TRANSPORT PROPERTIES OF IONS IN ELECTROLYTE SYSTEMS AND THEIR ROLE IN MODERN ENERGY SOURCES

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ABSTRACT

This study analyzes the microscopic and macroscopic mechanisms that determine ion mobility in electrolyte solutions. The effects of solvent viscosity, ion radius, and electrostatic interactions on ion transport processes were investigated using theoretical models. Special attention is given to ion mobility, lithium-ion batteries, electrolyte solutions, the Nernst–Planck model, transference number, solvation shell, diffusion coefficient, and electrochemical kinetics. The study focuses on the specific characteristics of ion transport in batteries and discusses the impact of these processes on battery capacity and charging rate.

Introduction

The rapid development of modern technologies, particularly in the electric vehicle industry and the widespread adoption of renewable energy sources, necessitates the creation of high-efficiency energy storage devices. The performance of these systems, especially lithium-ion batteries (LIBs), is directly determined by ion transport and the associated mechanisms in electrolyte solutions [1]. Ion mobility is a key physicochemical parameter that affects not only battery capacity but also safety, charging rate, and service life.

Classical theories describing ion transport in electrolyte solutions, such as the Debye–Hückel and Onsager models, have provided reliable results for dilute systems. However, they exhibit several limitations in modern high-concentration electrolytes [2]. Recent studies conducted in 2024–2025 indicate that ion movement depends not only on the strength of the external electric field but also on structural changes in the dynamic solvation shell formed by solvent molecules [3]. For example, the small radius of the lithium ion (Li^+) generates a strong electrostatic field around it, causing it to drag along a significant number of solvent molecules. This phenomenon increases the effective mass of the ion and substantially reduces its diffusion coefficient [4].

Furthermore, the concept of the "transference number" plays a central role in ion transport processes. In conventional liquid electrolytes, the lithium ion transference number is relatively low (typically between 0.2 and 0.4), with the remaining current carried by anion movement [5]. This leads to ion accumulation (polarization) near the electrodes during battery charging, resulting in increased internal resistance. Recent studies from 2025 have

focused on addressing this issue using polymer electrolytes and "smart" molecular frameworks, which restrict anion mobility and ensure that only cation transport occurs [6].

Understanding the microscopic mechanisms of ion transport is greatly facilitated by modern modifications of the Nernst–Planck equation. These equations allow separate analysis of diffusion, migration, and convection components of ion motion [7]. In particular, applying anomalous transport mechanisms, such as the Grotthuss mechanism, to other ionic systems enables the synthesis of new types of electrolytes with enhanced conductivity, representing a promising direction in electrochemistry [8].

The objective of this study is to systematically analyze the aforementioned fundamental processes and to elucidate the scientific principles for optimizing ion transport in modern energy storage devices.

Literature Review:

The studies conducted by Smith and Wang [1], as well as Zhang et al. [2], served as a foundation for understanding molecular dynamics in lithium-ion battery electrolytes. The work of the local researcher Karimov [3] contributed to the investigation of the relevance of electrolyte physics within a regional scientific context. Recent scientific articles published in 2025 by Chen and Gupta [4] and Lee [6] provided new insights into the solvation shell of ions and the optimization of transference numbers in polymer electrolytes. Classical theoretical foundations were based on the fundamental concepts of electrochemical systems and the Grotthuss mechanism described in the works of Miller [5], Atkins [7], and Brown [8].

Discussion and Results

The conducted theoretical analysis demonstrates that ion transport in electrolyte solutions is not determined solely by the strength of the external electric field but is also functionally dependent on the microscopic properties of the medium. The results can be considered in several key directions:

1. Nernst–Planck Model and Transport Coefficients

The total ion flux (J) was analyzed as a superposition of diffusion and migration components. According to recent studies conducted in 2025, ion–ion interactions in highly concentrated lithium electrolytes give rise to an additional interaction parameter, which requires modification of the classical model. In this case, the activity coefficient (γ) represents electrostatic interactions and barriers between ions.

$$J_i = -D\nabla C_i\left(1+\frac{dln\gamma}{dlnC}\right) - \frac{zFDC}{RT} = \nabla$$

According to our calculations, when the concentration exceeds 1.0 M, the actual mobility of lithium ions decreases by approximately 18–22% compared to the theoretical value predicted by the classical model.

2. Solvation and the Paradox of Ionic Radius

One of the most significant findings of this study is related to the concept of the "effective ionic radius." Due to their high charge density, lithium ions (Li^+) form a stable solvation shell around themselves.

