Turning Literature into Knowledge: AI-Driven Discovery of Solid-State Electrolytes

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Abstract

This study proposes an integrated discovery framework for next-generation battery applications, aimed at elucidating composition–structure–property relationships in sulfide solid electrolytes. The framework combines literature-derived data extraction, knowledge graph (KG) construction, large language model (LLM)–driven candidate material proposal, and validation through molecular dynamics (MD) simulations with machine-learning interatomic potentials. From 125 collected articles, 56 meeting quality criteria were converted into 146 normalized records that contained composition, space group, density, measurement temperature, and ionic conductivity, and 46 high-confidence entries were used to build the knowledge graph. Conditioning an LLM on the KG resulted in the identification of two novel candidate materials absent from the graph ($\mathrm{Li_{11}Si_2PS_{12}}$ and $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$). Diffusion simulations using GRACE and MACE over 600–1400 K, along with Arrhenius extrapolation, predicted activation energies of 0.21 and 0.20 eV and room-temperature ionic conductivities of 12.7 and 14.0 mS cm^{-1}, which are sufficiently high to be considered practically applicable. This end-to-end AI-driven framework is expected to establish a generalizable, data-centric paradigm for materials discovery that transcends conventional design limits, regardless of the targeted application domain.

1 Introduction

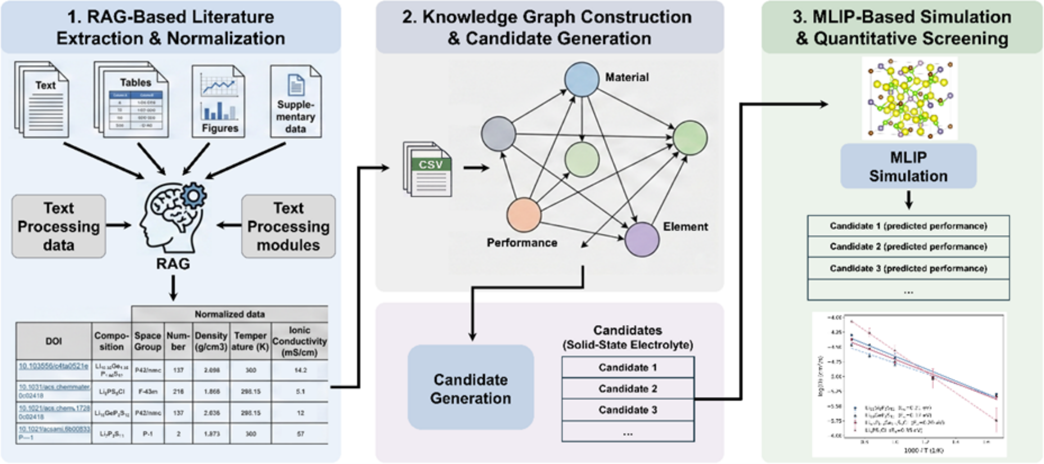
All-solid state batteries are emerging as a leading next-generation energy storage system capable of achieving both high energy density and safety [1]. Realizing their commercial potential requires the discovery of solid electrolyte materials that simultaneously satisfy conflicting requirements such as ionic conductivity, electrochemical stability, mechanical properties, and processability [2]. The primary challenge lies in the virtually infinite combinations of chemical compositions and crystal structures. Given this vast search space, traditional experimental trial-and-error methods face clear limitations due to excessive cost and time constraints.

To address these challenges, the materials science community has adopted high-throughput screening and artificial intelligence based on large-scale computational databases like the Materials Project and OQMD [3, 4, 5]. While these databases offer extensive data under unified protocols, they possess a critical limitation as they predominantly assume ideal crystal structures at absolute zero temperature without defects. In contrast, the actual performance of solid electrolytes is governed by realistic factors including operating temperatures, synthesis conditions, and grain boundary characteristics [6]. Consequently, this reality gap between idealized calculations and physical experiments becomes a major cause of failure during validation and undermines the reliability of data-driven exploration.

Scientific literature accumulated over decades represents the richest source of data capable of bridging this gap [7]. These documents contain actual ionic conductivity data across various synthesis conditions and temperatures. However, this information remains fragmented across unstructured text, tables, and figures using inconsistent unit systems [8]. Although human researchers can interpret these nuances, the structural limitations prevent artificial intelligence models from systematically learning or analyzing this knowledge. As a result, vast amounts of literature remain unutilized as data assets.

This study proposes an integrated framework that overcomes the unstructured nature of literature and combines it with computational science to present a new pathway for materials discovery (Fig. 1). Our primary contributions are summarized as follows:

- **Literature-Based Data Assetization:** We implemented Retrieval-Augmented Generation (RAG) to extract composition, temperature, and ionic conductivity from text and tables into a standardized schema with normalized units, converting literature into a machine-readable dataset and easing the data-availability bottleneck.
- **Structuring Condition-Performance Relations:** Beyond property lists, we organized the extracted data as a Knowledge Graph (KG) to capture structure–property links and preserve the context of processing conditions, enabling exploration under realistic conditions.
- **Knowledge Graph-Based Candidate Design:** We conditioned Large Language Models (LLMs) on KG-grounded literature evidence to propose new materials, reducing chemically invalid hallucinations and prioritizing feasible candidates consistent with established trends.
- **MLIP-Based Extended Validation:** To reduce DFT cost and move beyond 0 K assumptions, we performed large-scale simulations using Machine Learning Interatomic Potentials (MLIPs), enabling efficient evaluation of stability and ion diffusion at operating temperatures to shortlist promising candidates.

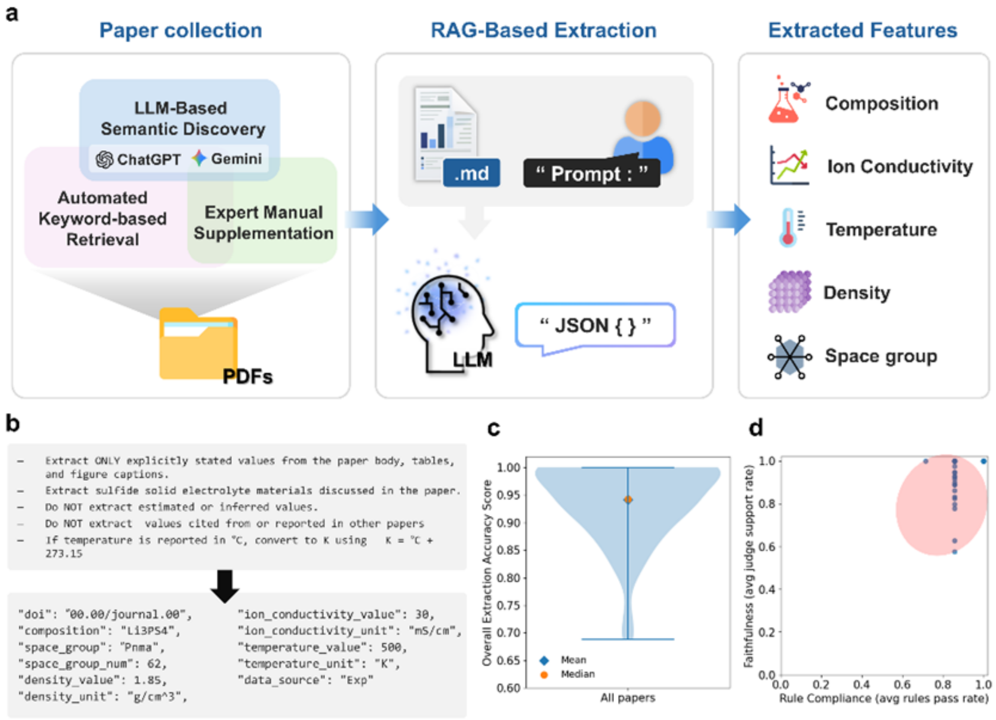

1. RAG-Based Literature Extraction & Normalization
Text
Tables
Figures
Supple-mentary data
Text Processing data
Text Processing modules
RAG
2. Knowledge Graph Construction & Candidate Generation
CSV
Material
Performance
Element
Candidate Generation
Candidates (Solid-State Electrolyte)
Candidate 1
Candidate 2
Candidate 3
...
3. MLIP-Based Simulation & Quantitative Screening
MLIP Simulation
Candidate 1 (predicted performance)
Candidate 2 (predicted performance)
Candidate 3 (predicted performance)
...
1000 / T (1/K)

		Normalized data				
DOI	Composition	Space Group	Number	Density (g/cm3)	Temperature (K)	Ionic Conductivity (mS/cm)
10.103556/c4ta0521e	$Li_{10.35}Ge_{1.35}P_{1.65}S_{12}$	P42/nmc	137	2.098	300	14.2
10.1031/acs.chemmater.0c02418	Li_6PS_5Cl	F-43m	216	1.868	298.15	5.1
10.1021/acs.chem.1728 0c02418	$Li_{10}GeP_2S_{12}$	P42/nmc	137	2.036	298.15	12
10.1021/acsami.6b00833 P—1	$Li_7P_3S_{11}$	P-1	2	1.873	300	57

Figure 1: Schematic of an integrated RAG-KG-MLIP framework for solid-state electrolyte discovery.

