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Perspective

Lithium bond chemistry in lithium batteries

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SUMMARY

The lithium bond is an essential weak interaction in lithium batteries, critically influencing ion transport, interfacial reactions, and electrochemical performance. Herein, the current understanding of lithium bond chemistry is systematically discussed across different lithium species and their associated electrochemical behaviors. We first discuss the lithium bonds formed between monomeric lithium ions and guest molecules, with an emphasis on their structural characteristics and functional roles in both liquid and solid phases. The discussion is then extended to lithium complexes, focusing on how the lithium bond drives short-range and long-range structure organization and corresponding functionality. Furthermore, the synergy between the lithium bond and strong ionic/covalent bonds is highlighted, emphasizing how their balance can inform the rational design of advanced lithium batteries. Finally, future research directions in lithium bond chemistry are outlined, aiming to accelerate the development of advanced lithium batteries and enrich the chemical understanding of weak interactions in the broader context of modern chemistry.

INTRODUCTION

The global energy revolution necessitates the advancement of efficient and reliable energy storage technologies to critically support sustainable development worldwide.[1] Lithium (Li) batteries, as a cornerstone of modern energy storage systems, play an indispensable role in enabling the integration of clean energy supply and consumption.[2] With their applications rapidly expanding from consumer electronics to electric vehicles and smart grids, the performance requirements of Li batteries have become increasingly stringent.[3–5] These requirements demand the simultaneous realization of high energy density, long cycle life, fast charging capability, intrinsic safety, and wide operational temperature tolerance.[6] Meeting these multidimensional and often competing objectives presents complex and interconnected challenges, underscoring the intrinsic limitations of existing Li battery technologies. Addressing these challenges requires a deeper fundamental understanding of the energy chemistry governing Li batteries.

At the core of Li battery operation lies the interaction between Li species and surrounding components, which constitutes the physicochemical basis of energy storage and conversion. Historically, research efforts have predominantly focused on strong chemical interactions such as ionic, covalent, and coordination bonds in battery systems (Figure 1A). These strong interactions play decisive roles in constructing electrodes and electrolytes, elucidating complicated electrochemical behaviors, and regulating bulk and interfacial processes for battery performance improvement. Accordingly, extensive studies on strong chemical bonds have driven substantial progress in battery chemistry and established a prevailing research paradigm centered on strong interaction engineering.[7]

In contrast to the well-studied strong interactions, weak interactions in Li batteries, including van der Waals forces, hydrogen bonds, and the emerging concept of Li bonds, remain less explored and insufficiently exploited. Despite their lower bond energies than conventional chemical bonds, the ubiquity and collective effects of these weak interactions can profoundly influence practical battery behaviors. For instance, in highly concentrated aqueous electrolytes, hydrogen-bond networks formed between water molecules and anions effectively suppress water decomposition and hydrogen evolution, thereby significantly expanding the electrochemical stability window.[8] Conversely, in layered electrode materials such as graphene and MXene, van der Waals force-induced stacking and agglomeration of nanosheets severely hinder ion transport, reducing active site availability and deteriorating rate capability.[9] These examples demonstrate that weak interactions play non-negligible and often decisive roles in regulating Li battery performances.

Against this backdrop, research interest has increasingly shifted from an exclusive emphasis on strong chemical bonds toward a broader exploration of weak interactions in Li batteries, with the lithium bond rapidly emerging as a new research frontier.[10,11] The concept of the Li bond was first proposed by Shigorin in 1959[12] and has been investigated for over six decades.[13,14] Broadly defined, the Li bond refers to a type of

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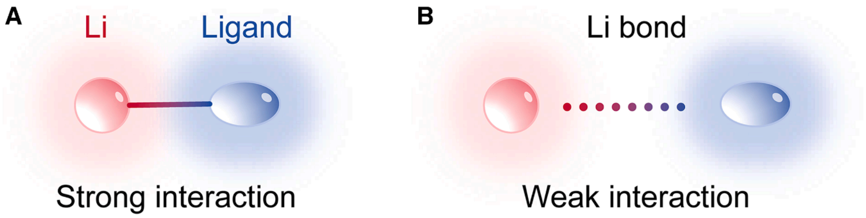

Figure 1. Interactions in Li batteries

(A) Schematic illustration of strong interactions, characterized by high bond energy, short interaction distance, and high stability.

