted using a range of input parameter values, and the results should be documented and reported in publications.
- *Peer Review*: Finally, This is an important step in improving the reproducibility of computational models, as it allows other researchers to evaluate the validity and accuracy of the model. Researchers should submit their work to peer-reviewed journals or conferences, and should ensure that their work is subject to rigorous peer review.

Overall, improving the reproducibility of computational models requires a combination of strategies, including documenting the methodology, using version control, sharing the code and data, using open-source software, conducting sensitivity analysis, and peer review. By following these strategies, researchers can ensure that their work is reliable, accurate, and useful to the broader scientific community.

# Conclusion 6

Ionic liquids have unique properties that make them suitable for use as electrolytes in lithium batteries. However, integrating them into existing battery designs may be challenging and require modifications. Continued research is needed to optimize the properties of ionic liquids and develop new types with improved characteristics. The interaction between cations and anions in ionic liquids is a delicate balance of forces. Researchers are exploring new battery designs or modifications to accommodate ionic liquid electrolytes.

The ion transport mechanism in ionic liquid electrolytes differs from traditional organic solvent-based electrolytes. High ionic conductivity and fast ion transport are crucial for high power output in applications like electric vehicles. The viscosity of the ionic liquid electrolyte affects ion transport and diffusion in batteries. Researchers are exploring ways to modify the ionic liquid structure or add co-solvents to reduce viscosity. Validating computational models for the electrode-ionic liquid interface requires experimental measurements, sensitivity analysis, consistency with physical principles, comparison with other models, reproducibility, and benchmarking. Careful consideration of limitations, challenges, strengths, weaknesses, and available experimental data is necessary for validating these models.

Managing and analyzing large amounts of data generated by simulations is a common challenge in computational modeling. To improve the reproducibility of computational models, researchers should document the methodology, use version control, share the code, conduct sensitivity analysis, and undergo peer review.

Improving the reproducibility of computational models is crucial for researchers. Strategies to achieve this include documenting the methodology, using version control, sharing the code and data, using open-source software, conducting sensitivity analysis, and undergoing peer review. These measures ensure that the work is reliable, accurate, and beneficial to the scientific community.

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