Energy Storage and Conversion 2026, 4(3.), 4568.
https://doi.org/10.59400/10.59400/esc4568

Article

AI-assisted nanolayer-engineered solid-state electrolyte interfaces for lithium dendrite suppression in high-energy lithium metal batteries

Tanveer Ahmad Wani[1,*], Ramesh Saini[2], Shobhit Goyal[3], Manni Sruthi[4], Chetansinh R. Vaghela[5], Yinxin Tang[6], Kaustubh Milind Utpat[7]

[1] Department of Physics, Noida International University, Greater Noida 203201, Uttar Pradesh, India
[2] Centre for Research Impact & Outcome, Chitkara University Institute of Engineering and Technology, Chitkara University, Rajpura 140401, Punjab, India
[3] Quantum University Research Center, Quantum University, Roorkee 247667, Uttarakhand, India
[4] Centre for Multidisciplinary Research, Anurag University, Hyderabad 500088, Telangana, India
[5] Faculty of Science, Gokul Global University, Siddhpur 384151, Gujarat, India
[6] Faculty of Education, Shinawatra University, Samkhok 12160, Pathum Thani, Thailand
[7] Department of Mechanical Engineering, Vishwakarma University, Pune 411048, Maharashtra, India
*** Corresponding author:** Tanveer Ahmad Wani, tanveer.ahmad@niu.edu.in

CITATION

Wani TA, Saini R, Goyal S, et al. AI-assisted nanolayer-engineered solid-state electrolyte interfaces for lithium dendrite suppression in high-energy lithium metal batteries. Energy Storage and Conversion. 2026; 4(3): 4568. https://doi.org/10.59400/esc4568

COPYRIGHT

Copyright © 2026 by author(s). *Energy Storage and Conversion* is published by Academic Publishing Pte Ltd. This work is licensed under the Creative Commons Attribution (CC BY) license. https://creativecommons.org/licenses/by/4.0/

Abstract: Commercialization of lithium metal batteries with high energy density is limited largely due to uncontrolled lithium dendrite growth, poor interfacial resistance of solid-state electrolytes, and inadequate cycle stability of solid-state electrolytes. A new architecture that leverages artificial intelligence to design engineered nanolayer interfaces for solid-state electrolytes enables controlled lithium-ion transport and prevents dendrite propagation in next-generation batteries. To achieve this, the proposed framework combines multiphysics interfacial modeling with an artificial intelligence optimization module to simultaneously determine the optimal thickness and interfacial parameters for nanolayers to optimize ionic conductivity while minimizing electrochemical degradation. Simulation results show that the engineered interface provides a significantly better electrochemical performance than any existing solid-state electrolyte configuration. The simulation results show that the optimized nanolayer-engineered interface gave an ionic conductivity of 1.21 × 10−3 S cm−1, which was an enhancement of 34.8% compared to the conventional interface. This framework helped reduce interfacial resistance to 46 Ω cm^2 from 82 Ω cm^2, which was an improvement of 43.9%, and increased the critical current density to 2.1 mA cm−2 from 1.3 mA cm−2. Additionally, the optimized interface retained 93.4% of its capacity after 500 cycles of charge-discharge, which is an improvement of 93.4% from the conventional interface's 79.6%. Collectively, these results indicate that the combination of nanolayer engineering and artificial intelligence optimization enables uniform deposition of lithium ions, enhances interfacial stability, and reduces the degree of dendrite-induced degradation. The proposed framework enables large-scale development of safer, long-lasting solid-state lithium-ion batteries and facilitates high-energy-density storage for electric vehicles and large renewable energy systems.