(B) Schematic illustration of Li bonds as weak interactions, exhibiting low bond energy, long interaction distance, and dynamic characteristics with facile formation and dissociation.

secondary weak interaction formed between host Li species and electron-donating atoms or functional groups of guest molecules.[15] Characterized by relatively low bond energy, longer interaction distance, and dynamic behaviors that favor facile formation and dissociation (Figure 1B), the lithium bond critically influences the solvation structure of Li ions, the energy barrier of ion transport in electrolyte or electrodes, and the thermodynamics and kinetics of interfacial electrochemical processes. A systematic investigation of the formation principles, dynamic evolution, and regulation methodology of the Li bond under practical battery operating conditions is therefore highly desirable, not only to expand the theoretical framework of energy chemistry but also to provide new avenues for overcoming key challenges in contemporary Li batteries.

In this perspective, we focus on lithium bond chemistry in Li batteries and aim to elucidate the mechanisms and functions of the Li bond across different Li species. We begin by discussing Li bonds formed between monomeric Li ions and electron-rich guest molecules, highlighting their roles in regulating liquid-solid interfacial behaviors and ion transport in the solid phase. The discussion is then expanded to Li-containing complexes, emphasizing the critical functions of lithium-bond-induced short- and long-range structures across diverse electrochemical processes. Finally, we present an outlook on the synergy between strong and weak interactions in battery systems, underscoring the pivotal role of Li bond chemistry in advancing next-generation high-performance Li batteries.

LI BOND OF MONOMERIC LI IONS

In Li battery systems, the interaction between monomeric Li ions and surrounding guest molecules critically determines the fundamental physicochemical properties of Li-containing species. In typical liquid-phase electrolytes, conventional strong interactions lead to tightly bound solvation structures between Li ions and guest species, characterized by high bond energy and high coordination number, which enhance structural stability (Figure 2A). Such solvation structures substantially increase the energy barrier for Li ion desolvation, which in turn limits the fast-charging capability of Li batteries.[16,17] On the contrary, introducing weakly solvating solvents enables the construction of solvation structures dominated by the Li bond. The Li-bond-dominated configurations exhibit lower bond energy and reduced coordination number, resulting in more facile dissociation and reorganization and thereby facilitating fast-charging Li batteries. For instance, Yao et al. employed 1,4-dioxane as a weakly solvating solvent to create an anion-dominated Li-bond-rich solvation structure.[18] The relatively weak Li-solvent/anion interactions significantly reduce the energy barrier associated with Li ion desolvation and transport across the solid electrolyte interphase (SEI). As a result, graphite anodes retain 54% of their capacity even under a high rate of 4 C. Moreover, the anion-derived inorganic-rich SEI effectively suppresses solvent co-intercalation, thereby enhancing battery cycling stability as well. Similarly, the use of sterically bulky or charge-delocalized anions establishes weakly coordinated and Li-bond-rich microenvironments that accelerate charge transfer kinetics at the electrode-electrolyte interface, collectively improving high-rate performances.[19]

Under extremely low-temperature conditions, strongly solvating electrolytes often induce Li dendrite growth and rapid capacity decay due to elevated desolvation energy barriers and increased interfacial impedance.[20] By contrast, the inherent weak and dynamic nature of the Li bond facilitates fast kinetics even at low temperatures.[21,22] A representative strategy involves incorporating oxygen-free solvents such as n-hexane with monoethers such as hexyl methyl ether, which effectively reduce the electron-donating ability of solvent molecules and weaken Li ion-solvent interactions.[23] Such a configuration allows the electrolyte to maintain an ultralow desolvation barrier at -30°C and promotes uniform Li deposition without dendrite formation, clearly demonstrating the advantages of Li bond regulation in extending battery operation across wide temperature ranges. Notably, excessively weakening solvation interactions may hinder effective Li bond formation and compromise bulk ionic conductivity. Therefore, solvents with moderate solvation ability, such as fluorinated esters[24] or ethoxy-side-chain difluoro-substituted solvents,[25] are more favorable to form Li bonds, simultaneously supporting fast ion transport and suitable interfacial properties in working Li batteries.