2 RAG-based Data Extraction

As shown in Fig. 2a, the overall workflow begins with a literature acquisition stage that integrates multiple search strategies and then expands into RAG-based automated information extraction and quantitative evaluation. We collected more than 100 papers on sulfide solid-state electrolytes via a multi-path acquisition protocol and selected 56 papers that satisfy pre-defined quality criteria as the final analysis set. Papers not directly relevant to sulfide solid electrolytes or lacking sufficient quantitative data were excluded. The same curated corpus was used consistently across all subsequent automated extraction and evaluation steps. Additional details of the acquisition strategy are provided in the Appendix. For knowledge graph construction and downstream new-material prediction, we define the target feature set to capture properties and structural information most directly linked to ionic conductivity in sulfide electrolytes. Concretely, we use LLM-guided feature selection step using ChatGPT-5.2 and Gemini-3, and finalize the extracted fields such as: DOI, composition, space group, space group number, density, ionic conductivity, temperature, and data source (calculation vs. experiment).



```
–   Extract ONLY explicitly stated values from the paper body, tables,
    and figure captions.
–   Extract sulfide solid electrolyte materials discussed in the paper.
–   Do NOT extract estimated or inferred values.
–   Do NOT extract  values cited from or reported in other papers
–   If temperature is reported in °C, convert to K using   K = °C +
    273.15
```

```
"doi": "00.00/journal.00",            "ion_conductivity_value": 30,
"composition": "Li3PS4",              "ion_conductivity_unit": "mS/cm",
"space_group": "Pnma",                "temperature_value": 500,
"space_group_num": 62,                "temperature_unit": "K",
"density_value": 1.85,                "data_source": "Exp"
"density_unit": "g/cm^3",
```

Figure 2: (a) LLM-RAG–based data collection pipeline for sulfide solid electrolytes. (b) Examples of the document-grounded extraction setup and structured outputs. (c) Distribution of extraction accuracy across all analyzed papers. (d) Relationship between rule compliance and faithfulness for individual documents.

Feature extraction from each paper is performed using a document-grounded extraction RAG setup, where a single document is mapped to a structured JSON record. Specifically, we convert each PDF into markdown text and provide it to the model together with a pre-defined prompt. The model is instructed to generate structured outputs only from information explicitly stated in the provided text, enforcing document-grounding and reducing unsupported inference. We implement this pipeline using LangChain [9] and Gemini-2.5-Flash and the average processing cost is approximately 24.3 KRW per PDF, and the average processing time is approximately 1 minute per PDF. Using this pipeline, we extract a total of 146 independent data records from the curated literature set. Fig. 2b presents the prompt template used in our extraction pipeline and a corresponding example of the structured output.

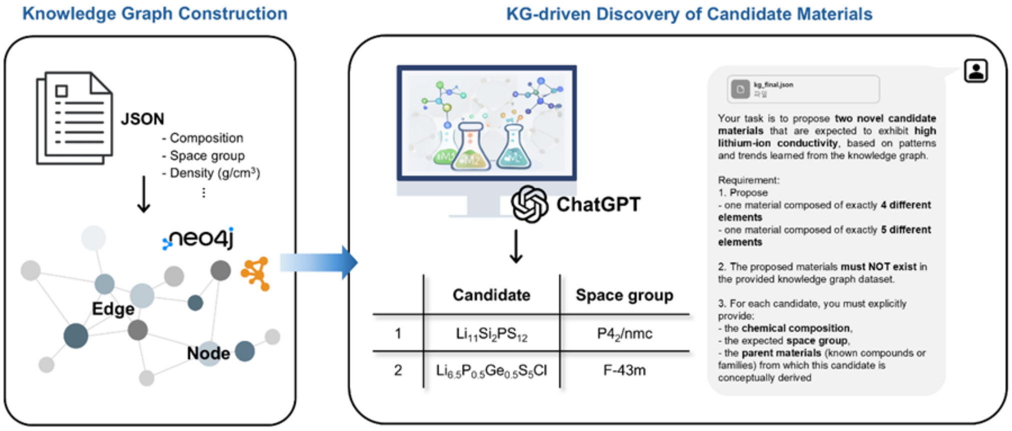
To assess the quality of the extracted records, we apply (i) rule-based validation that checks whether each output satisfies the required structural constraints, and (ii) an LLM-as-judge protocol to evaluate faithfulness, i.e., whether each extracted value is supported by evidence in the source document. This evaluation procedure is designed following a recently proposed reliability evaluation framework for RAG systems [10]. Fig. 2c summarizes the distribution of extraction accuracy computed over the full set of papers. We compute the accuracy as follows.

$$A_{\text{overall}} = 0.4\,A_{\text{rule}} + 0.6\,A_{\text{faith}}$$

The mean and median of the overall extraction accuracy are 0.942 and 0.943, respectively, indicating a highly concentrated score distribution in the high-accuracy regime. This suggests that the extraction performance exhibits neither strong systematic skews nor a large number of catastrophic failure cases. Fig. 2d shows a scatter plot of rule compliance versus faithfulness at the paper level. The average rule compliance and faithfulness are 0.918 and 0.957, respectively, and all analyzed papers lie in the upper-right region. This indicates that the outputs not only satisfy the structural constraints, but that the extracted numerical values are also explicitly supported by the source text.

After extraction, we apply an additional preprocessing filter to improve downstream reliability by removing records that do not explicitly report both ionic conductivity and density. This criterion is designed to minimize error propagation caused by incomplete inputs in subsequent stages, including knowledge graph construction, generative structure proposal, and MLIP-based physical validation. From 146 initially extracted records, after filtering, we obtained a final dataset of 46 sulfide solid-state electrolyte property records with clear provenance and improved numerical reliability.

3 Knowledge Graph Construction and KG-guided Materials Proposal



	Candidate	Space group
1	$Li_{11}Si_2PS_{12}$	$P4_2/nmc$
2	$Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl$	F-43m

Your task is to propose **two novel candidate materials** that are expected to exhibit **high lithium-ion conductivity**, based on patterns and trends learned from the knowledge graph.

Requirement:
1. Propose
- one material composed of exactly **4 different elements**
- one material composed of exactly **5 different elements**

2. The proposed materials **must NOT exist** in the provided knowledge graph dataset.

3. For each candidate, you must explicitly provide:
- the **chemical composition**,
- the expected **space group**,
- the **parent materials** (known compounds or families) from which this candidate is conceptually derived

Figure 3: Construct a Neo4j knowledge graph from RAG-extracted JSON records, then use the KG as context to propose novel electrolyte compositions with space-group hypotheses, excluding compositions already present in the KG.