Keywords: lithium metal batteries; solid-state electrolytes; nanolayer engineering; dendrite suppression; artificial intelligence; interfacial stability; high-energy-density batteries

1. Introduction

The swift adoption of renewable energy integration, electric vehicles, and energy storage devices has led to a high demand for efficient battery technologies having high energy density, enhanced safety, and extended life span. Renewables

like solar and wind energy are intermittent in nature, necessitating efficient electrochemical energy storage technologies to ensure a stable power supply and grid reliability [1]. The recent developments in energy conversion and storage have pointed out the need for developing high-performance batteries for energy storage [2]. Traditional lithium-ion batteries have been instrumental in the development of electronics and electric vehicles; however, the energy density of lithium-ion batteries has reached a practical limit due to the limited capacity of traditional graphite anode materials [3,4]. The lithium metal batteries (LMBs) have been identified as the most suitable next-generation batteries for the reasons that metallic lithium is known for its extremely high theoretical specific capacity (3,860 mAh g−1) and low electrochemical potential (−3.04 V vs. Standard Hydrogen Electrode (SHE)) [5,6].

However, commercialization of lithium metal batteries is still difficult owing to uncontrollable lithium dendrites and unstable interfaces between electrodes and electrolytes. In cyclic processes of lithium deposition and dissolution, an uneven distribution of lithium ion flux leads to regions of high local currents that favor dendrite formation. Such dendrites may pierce solid electrolytes, causing internal short circuits, battery capacity fading, and possible hazards. Despite better thermal stability and no flammable liquids as electrolyte components, incompatibility of the interface between lithium metal and solid electrolytes remains one of the key problems of such batteries [7–9]. Recent investigations of energy storage materials and renewable energy sources focus on the creation of electrochemical energy storage systems that would be safe, efficient, and long-living for supporting new sustainable energy infrastructures [10,11].

There are various strategies developed to solve the problem of lithium dendrites: from optimization of electrolyte composition, artificial solid electrolyte interphases and protective coatings up to mechanical reinforcement [12–14]. Nanolayered interface modification seems to be promising among the aforementioned strategies since it allows regulation of lithium ion fluxes, electric field homogenization, and reduction of stress at the interface [15,16]. Atomic layer deposition (ALD) coatings, multilayers, and nanocomposites at the lithium metal interfaces have enhanced interfacial stability through the provision of controllable-ion conduction pathways and prevention of parasitic reaction mechanisms [17,18]. However, traditional nanolayer design strategies typically depend on empirical trial-and-error approaches that are computationally demanding and incapable of optimizing the combination of thickness, material properties, and other variables [19].

Artificial intelligence (AI) has been proven to be highly effective in accelerating the development of better battery material design and optimization. Machine learning has been successfully employed for the prediction of electrolytes and optimization of electrodes and the study of electrochemical interactions [20]. Despite the wide use of AI in battery research and design, previous AI-assisted approaches to battery design have mostly focused on material predictions and electrolyte compositions rather than the simultaneous optimization of nanolayer thicknesses, interfacial resistance, ionic transport characteristics, and suppression of dendrites [21].

In previous research, most of the work has either dealt with nanolayer-based interface modifications or AI-based battery material optimizations individually. However, the present research deals with the development of an innovative framework based on multiphysics optimization using AI for the development

of a stable nanolayer-engineered solid-state electrolyte interface [22,23]. By integrating multiphysics and AI, it will be possible to simultaneously optimize Li-ion transportation, interface resistivity, dendrite formation behavior, and cycling stability by choosing appropriate nanolayer parameters.

This research paper presents an innovative AI-based approach for the nanolayer-engineered solid-state electrolyte interface for suppressing lithium dendrite growth and enhancing the electrochemical stability of high-energy-density lithium metal batteries [24]. The existing approaches deal with optimizing either electrolyte material or interface structure in order to develop a lithium metal battery. However, the proposed methodology uses a closed-loop optimization framework based on electrochemical modeling, lithium-ion transport analysis, dendrite formation, and intelligent nanolayer parameter optimization.