In the solid phase, the Li bond also plays a critical role in regulating ion-transport behaviors (Figure 2B). In conventional crystalline solid electrolytes, Li ions are confined to specific lattice sites by strong coordination within rigid anionic frameworks, resulting in high migration energy barriers and limited ionic conductivity. By constructing Li-bond-dominated coordination environments, these constraints can be effectively circumvented, enabling rapid ion conduction. A representative example is provided by halide-based superionic conductors developed by Prof. Sun's group, where a tailored anionic arrangement promotes the formation of low-coordination and distorted [$LiCl_x$] configurations characteristic of Li-bond-rich environments.[26] This structure provides sufficient localization to stabilize Li ions while substantially lowering the energy barrier for Li ion hopping between adjacent sites, thereby enabling rapid "hop-and-migrate" conduction and underscoring the vital role of the Li

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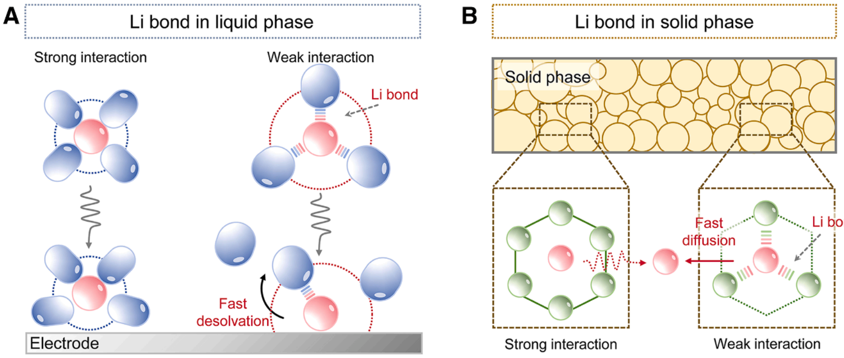

Figure 2. Li bond formed by monomeric Li with guest species

(A) Solvation structures in liquid phase formed via strong interactions or a Li bond. The loose Li-bond-induced structures lower the Li ion desolvation barrier, enabling faster interfacial reactions.

(B) Solid-phase structures formed through various interactions. The Li-bond-dominated unsaturated coordination reduces the Li ion migration barrier, facilitating rapid bulk transport.

bond in achieving superionic conductivity in amorphous systems.

Similarly, in polymer-based solid electrolytes, Li bond regulation contributes to enhanced ion transport and interfacial stability.[27] Introducing solvents with moderate solvation ability weakens otherwise strong interactions between Li ions and anions or polymer segments. Such Li-bond-dominated structures accelerate ion migration kinetics and promote the formation of a thin and uniform SEI or cathode-electrolyte interphase (CEI) rich in inorganic components, thereby significantly improving interfacial stability and ion-transport efficiency.[28] Building on these principles, Prof. Zhang's team at Tsinghua University fabricated a solid-state polymer electrolyte pouch cell with an actual energy density exceeding 600 Wh kg^{-1} while maintaining exceptional safety performance.[29] This achievement underscores the substantial potential of Li bond regulation in guiding the development of next-generation high-energy-density and safe solid-state batteries.

LI BOND IN LI COMPLEXES

Li species in battery systems also exist as Li complexes, including solvated Li ions; anion-induced contact ion pairs (CIPs) and aggregates (AGGs); and molecular Li compounds such as Li polysulfides (LiPSs). It is therefore essential to treat these Li complexes as integral entities and analyze the Li bond interactions with surrounding guest species, including solvents, anions, and functional groups on electrode surfaces. The ability of a Li complex as a Li bond donor is fundamentally governed by its intrinsic molecular dipole moment, which originates from the pronounced electronegativity difference between electropositive Li and the electronegative atoms to which it is bonded. When a compatible dipolar guest species is present, the Li complex may serve as the host for Li bond formation through dipole-dipole interaction, a mechanism distinct from hydrogen bonding. Such dipole-dipole interaction differs from traditional coordination bonding by one electron donor and one electron acceptor. The dipole structure and dipole-dipole interaction play a key role in forming the Li bond.