In this section, we briefly describe how we use the constructed knowledge graph to propose new sulfide solid-state electrolyte candidates. As illustrated in **Fig. 3**, converting literature-extracted information into a KG provides a structured context that captures relationships among composition, crystallographic descriptors, properties, and measurement conditions, which in turn helps define a principled search space for candidate exploration. We leverage this KG context to guide an LLM to propose novel compositions that are not present in the curated dataset, and to provide a plausible space-group hypothesis for each candidate together with a brief rationale grounded in related compositional families observed in the KG. We emphasize that this section focuses on candidate proposal (composition and structural hypothesis), while the concrete procedure for crystal structure generation and subsequent physical validation is described in the following sections.

3.1 Element Frequency Analysis

We analyze the sulfide solid-state electrolyte dataset extracted via our RAG pipeline. We first compute the frequency of constituent elements and observe that Li, P, and S dominate the corpus (Fig. 4a). This reflects the fact that the most fundamental compositional family in sulfide electrolytes is the Li_2S–P_2S_5 (LPS) system, and that a substantial fraction of prior work has been developed around LPS-derived formulations [11, 12].

Among the next most frequent elements, Ge appears with relatively high prevalence, which we attribute to the influence of studies on $Li_{10}GeP_2S_{12}$ (LGPS)-type electrolytes [13, 14]. In addition, among halogens, Cl and I show meaningful occurrence, consistent with the prominence of argyrodite-structured sulfide electrolytes in the [15].

This elemental distribution indicates that prior studies on sulfide solid-state electrolytes have predominantly focused on a limited compositional domain. The elements identified are mainly drawn from the p-block, whereas transition metals are only rarely observed. This trend aligns with prior observations that transition metals can introduce electronic conduction pathways or trigger undesirable redox activity, thereby limiting their suitability as constituent elements in solid electrolytes [16]. Overall, our element-frequency analysis not only quantitatively confirms that sulfide solid-state electrolyte research largely progressed within a relatively constrained compositional subspace centered on LPS-derived chemistries.

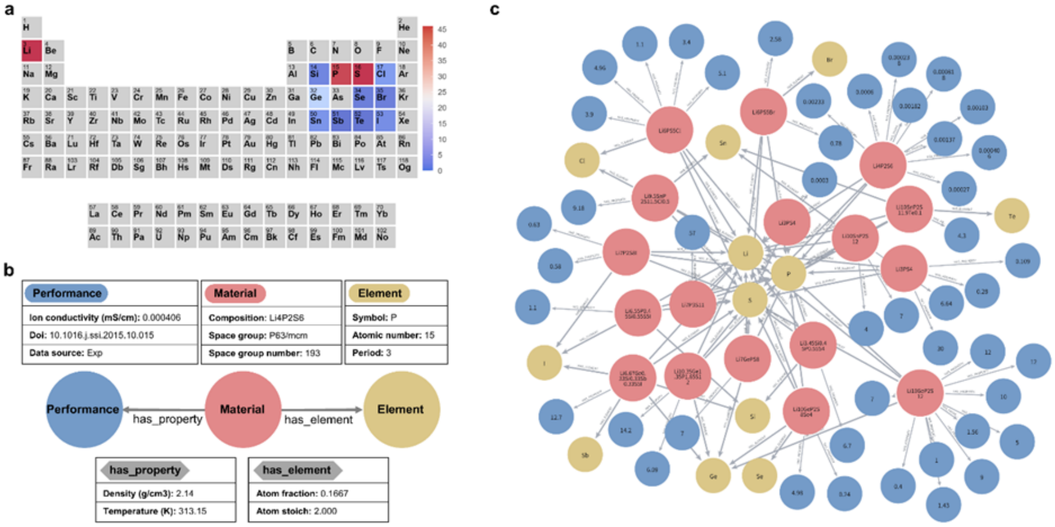


Figure 4: (a) Element frequency distribution of the constituent elements in the sulfide solid-state electrolyte dataset. (b) Knowledge graph schema, including definitions of node types and edge relations. (c) Overall structure of the knowledge graph constructed from the curated sulfide solid-state electrolyte dataset.

3.2 Knowledge Graph Construction

While element frequency analysis is useful for characterizing how individual elements are used, it is limited in capturing relationships across elements, compositions, and properties. To visualize and represent the complex interactions embedded in the sulfide solid-state electrolyte dataset in an inference-friendly form, we construct a knowledge graph (Fig. 4b, c). Methodologically, our knowledge graph differs from many prior studies that predominantly focus on bibliographic linking or simple element-material associations. By introducing sample-level material nodes, explicit measurement-condition nodes, and distinct performance nodes, our graph structurally decouples intrinsic compositional and structural effects from extrinsic measurement factors. This topology transcends flat correlation networks, enabling subgraph-level reasoning and message-passing inference along composition-structure-condition-property pathways. Consequently, it unveils latent design patterns that remain obscured in frequency analyses or simple pairwise statistics.

In the resulting graph, the element nodes Li, P, and S act as central hubs with the highest degrees, and most material nodes form a radially connected structure around them. This observation is consistent with the element-frequency analysis and suggests that performance improvements in sulfide solid electrolytes have largely been pursued through compositional tuning and structural variations within a constrained backbone chemistry, rather than by exploring fundamentally different elemental families.

The Ge node exhibits relatively high connectivity, and we also observe limited connections for Si and Sn, which are group-14 congeners of Ge. This pattern reflects emerging attempts to substitute within the same group to reduce cost and/or improve stability [17]. However, the substantially lower connectivity of Si and Sn compared to Ge suggests that such substitution strategies remain only partially explored in the current literature. For the halogens Cl, Br, and I, we find that these nodes connect selectively to material nodes belonging to specific structural families, such as argyrodites.

Among them, Cl shows the highest connectivity, which we attribute to its ionic-radius compatibility with S, enabling effective substitution on S sites with minimal lattice distortion [18].

Additional elements such as Sb, Se, and Te are also observed in the dataset; however, their corresponding nodes do not exhibit strong connectivity to the major compositional families. This suggests that, although these elements have been discussed as potential levers for performance improvement, they have not yet emerged as broadly adopted design variables in sulfide solid electrolytes.

Overall, the constructed knowledge graph provides an integrated representation that links compositional information with property signals such as ionic conductivity. By reassembling fragmented literature knowledge into a connected relational form, the KG offers a machine-interpretable substrate for capturing and reasoning over element-composition-property relationships in sulfide solid-state electrolytes.

3.3 Knowledge Graph-guided Candidate Proposal

Knowledge graphs serve as an effective tool for visualizing compositional biases reported in sulfide-based solid electrolyte research as well as the relational structures among materials, crystal structures, and ionic transport properties. However, because such representations are inherently limited to existing data, they face fundamental constraints in directly discovering novel compositional combinations that remain insufficiently explored. In contrast, LLMs possess the capability to perform combinatorial exploration and generation based on extensive literature-derived knowledge and relational reasoning.

In this study, we propose a framework that leverages a knowledge graph as structured input to an LLM in order to systematically identify new candidate sulfide solid electrolytes located in relatively unexplored regions of compositional space while remaining consistent with existing research trends. Specifically, relationships among material compositions, crystal structures, and ionic conductivities encoded in the knowledge graph were provided to the LLM, enabling the prioritized generation of new compositions that have not been reported in existing databases but are expected to exhibit high lithium-ion conductivity.

As a result, the LLM proposed two novel candidate compositions consisting of four and five elements, respectively. The first candidate, $\mathrm{Li_{11}Si_2PS_{12}}$, adopts an LGPS-type structure with a tetragonal $P4_2/nmc$ space group. Knowledge graph analysis revealed that LGPS-type structures constitute a representative structural family that repeatedly exhibits high ionic conductivity across the literature, and that LGPS compositions containing Si or Ge tend to show statistically superior transport performance. Moreover, multiple Li-Si-P-S compositions have already been reported within the same structural family. Based on these compositional distributions and property trends, the LLM derived the present candidate as an extension of the Si-based LGPS compositional space.

The second candidate, $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$, crystallizes in the cubic $F\bar{4}3m$ argyrodite structure. The knowledge graph indicates that numerous halide-containing argyrodite materials, including $\mathrm{Li_6PS_5Cl}$, as well as compositions featuring partial substitution of P by Ge, Si, or Sb, have been reported, with many of these exhibiting relatively high room-temperature ionic conductivity. After learning these composition-structure-property correlations, the LLM proposed a new candidate composition that preserves the Cl-based argyrodite framework while partially substituting Ge for P and adjusting the lithium content, thereby extending existing research trends into a previously unreported compositional regime.