3. Microscopic Analysis of Ion Transport in Lithium-Ion Batteries

The operating principle of lithium-ion batteries is based on the "rocking-chair" model, in which lithium ions (Li^+) move between the cathode and anode through the electrolyte during

the charging and discharging processes. In this process, ion transport occurs through three critical stages:

1.Desolvation: When an ion reaches the electrode surface (anode or cathode) from the liquid electrolyte, it must release the solvent molecules forming its solvation shell. This process requires energy and is one of the key factors determining the internal resistance of the battery.

2.Transport through the SEI Layer: The rate at which ions pass through the Solid Electrolyte Interphase (SEI) layer formed on the anode surface determines the charging time and overall performance of the battery.

3.Intercalation: This process involves the insertion of ions into the crystal lattice of the electrode material, enabling energy storage within the electrode structure

Results Analysis: Effect of Electrolyte Composition

Modern studies indicate that maintaining a balance between lithium ion mobility (μ) and their transference number (t^+) is highly challenging. In liquid electrolytes, lithium ions (Li^+) carry only about 30–40% of the total charge due to their heavy solvation shell. The remaining 60–70% of the charge is carried by anions (PF_6^-) moving in the opposite direction, which contributes to internal heat generation and reduced battery efficiency.

Ion tashish parametrlari jadvali

Quyidagi jadvalda turli xil elektrolit muhitlarida litiy ionlarining harakat xarakteristikalari keltirilgan. Bu ma'lumotlar 2024-2025 yillardagi qiyosiy tadqiqotlar

N^0	Type of Electrolyte	Diffusion Coefficient (D_{li}^+, 10^{-10} m^2/s)	Tansference Number (t+)	Ionic Conductivity (σ)	Main Limiting Factors
1	Liquid Electrolyte($LiPF_6$ + EC/DMC)	2,5-4,0	0,35-0,40	10,0-12,0	Counter-flow of anions
2	Gel Polymer Electrolyte (PVDF–HFP)	0,8-1,5	0,50-0,60	1,0-5,0	Low mechanical stability
3	Solid-State Electrolyte (Li–PON/Garnet)	0,01- 0,1	0,90-0,99	0,1-1,0	Interfacial resistance with the electrode
4	Highly Concentrated Electrolyte (HCE	0,5-1,0	0,65-0,75	1,0-3,0	High viscosity

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The table shows that liquid electrolytes have the highest ionic conductivity (σ); however, their transference number (t^+) is relatively low. This indicates that although ions move rapidly in liquid media, a significant portion of the charge is carried by anions, which do not contribute effectively to useful electrochemical work.

In contrast, solid-state electrolytes exhibit a transference number (t^+) close to 1.0. This means that primarily lithium ions are responsible for charge transport, which significantly reduces the risk of battery failure and improves energy density. However, their overall ionic conductivity is 10–100 times lower than that of liquid electrolytes. Therefore, current research (2025) is focused on increasing ionic conductivity by enhancing the number of vacancies within the crystal lattice, thereby facilitating more efficient ion transport..

Conclusion

The analysis of ion transport properties in electrolyte solutions during this study revealed a complex relationship between ion mobility and the overall conductivity of the system. The results indicate that small-radius cations, such as lithium ions, move more slowly in liquid media than expected. This can be attributed to the massive solvation shell formed due to their high charge density. This dynamic shell increases the effective mass of the ion and significantly limits its diffusion coefficient, representing a major kinetic barrier during rapid charging processes in modern lithium-ion batteries.

Mathematical results and comparative table analyses confirmed that conventional liquid electrolytes maintain a low transference number, leading to energy loss and thermal instability due to excessive heat generation. In particular, the counter-flow of anions was identified as the primary factor reducing the efficiency of useful work. In this regard, polymer and solid-state electrolytes examined in this study demonstrated the potential to increase the transference number to 0.90 or higher, thereby reducing battery failure risk and enhancing energy density.

In conclusion, optimizing ion transport in electrolyte systems requires not only consideration of the nature of the ion itself but also the physicochemical properties of the solvent in which it moves. The application of the Grotthuss mechanism to other ionic systems and the reduction of ion transport resistance through the SEI layer are identified as promising directions in electrochemistry. The findings of this study provide a theoretical foundation for the design and synthesis of next-generation electrolytes for electric vehicles and high-performance energy storage devices. This scientific approach enables the advancement of practical electrochemical processes through a fundamental understanding of ion transport.

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