Li bond interactions between Li complexes and guest species give rise to distinct short-range structures (Figure 3A). Owing to their weak and dynamic nature, these Li bond configurations achieve a balance of dynamic stability, avoiding both ineffective binding and excessive rigidity.[30] In Li-sulfur (S) batteries, for instance, where the shuttle effect of LiPSs severely compromises battery cycling stability, introducing polar electrocatalysts capable of forming moderate-strength Li bonds with LiPSs allows for precise modulation of adsorption strength.[10,31,32] This approach effectively anchors LiPSs to suppress shuttle while preserving rapid diffusion and conversion kinetics owing to the dynamic and reversible character of the Li bond, thereby achieving optimized adsorption-conversion synergy.[33,34]

A similar Li-bond-guided strategy is employed to optimize Li metal anodes to promote uniform Li deposition. Featuring dipole structures formed by electron-donating pyridinic and pyrrolic nitrogen and electron-accepting skeleton carbon, heteroatom-doped carbon substrates establish moderate Li bonds with solvated Li complexes during Li deposition.[35] Spectroscopic and computational analyses reveal that these Li-bond-induced short-range structures reduce the nucleation barrier recognized as lithiophilicity. These lithiophilic sites guide uniform Li nucleation and ultimately yield dense and dendrite-free Li deposition, which is favorable for achieving high Coulombic efficiency and long cycling stability in Li metal batteries.

When the spatial configuration and interaction capability of the Li complexes are well matched, the Li bond can further extend to form long-range dynamic network structures (Figure 3B). In high-concentration electrolytes (HCEs) and localized HCEs (LHCEs) where anion-Li^{+} coordination predominates, large solvated micelles corresponding to CIPs and AGGs emerge. Within these systems, the Li bond forms between adjacent micelles to stabilize the system against precipitation into the solid phase, thereby maintaining homogeneity and long-term stability.[36,37] Beyond conventional electrolyte systems, long-range Li bond networks also provide a plausible explanation for distinctive phenomena observed in specialized systems. For example, recent phase-diagram studies of Li–S batteries indicate that LiPSs form gels rather than precipitate as solids at ultrahigh concentrations, most likely arising from a three-dimensional network stabilized by the Li bond formed among LiPSs or between LiPSs and guest species.[38] Such LiPS gelation impedes ion transport and accelerates battery failure, indicating that suppressing the formation of such long-range Li bond networks is essential for designing high-energy-density Li–S batteries.[39]

SYNERGISTIC EFFECTS BETWEEN LI BOND AND STRONG INTERACTIONS

In the complex chemical environment of Li batteries, strong interactions (e.g., ionic and covalent bonds) and weak interactions (e.g., Li

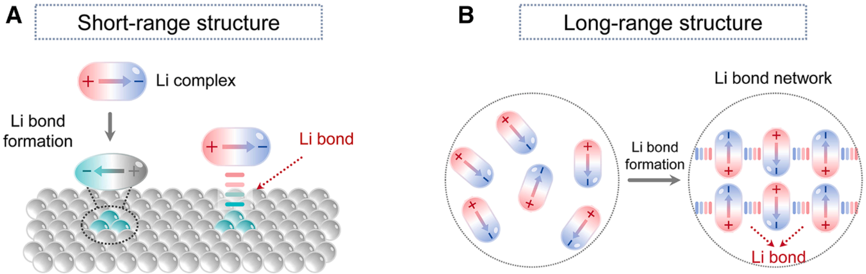

Figure 3. Li bond formed between Li complexes and guest species

(A) Schematic diagram of short-range structures formed by a Li bond between a Li complex and a guest species.

(B) Schematic diagram of long-range structures formed by a Li complex with itself or with other guest species.

bonds) coexist and function synergistically, collectively determining the overall battery performance. The comprehensive understanding and deliberate regulation of the synergy between these two types of interactions represents a critical paradigm for developing next-generation high-performance Li batteries (Figure 4).

The fundamental principle underlying this synergy is the use of strong interactions to establish stable structures while utilizing Li bonds to facilitate dynamic processes. Strong interactions, such as metal–oxygen bonds in electrode materials, form the structural skeleton of battery systems. They provide mechanical integrity and robustness during repeated cycling. However, overly rigid and strong interactions may impair kinetic performance. In this context, Li bonds act as dynamic “joints.” Their low bond energy and rapid reorganization capability generate low-energy-barrier hopping sites or efficient interfacial transport pathways without compromising structural stability. For instance, in solid-state electrolytes, strong interactions maintain a stable crystalline or molecular framework, while Li bonds formed between Li ions and certain framework atoms (e.g., halogens) establish a dynamic and continuous coordination environment. This synergistic combination significantly lowers the activation energy for Li ion migration, achieving high ionic conductivity without sacrificing structural stability.