4 Structural Construction and Ionic Transport Properties of KG-LLM Proposed Materials

4.1 Structural Construction of Candidate Materials

Based on the compositions and space groups proposed by the LLM, we constructed crystal structure models for each candidate material. In this process, the crystal structure files (POSCAR format) of the corresponding parent materials, which explicitly contain lattice parameters and atomic coordinates, were obtained from the Materials Project database and provided as input structures. The LLM then performed atomic substitutions and compositional adjustments directly on these frameworks to generate the structures of the proposed candidates. Specifically, experimentally reported sulfide solid electrolytes with well-established structural stability were adopted as reference frameworks, and their

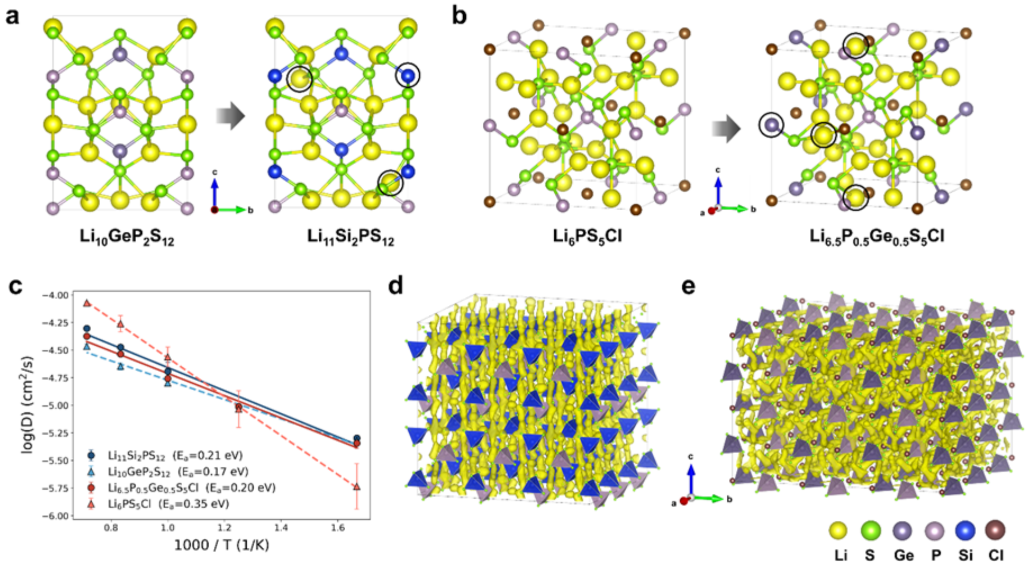


Figure 5: (a) Structural modification from $\mathrm{Li_{10}GeP_2S_{12}}$ to $\mathrm{Li_{11}Si_2PS_{12}}$ (LGPS-type). (b) Structural modification from $\mathrm{Li_6PS_5Cl}$ to $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ (argyrodite-type). (c) Arrhenius plots of ionic conductivity from MLIP-based simulations. (d) Li-ion diffusion pathways in $\mathrm{Li_{11}Si_2PS_{12}}$ at 300 K. (e) Li-ion diffusion pathways in $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ at 300 K.

structures were automatically modified by the LLM to satisfy the target compositions, resulting in the generation of POSCAR files for the candidate materials.

For the four-element candidate $\mathrm{Li_{11}Si_2PS_{12}}$, the POSCAR file of the LGPS-type structure [19] with the $P4_2/nmc$ space group was used as the parent framework. The LLM replaced the Ge atoms occupying the tetrahedral sites with Si atoms while preserving the lattice symmetry and the fundamental structural skeleton, and adjusted the Li occupancy to match the target stoichiometry, thereby generating a crystal structure model corresponding to the new composition (Fig. 5a).

For the five-element candidate $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$, the POSCAR file of the argyrodite-type $\mathrm{Li_6PS_5Cl}$ structure [20] with the $F\bar{4}3m$ space group was adopted as the reference. In this case, a partial substitution of Ge for P at the tetrahedral sites was introduced, and the Li occupancy was re-adjusted accordingly to construct a structure consistent with the proposed composition using the LLM (Fig. 5b). Throughout this procedure, the characteristic anion framework of the argyrodite structure and the connectivity of the Li sublattice were preserved.

4.2 MLIP-Based Analysis of Ionic Transport Properties

The optimized structures of the two candidate materials obtained from density functional theory (DFT) calculations were expanded into $3 \times 3 \times 2$ supercells and subjected to molecular dynamics simulations using two machine-learning interatomic potential models: Graph Representation and Atomic Simulation Engine (GRACE[21]) and Materials-Aware Atomic Cluster Expansion (MACE[22]). Under identical simulation conditions, using an NVIDIA RTX 4090 GPU, the computational cost for 100 ps of simulation was approximately 1.93 h for MACE(MPA-0) and 1.17 h for GRACE(2L-OAM-L), indicating that GRACE provides higher computational efficiency. For each material, ionic diffusion behavior was evaluated over a temperature range of 600–1400 K, and the room-temperature ionic conductivity was estimated through Arrhenius analysis. To benchmark the performance of the candidate materials, identical simulations were also performed for the parent compounds, LGPS and $\mathrm{Li_6PS_5Cl}$, under the same conditions. The mean squared displacement (MSD) curves of lithium ions obtained from both MLIP models for all materials are provided in the Appendix (Fig. 8), where stable diffusion behavior and consistent trends between the two models are observed across the entire temperature range. Fig. 5c presents the Arrhenius plots for both the candidate and parent materials. The reported values correspond to averages over the two MLIP models, with the standard deviations shown as error bars to represent model-to-model variability. All materials exhibit clear Arrhenius-type temperature dependence, and similar conductivity trends are reproduced by both MLIP models, confirming the consistency of the predictions.

Quantitatively, the four-element candidate $\mathrm{Li_{11}Si_2PS_{12}}$ exhibits an activation energy of 0.21 eV and a room-temperature ionic conductivity of 12.7 mS cm^{-1}, which is slightly higher in activation energy than its parent material $\mathrm{Li_{10}GeP_2S_{12}}$ (0.17 eV, 19.0 mS cm^{-1}), yet still maintains a high conductivity exceeding 10 mS cm^{-1}. In contrast, the five-element candidate $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ shows an activation energy of 0.20 eV and a room-temperature ionic conductivity of 14.0 mS cm^{-1}, representing a substantial improvement over the parent compound $\mathrm{Li_6PS_5Cl}$ (0.35 eV, 0.34 mS cm^{-1}), with a pronounced reduction in activation energy and an enhancement in conductivity by nearly two orders of magnitude. These results indicate that, particularly for the argyrodite family, partial cation substitution combined with Li stoichiometry tuning can effectively lower migration barriers and significantly enhance room-temperature ionic conductivity. Furthermore, the LGPS-type candidate demonstrates that Ge-free compositions can retain conductivity levels comparable to those of conventional LGPS, suggesting a promising alternative from both performance and resource-efficiency perspectives. In particular, replacing Ge with Si avoids the use of a relatively scarce and costly element, which is expected to reduce raw material costs and supply-chain constraints in large-scale electrolyte production. Overall, these findings quantitatively demonstrate that the integration of knowledge-graph-based compositional trend analysis with LLM-driven combinatorial design can successfully identify new sulfide solid electrolyte candidates exhibiting high ionic conductivity.