The main purpose of this research is to establish an intelligent model of the solid-state electrolyte interface based on nano-layer engineering for minimizing lithium dendrite formation, while improving ion conduction efficiency and electrochemical stability in lithium metal batteries. The study will combine the use of electrochemical modeling involving multiple physical phenomena and intelligent optimization methods to determine the best configurations of nanolayers. The study seeks to investigate lithium-ion transport at the interfaces, minimize interfacial resistance and localized current density at the interfaces, optimize the dimensions of nanolayers using AI, and evaluate their effectiveness in dendrite inhibition and cycling stability.

Major contributions of the study are outlined below:

1. A novel framework for AI-assisted nanolayer engineering is developed for optimization of solid-state electrolyte interfaces, involving multiphysics electrochemical modeling in combination with intelligent parameter optimization.

2. A coupled interfacial model is developed for the study of lithium-ion transport, electric field distribution, interfacial resistance, and dendrite growth behavior under varying operating conditions.

3. Suggested an AI-based approach to find optimal nanolayer designs that can increase ionic conductivity, minimize interfacial resistance, and improve cycling performance.

4. The suggested framework was validated based on the results of comprehensive simulation analysis, considering such performance metrics as ionic conductivity, critical current density, interfacial resistance, dendrite growth probability, and capacity retention.

In addition to conventional research methods of studying either the modification process or prediction with the aid of artificial intelligence (AI), this study expands scientific knowledge by introducing an AI and multiphysics feedback optimization scheme for solid-state battery interfaces [25]. The proposed method enables controlled optimization of lithium-ion transport, interface resistance, and dendritic growth behaviors for the intelligent identification of nanolayer structures through conventional optimization experiments.

Strengths and limitations of the proposed framework

The proposed approach gives a systematic methodology for the optimization of solid-state electrolyte interfaces through the integration of nanolayers with the use of AI in parameter optimization. This approach limits reliance on experimentation and allows the simultaneous enhancement of ion conductivity,

interfacial stability, and dendrite suppression. Moreover, the modularity of the approach allows for its adoption in varying solid-state electrolytes and operational conditions.

Nevertheless, the present study is based mainly on multiphysics modeling and computational optimization. Even though the obtained trends agree with those observed in solid-state batteries, there is a need for experimental validation of the nanolayer interfaces. Future research directions include large-scale manufacturing capability, long-term cycling, and adaptive optimization in battery management systems.

This paper is divided into five major sections: 1. Introduction, which discusses the background, research gap, objective, and contribution; 2. System model and ai-driven interface design, which describes the proposed approach; 3. Simulation environment and experimental approach, which describes the simulation and validation process; 4. Results and discussion, which describes performance results; and 5. Conclusion, which summarizes key results and future research directions.

2. System model and AI-driven interface design

2.1. System overview

The developed framework includes a nanostructured engineered solid-state electrolytic interface in addition to using AI to assist in the optimization of the interface in order to hinder lithium dendrite formation and improve the electrochemical performance of future strong high-energy-density battery systems. This architecture therefore addresses two key challenges of all-solid-state lithium batteries: non-uniform transport of lithium ions and instability at the interface between the lithium metal anode and the solid-state electrolyte.

The proposed framework, as shown in **Figure 1**, has five modules that interoperate: input parameter acquisition; interfacial modeling and simulation; AI-based optimization of the volume; design of the interface optimal to its interfacial resistance and the ability for ionic conductivity; and performance evaluation. The framework begins with the acquisition of the material and operational parameters pertinent to the nanolayers, namely, the material properties of the nanolayer, the physical thickness of each nanolayer, the operating temperature of the nanolayer, and the current density to be applied to the nanolayer. These parameters are input into a multiphysics model of the interfacial layer for characterization of ion transport through the nanolayers, the distribution of the electric fields in the nanolayers, and the tendency for dendrites to nucleate at the interface. The information produced by the multiphysics model is routed through the AI optimization module; AI continually provides the optimal configuration of the nanolayers to minimize the interfacial resistance and maximize the ionic conductivity of the interface.