SUMMARY AND OUTLOOK

This perspective elucidates the pivotal role of the Li bond as an essential secondary weak interaction in Li batteries, offering a renewed theoretical framework for the rational design of high-performance battery systems. The mechanistic functions of Li bonds are analyzed across two distinct domains: at the level of monomeric Li species, the Li-bond-facilitated dynamic structures significantly enhance desolvation kinetics at electrode-electrolyte interfaces and promote rapid ion transport within solid phases; at the level of Li complexes, the Li-bond-induced short-range and long-range structures establish a theoretical basis for regulating interfacial electrochemical processes and stabilizing high-concentration systems. Furthermore, this perspective highlights that the synergistic interplay between strong interactions and Li bonds is crucial for developing advanced batteries capable of addressing multifaceted performance requirements. Beyond the notable advances in Li bond research, this emerging research field continues to present fundamental challenges that warrant deeper exploration.

In terms of structural characterization, the anomalous ^{7}Li-nuclear magnetic resonance (NMR) chemical shift has emerged as preliminary experimental evidence for Li bond formation,[40] while the Li coordination number has been proposed as a quantitative descriptor.[41] Future efforts should prioritize the development of more accurate and sensitive *in situ* or *operando* characterization techniques (e.g., synchrotron X-ray absorption spectroscopy), integrated with high-throughput computational screening and *ab initio* molecular dynamics simulations. Such approaches will enable the systematic resolution of Li bond parameters, including bond energy, bond length, directionality, and dynamic evolution, revealing their structure-activity relationships at the atomic scale and strictly distinguishing them from other Li-containing interactions.

The integration of artificial intelligence (AI) offers transformative potential for Li bond research. Beyond identifying and analyzing Li bond features, employing physicochemical parameters such as bond energy, bond length, symmetry, and electron cloud density of the Li bond as descriptors in machine learning may inversely guide electrolyte formulation, additive molecule design, and interface engineering strategies, which promise to significantly shorten development cycles and accelerate innovation in battery technology.

With respect to the broader expansion of Li bond chemistry, current research is largely focused on Li battery systems. Whether the “weak interaction with strong functional effect” represented by the Li bond is a universal phenomenon across diverse chemical systems remains an open question.[42,43] For instance, incorporating Li bond networks into polymer elastomers yields materials that simultaneously exhibit high toughness, self-healing capability, and ionic conductivity.[44,45]

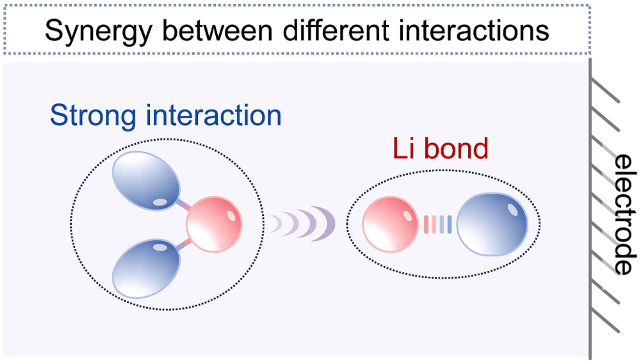

Figure 4. Synergistic effects between a Li bond and other strong interactions in Li batteries

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Exploring the universality of Li bonds across diverse systems, such as other alkali metal battery systems or broader fields, may unlock new directions in chemistry.

In conclusion, deepening the understanding of Li bond chemistry is expected to enrich the broader framework of weak interaction chemistry and advance modern chemical bond theory. The exploration of Li bonds aims not only to enable superior Li batteries but also to address a fundamental objective of chemistry: understanding and controlling microscopic interactions in matter.

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AUTHOR CONTRIBUTIONS

Conceptualization, Q.Z.; writing – original draft, J.Z.; writing – review & editing, J.Z., M.Z., X.-Y.L., B.-Q.L., and Q.Z.; funding acquisition, M.Z., B.-Q.L., and Q.Z.; resources, M.Z., B.-Q.L., and Q.Z.; supervision, Q.Z.

DECLARATION OF INTERESTS

The authors declare no competing interests.

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