To elucidate the room-temperature ionic transport mechanisms of the candidate materials, additional MLMD simulations were performed for each candidate supercell at 300 K for 2 ns, and the spatial occupation and migration pathways of lithium ions were analyzed. As a result, long-range interconnected lithium-ion conduction networks were observed in both candidate materials, and representative visualizations of the diffusion pathways are shown in Fig. 5d and 5e. For the LGPS-type structure $\mathrm{Li_{11}Si_2PS_{12}}$, lithium ions preferentially migrate along well-defined channels oriented primarily along the crystallographic c-direction, followed by inter-channel hopping that enables continuous long-range diffusion (Fig. 5d and Fig. 9a). This behavior indicates that the channel-based diffusion mechanism commonly reported for LGPS-type electrolytes is preserved in the newly proposed composition. In contrast, for the argyrodite-type structure $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$, lithium ions form more isotropic three-dimensional interconnected pathways throughout the structure, consistent with a typical cage-to-cage hopping mechanism (Fig. 5e and Fig. 9b). Notably, in both candidates, the lithium occupation density forms continuous networks without fragmentation, demonstrating that meaningful long-range diffusion can occur even at room temperature. These pathway-based observations are qualitatively consistent with the low activation energies and high room-temperature ionic conductivities obtained from the Arrhenius analysis.

5 Conclusion

5.1 Conclusion

In this study, we proposed an integrated computational materials discovery framework that combines literature-based information extraction via retrieval-augmented generation (RAG), knowledge graphs (KG), large language models (LLMs), and machine-learning interatomic potentials (MLIPs) to systematically exploit composition–structure–property relationships in sulfide solid electrolytes. Unlike conventional computational screening approaches that rely primarily on high-cost density functional theory (DFT) calculations or random compositional sampling, the present strategy enables efficient identification of physically plausible and explainable candidate materials by structuring accumulated literature knowledge and incorporating it into generative models.

Specifically, key information such as chemical compositions, space groups, densities, measurement temperatures, and ionic conductivities was automatically extracted from the literature using an RAG-based pipeline and organized into a knowledge graph, enabling quantitative analysis of correlations among composition, structure, and performance. By providing this structured KG information as input to the LLM, two promising sulfide solid electrolyte compositions—$\mathrm{Li_{11}Si_2PS_{12}}$ (LGPS-type) and $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ (argyrodite-type)—were generated as candidates with high expected lithium-ion conductivity.

Although $\mathrm{Li_{11}Si_2PS_{12}}$ has been reported in previous experimental studies [23, 24], it was not included in the literature corpus used to construct our knowledge graph and was therefore treated as an out-of-graph composition by the model. This result indicates that the framework can systematically recover high-performance compositions that are consistent with learned composition–structure–property trends, even when such materials are absent from the training knowledge graph, rather than relying on direct memorization. In contrast, to the best of our knowledge, the argyrodite-type candidate $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ has not been previously reported, demonstrating that the proposed approach can also generate genuinely unexplored compositions within known structural classes.

The LLM-generated structural models were subsequently optimized using DFT and quantitatively validated through molecular dynamics simulations based on two independent MLIP models, GRACE and MACE. The results demonstrate that both candidates exhibit high room-temperature ionic conductivities of 12.7 mS $\mathrm{cm^{-1}}$ and 14.0 mS $\mathrm{cm^{-1}}$, respectively. Notably, the argyrodite candidate shows an improvement of nearly two orders of magnitude compared to its parent compound, while the LGPS-type candidate maintains conductivity comparable to conventional LGPS despite being free of Ge, highlighting its potential advantage in terms of resource efficiency.

Furthermore, long-timescale MLMD simulations at 300 K revealed that the channel-based diffusion mechanism along the crystallographic c-axis is preserved in the LGPS-type candidate, whereas the argyrodite candidate retains a three-dimensional cage-to-cage diffusion network. These diffusion characteristics are consistent with the low activation energies and high ionic conductivities obtained from Arrhenius analysis, providing a coherent physical interpretation of the observed transport behavior.

Overall, this work demonstrates that integrating structured literature knowledge (KG), generative reasoning (LLM), and large-scale property validation (MLIP) enables an explainable, reproducible, and computationally efficient pipeline for discovering high-performance solid electrolytes. The proposed framework is not limited to sulfide systems and can be readily extended to oxide, halide, and other functional materials, offering a general strategy to accelerate next-generation materials discovery when combined with targeted model refinement and experimental validation.

5.2 Limitation

Despite the advantages of the proposed framework, several limitations should be acknowledged. First, parts of the literature acquisition process still require manual intervention, as downloading and organizing full-text PDFs cannot be fully automated due to heterogeneous publisher access policies. Second, the constructed dataset and knowledge graph are inherently shaped by existing literature, resulting in denser coverage of well-studied material systems and literature-induced bias. This bias can limit the discovery of structurally or chemically underrepresented materials, including metastable or unconventional compositions. The dataset and knowledge graph are also not directly reusable across material domains, requiring reconstruction and prompt redesign for each new material class.

Methodologically, candidate discovery is constrained to substitutional exploration around known prototype structures. LLM-based structure generation relies on provided prototype POSCAR files and produces modified structures through compositional substitution or limited structural variation. While the current dataset size is sufficient for substitution-based exploration, it is not large or diverse enough to enable reliable prediction of entirely novel crystal structures beyond known motifs. Future work will address this limitation by expanding the dataset with experimental and computational structures, enabling exploration beyond local prototype substitutions. Moreover, the framework assumes that the extracted literature information is accurate, and any inaccuracies may propagate through the knowledge graph and affect downstream screening.

Finally, although MLIP-based molecular dynamics enable efficient large-scale screening, the use of pre-trained MACE and GRACE models introduces domain bias and uncertainty, particularly when extrapolating to unexplored compositions. Moreover, the simulations are limited to ideal crystalline structures and neglect microstructural effects, thermodynamic stability, and experimental synthesizability, collectively leading to a realism gap between predicted and experimentally observable behavior. Future work will focus on reducing this gap through targeted domain adaptation using system-specific training data and by incorporating stability- and disorder-aware modeling strategies, thereby improving transferability and practical relevance.

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Appendix / supplemental material

A LLM-Based Problem Formulation and Research Question Derivation

A.1 Multi-LLM Workflow: Setup, Integration, and Cross-Checking

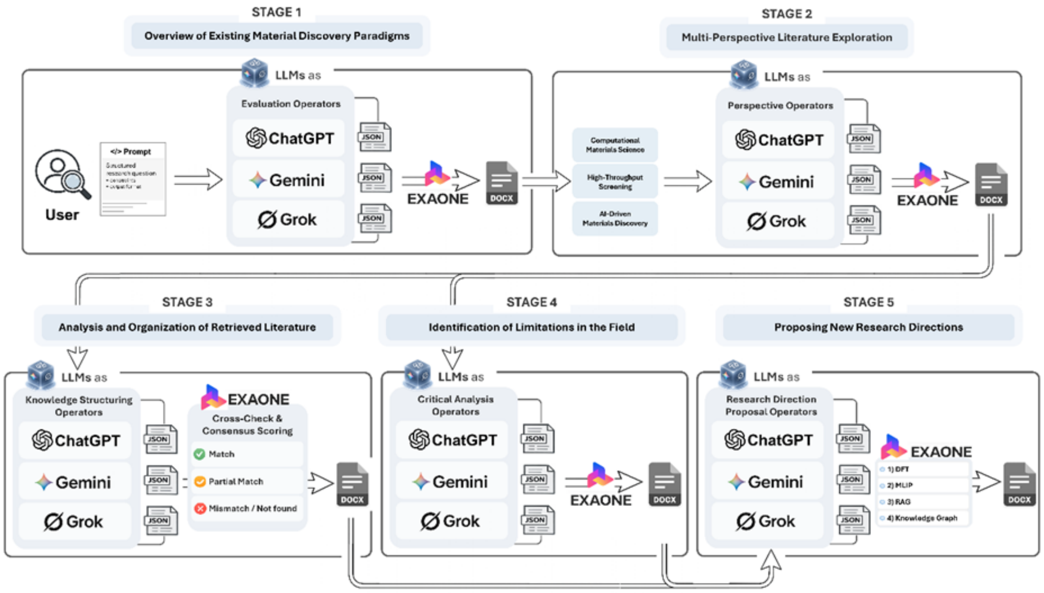
STAGE 1
Overview of Existing Material Discovery Paradigms
LLMs as
Evaluation Operators
ChatGPT
Gemini
Grok
JSON
User
</> Prompt
EXAONE
DOCX
STAGE 2
Multi-Perspective Literature Exploration
LLMs as
Perspective Operators
Computational Materials Science
High-Throughput Screening
AI-Driven Materials Discovery
STAGE 3
Analysis and Organization of Retrieved Literature
LLMs as
Knowledge Structuring Operators
EXAONE
Cross-Check & Consensus Scoring
Match
Partial Match
Mismatch / Not found
STAGE 4
Identification of Limitations in the Field
LLMs as
Critical Analysis Operators
STAGE 5
Proposing New Research Directions
LLMs as
Research Direction Proposal Operators
1) DFT
2) MLIP
3) RAG
4) Knowledge Graph

Figure 6: Multi-LLM workflow for Stages 1–3 (topic selection to literature analysis). ChatGPT, Gemini, and Grok generate independent, structured JSON outputs; EXAONE integrates them into a single Korean DOCX deliverable while enabling cross-checking and standardization.

In this appendix, we describe the detailed setup and integration procedure of the multi-LLM workflow used in Stages 1–3 (**Fig. 6**). In §A.1.1, we specify the prompting strategy and the structured output (JSON) schema. In §A.1.2, we describe the stage-wise execution procedure and the EXAONE-based integration process. In §A.1.3, we present the cross-check protocol and consensus labeling rules used in Stage 3.

A.1.1 Prompting and Structured Output Schema

Across all stages, we use role-specific instructions (e.g., evaluation, perspective exploration, and knowledge structuring). To ensure comparability across models, we constrain outputs to a pre-defined JSON schema. Each JSON record contains: (i) stage and role identifiers, (ii) core claims and supporting rationale, and (iii) provenance fields that indicate which model produced each item. This structured interface enables downstream integration and facilitates auditing when needed.

A.1.2 Stage-wise Procedure and Integration (Stages 1-5)

Stage 1 (Paradigm overview). We run ChatGPT, Gemini, and Grok as evaluation operators under the same prompt conditions. Each model independently summarizes existing materials discovery paradigms and produces a structured JSON output. We then consolidate these outputs using EXAONE to generate a single DOCX artifact that standardizes terminology and merges overlapping points while preserving provenance.

Stage 2 (Multi-perspective literature exploration). Using the domain axes obtained in Stage 1, we perform multi-perspective literature exploration by running the same three LLMs as perspective operators. Each model proposes candidate papers and returns structured entries (e.g., title/venue/year/DOI when available) in JSON. EXAONE merges the union of candidate lists, removes duplicates, and produces a consolidated literature list in DOCX form.

Stage 3 (Analysis and organization of retrieved literature). For each retrieved paper, we request independent analyses from multiple LLMs and enforce JSON outputs. EXAONE performs cross-checking by aligning paper identity (preferably via DOI; otherwise via normalized title matching) and aggregates model-level summaries into a unified record per paper. The final output is a DOCX report that includes both the merged analysis and model agreement signals.

Stage 4 (Identification of limitations in the field). Based on Stage 1–3 outputs, we run ChatGPT, Gemini, and Grok as critical analysis operators to extract recurring bottlenecks and failure modes in the target research area. Each model produces a structured JSON that separates (i) methodological limitations (e.g., assumptions, missing physics, evaluation gaps), (ii) data limitations (e.g., bias, coverage, label noise, reproducibility), and (iii) deployment limitations (e.g., scalability, robustness, integration barriers). EXAONE consolidates these limitation inventories into a single DOCX report, while retaining per-item provenance to enable traceable auditing of where each limitation originated.

Stage 5 (Proposing new research directions). Using the consolidated limitation report (Stage 4) as constraints, we run the three LLMs as research direction proposal operators to generate actionable research directions and testable research questions. Outputs are again serialized in JSON with fields such as: (i) proposed direction, (ii) hypothesis and expected mechanism, (iii) required resources/data, (iv) evaluation protocol and success criteria, and (v) risks/ablation plans. EXAONE integrates proposals into a single DOCX and additionally maps each direction onto an execution pathway (e.g., DFT, MLIP, RAG, and Knowledge Graph) to explicitly connect ideation with implementation modules and verification routes.

A.1.3 Cross-check Protocol and Consensus Labels

To reduce hallucination risk and ensure traceability, we assign a consensus label to each paper-level record. We use four categories—Match, Partial match, Mismatch, and Not found—based on (i) paper identity resolution (DOI/title) and (ii) agreement on the extracted core technical claims. The final DOCX report stores the consensus label together with per-model evidence fields, enabling manual verification when needed.

A.2 Multi-Agent Deliberation Protocol for Pipeline Synthesis

This appendix describes the design-time mechanism we used to synthesize the end-to-end discovery pipeline shown in Fig. 7. The core idea is to treat pipeline design as a structured deliberation problem: multiple role-specialized LLM agents iteratively propose, critique, and revise a candidate workflow until a verifiable and resource-aware specification is produced. We implement the interaction using an AutoGen-style multi-agent framework, with explicit turn-taking and grounding tools to reduce unsupported reasoning.

A.2.1 Agent Committee and Grounding Tools

We instantiate a small committee of LLM agents, each constrained to a distinct responsibility: (i) coordination and decision arbitration, (ii) target-property specification (e.g., ionic conductivity and stability), (iii) unstructured-data processing and representation, (iv) AI-method design, and (v) physics/validation constraints. The committee is equipped with web retrieval, enabling agents to fetch recent references during discussion rather than relying solely on parametric memory. Retrieved evidence is used to justify critiques, resolve disagreements, and update the evolving pipeline specification.

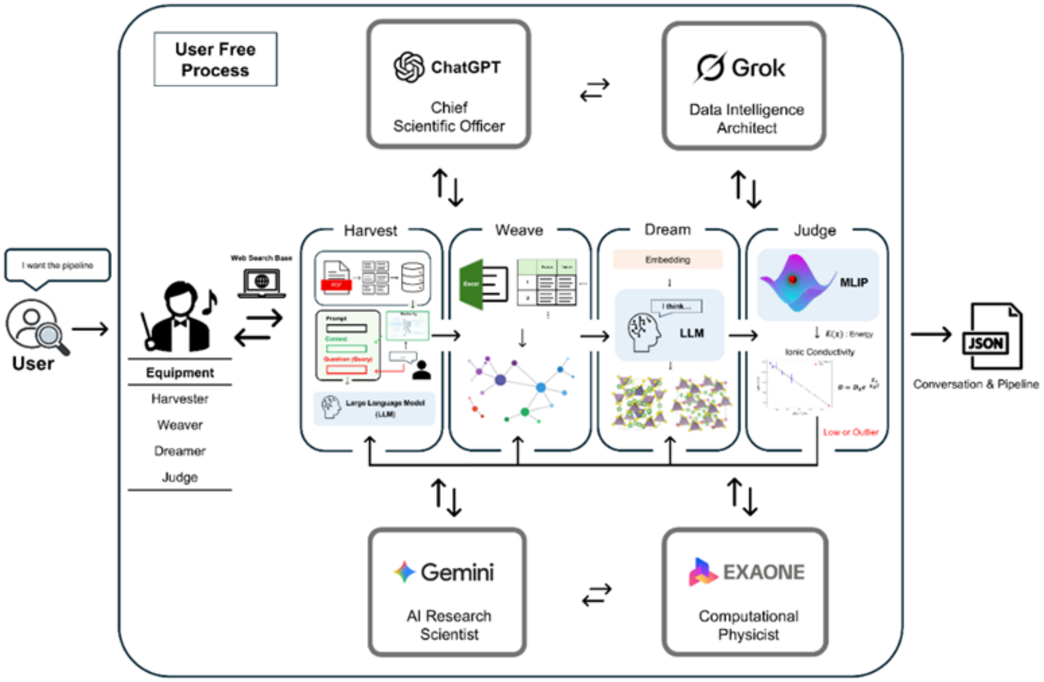

Figure 7: Multi-agent, web-grounded deliberation used to synthesize a closed-loop discovery pipeline (Harvest-Weave-Dream-Judge), with role-specialized agents interacting via round-robin critique and exporting a structured JSON specification.

A.2.2 Round-Robin Adversarial Refinement

The committee follows a round-robin deliberation protocol. Each proposal must be followed by a critique from the next agent, enforcing systematic stress-testing of assumptions (data availability, evaluation validity, physical consistency, and feasibility under compute constraints). We run multiple critique–revision rounds (≥ 5) and terminate when the pipeline description becomes (i) internally consistent, (ii) grounded with supporting evidence where applicable, and (iii) executable within the project's practical constraints. Importantly, the goal of this process is not to maximize creativity, but to converge to a pipeline with explicit checks against hallucinated steps and unverifiable claims.

A.2.3 Output Artifact and Reproducibility

Upon termination, the system exports the deliberation trace and the finalized pipeline as a structured JSON artifact. The JSON includes role-tagged messages, intermediate revisions, and the final stage definitions, enabling auditability of "why" each stage exists and what constraints motivated it. This makes the pipeline derivation reproducible as a controlled protocol, rather than a one-off design decision.

A.2.4 Resulting Four-Stage Loop

The deliberation produces a four-stage cyclic workflow (Harvest–Weave–Dream–Judge) that connects: (1) literature-scale extraction via retrieval and structured parsing, (2) relational consolidation into a knowledge graph, (3) KG-conditioned candidate suggestion, and (4) fast physics-oriented filtering via MLIP-based evaluation. Structural construction details for candidates are intentionally deferred to later sections; here we only document how the pipeline itself is synthesized and serialized.

B Method: Document-grounded Literature Collection and Extraction

We acquired sulfide solid-state electrolyte papers using a multi-route collection strategy that combines three complementary pathways. First, we used an LLM for semantic recommendation to gather relevant paper DOIs. Second, we performed keyword-based automated DOI collection using OpenAlex. Third, we manually supplemented the resulting list to recover papers that may be missed by specific keywords or by the automated retrieval process. All collected papers were standardized to PDF format and organized under a single directory to enable consistent use in the downstream automated extraction pipeline.

We extract information from each paper using a document-grounded extraction RAG setup that maps a single document to a structured JSON record. During extraction, we restrict evidence strictly to numerical values explicitly stated in the paper as primary results. In particular, we exclude values that appear only in narrative background or review text, values cited from other papers, and values obtained via inference, interpolation, or extrapolation. Only values that are directly measured by the authors or explicitly computed are permitted. To ensure format consistency, we normalize temperature to K and ionic conductivity to mS/cm. When a single composition is reported under multiple temperature conditions or with multiple conductivity values, we do not aggregate them (e.g., by averaging); instead, we store them as separate records to preserve condition-specific context.

C Machine Learning Interatomic Potentials

C.1 Simulation Settings

DFT was performed using the Vienna *Ab initio* Simulation Package (VASP). The core–valence interactions were treated using the projector-augmented wave (PAW) method. Spin-polarized DFT calculations employed the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) functional. A kinetic energy cutoff of 500 eV was applied, and the Brillouin zone was sampled using a Γ-centered $3 \times 3 \times 3$ k-point grid. The electronic energy was converged to within 10^{-5} eV, and ionic relaxations were performed until the forces on all atoms were below 0.02 eV Å^{-1}.

Following the DFT structural optimization, each primitive unit cell was expanded into a $3 \times 3 \times 2$ supercell to construct large-scale atomic models for subsequent molecular dynamics simulations. As a result, the simulation cell for $\mathrm{Li_{11}Si_2P_2S_{12}}$ contained 936 atoms, while that for $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ comprised 972 atoms.

To evaluate lithium-ion diffusion behavior with high computational efficiency while maintaining reliable accuracy, molecular dynamics simulations based on machine-learning interatomic potentials (MLMD) were performed using two state-of-the-art models, GRACE and MACE, as implemented in the LAMMPS simulation package. For each candidate material, simulations were conducted at five different temperatures ranging from 600 K to 1400 K in increments of 200 K, and MD trajectories of 100 ps were generated at each temperature for Arrhenius analysis. In addition, to investigate lithium-ion transport mechanisms under operating conditions, extended MLMD simulations were carried out at 300 K for 2 ns for each candidate material. All MLMD simulations were performed using a time step of 2 fs under the NVT ensemble. The resulting trajectories were analyzed and visualized using VESTA to examine the structural and dynamic evolution of the systems.

C.2 Transport Property Analysis

The lithium-ion diffusion coefficients D were calculated from MLMD trajectories using the mean squared displacement (MSD) method. The MSD is defined as

$$\mathrm{MSD}(t) = \left\langle |\mathbf{r}_i(t) - \mathbf{r}_i(0)|^2 \right\rangle, \tag{1}$$

where $\mathbf{r}_i(t)$ denotes the position of the i-th lithium ion at time t, and $\langle \cdots \rangle$ represents an average of all mobile lithium ions and different time origins.

The diffusion coefficient D was obtained from the slope of the MSD curve according to the Einstein relation,

$$D = \frac{1}{2d}\frac{d}{dt}\mathrm{MSD}(t), \tag{2}$$

where $d = 3$ is the dimensionality of the diffusion space. In practice, D was extracted by linear fitting of the MSD curve within the time window exhibiting diffusive behavior, where the MSD increases linearly with time.

For each material, diffusion coefficients were evaluated at five temperatures ranging from 600 to 1400 K using two independent machine-learning interatomic potential models, GRACE and MACE. Arrhenius plots were constructed by fitting the temperature-dependent diffusion coefficients to

$$D(T) = D_0 \exp\left(-\frac{E_a}{k_{\mathrm{B}}T}\right), \tag{3}$$

where D_0 is the pre-exponential factor, E_a is the activation energy, k_{B} is the Boltzmann constant, and T is the absolute temperature. For each material, the final Arrhenius parameters were obtained by averaging the results from the two MLIP models.

The ionic conductivity σ_T was subsequently estimated using the Nernst–Einstein relation,

$$\sigma_T = \frac{nz^2F^2D}{RT}, \tag{4}$$

where n is the lithium-ion concentration, z is the ionic charge number ($z = 1$ for Li^+), F is the Faraday constant, and R is the ideal gas constant.

The same analysis procedure was applied to both the proposed candidate materials and their corresponding parent compounds to enable direct comparison of transport properties under identical simulation conditions.

C.3 Lithium-Ion Probability Density and Diffusion Pathway Analysis

To visualize lithium-ion migration pathways in the proposed candidate solid electrolytes, lithium-ion probability density distributions were constructed from MLMD trajectories at 300 K for $\mathrm{Li_{11}Si_2PS_{12}}$ and $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$.

During the simulations, the supercell was discretized into a three-dimensional grid, and the number of occurrences of lithium ions within each grid voxel was accumulated over the entire trajectory. The local probability density P was computed as

$$P = \frac{N}{V},$$

where N is the number of lithium-ion occurrences within a voxel and V is the voxel volume. The average probability density over the simulation cell is denoted as P_0.

Three-dimensional isosurfaces of lithium-ion probability density were generated at multiple threshold values ranging from $2P_0$ to $6P_0$ to identify dominant diffusion channels as well as secondary migration pathways. Regions with higher probability density correspond to frequently occupied lithium sites, whereas lower isovalues reveal extended connections between neighboring sites, representing long-range diffusion networks.

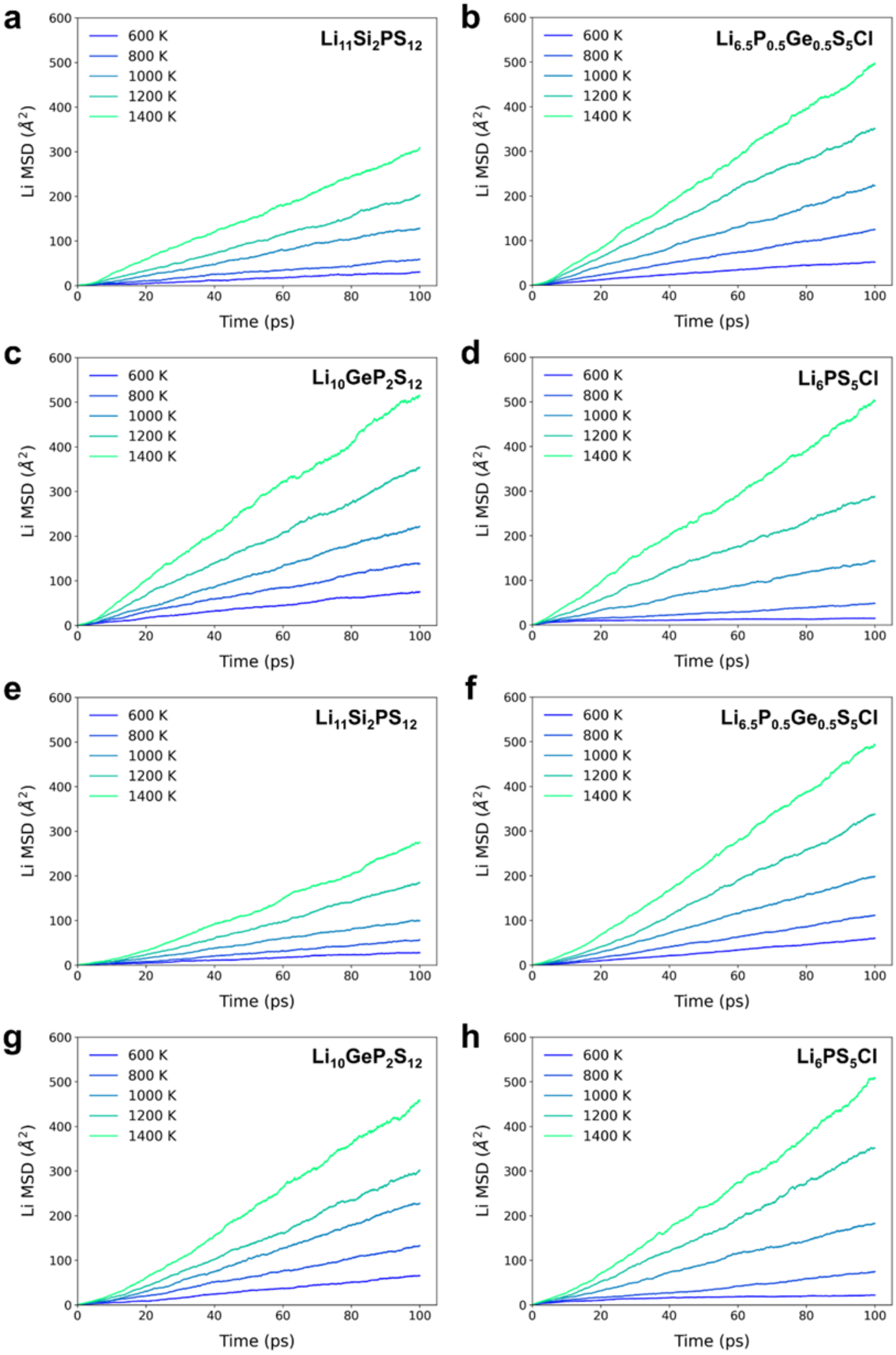

Figure 8: Lithium-ion MSD plots at 600-1400 K calculated using the MACE (a-d) and GRACE (e-h) models for the candidate materials and their parent compounds.

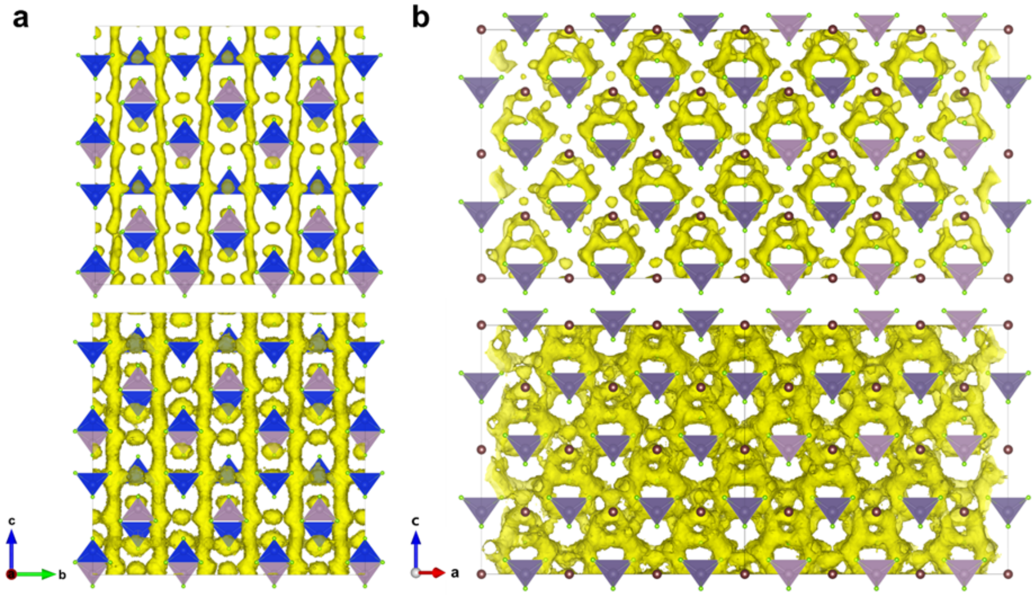

Figure 9: Lithium-ion probability density isosurfaces at 300 K for (a) $\mathrm{Li_{11}Si_2PS_{12}}$ and (b) $\mathrm{Li_{6.5}P_{0.5}Ge_{0.5}S_5Cl}$ obtained from MLMD simulations. The upper panels correspond to an isovalue of $6P_0$, highlighting the most frequently occupied lithium sites, while the lower panels show an isovalue of $2P_0$, revealing extended diffusion pathways. Yellow isosurfaces indicate regions of high lithium occupation probability, and tetrahedral units are shown as polyhedra for structural reference.

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The checklist is designed to encourage best practices for responsible machine learning research, addressing issues of reproducibility, transparency, research ethics, and societal impact. Do not remove the checklist: **The papers not including the checklist will be desk rejected.** The checklist should follow the references and follow the (optional) supplemental material. The checklist does NOT count towards the page limit.

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The checklist answers are an integral part of your paper submission. They are visible to the reviewers, area chairs, senior area chairs, and ethics reviewers. You will be asked to also include it (after eventual revisions) with the final version of your paper, and its final version will be published with the paper.

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   Question: Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope?

   Answer: [Yes]

   Justification: The main claims are explicitly stated in the Abstract and Section 1 (Introduction) and are consistent with corresponding sections of the paper: RAG-based literature-to-dataset construction in Section 2, evidence-preserving knowledge graph construction and KG-grounded candidate proposal in Sections 3.2 and 3.3, and MLIP-based screening of ionic transport properties in Section 4.2.

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2. **Limitations**

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   Answer: [Yes]

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  (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
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   Answer: [No]

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   - The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
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   Answer: [No]

Justification: The paper provides detailed and reproducible descriptions of the molecular dynamics simulation and analysis settings, including the MLIP models (MACE and GRACE), system sizes, temperature ranges, and transport-property evaluation procedures (Section 4.2 and Appendix C). However, the detailed configurations of the LLM-based literature processing pipeline, such as prompt templates, inference parameters, and model-specific settings, are not fully specified. As a result, not all experimental settings necessary to fully reproduce the entire pipeline are disclosed.

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- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
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7. **Experiment Statistical Significance**

   Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

   Answer: [Yes]

   Justification: Statistical variability is explicitly reported using error bars to quantify model-to-model uncertainty. For each material, ionic transport properties were evaluated using two independent MLIP models (MACE and GRACE) under identical simulation conditions. The reported values correspond to averages over the two models, with error bars representing the standard deviation between model predictions (Fig. 5). Consistent lithium diffusion behavior is observed across the full temperature range, as confirmed by the MSD curves provided in the Appendix (Fig. 8). The agreement in Arrhenius trends between the two models supports the robustness and consistency of the reported results.

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