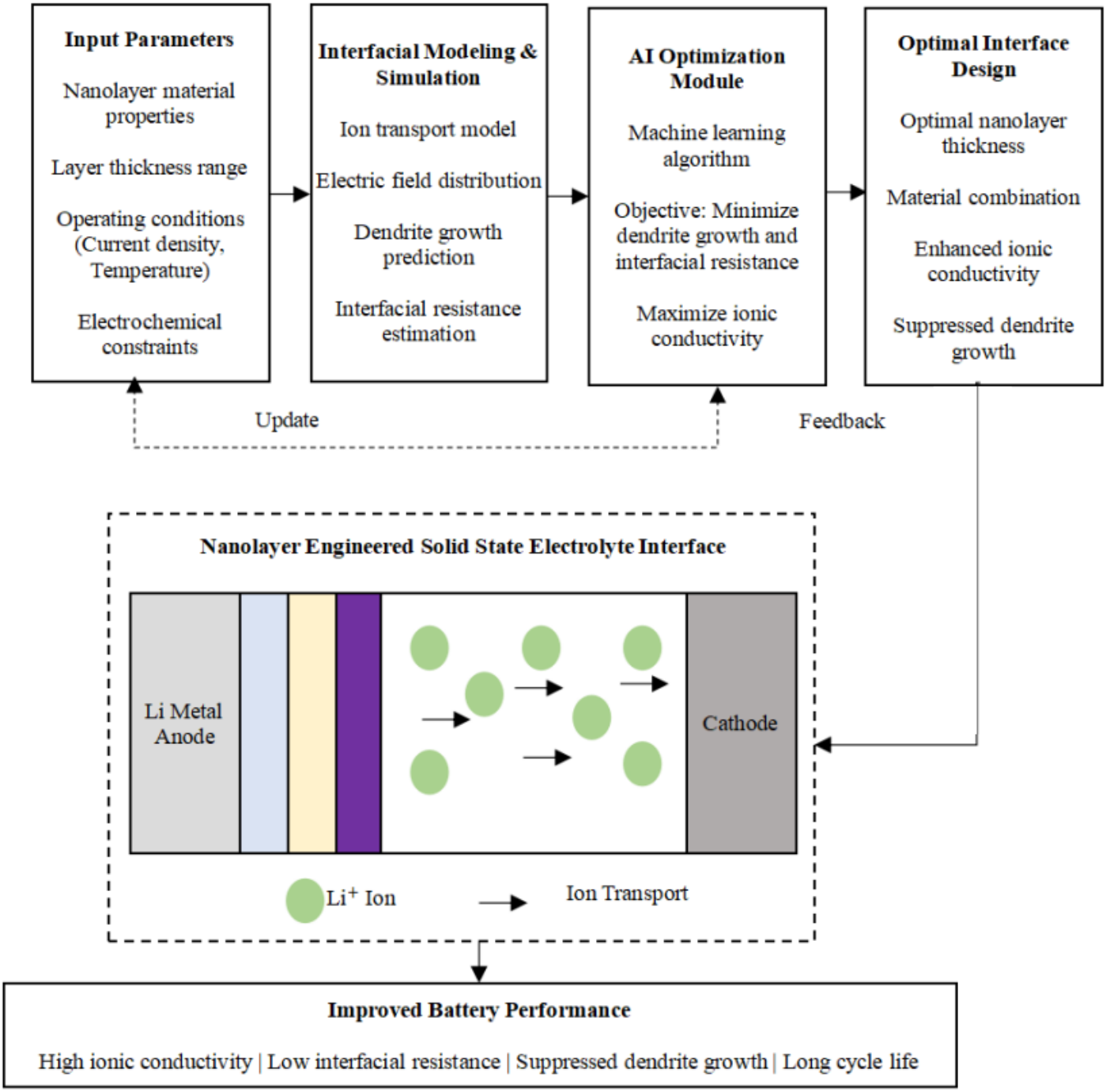


Figure 1. AI-driven control architecture for nanolayer-engineered solid-state electrolyte interfaces.

After the optimal shape of the interface has been determined, it is used in a solid-state battery model, where how the new design affects the movement of lithium ions and stops dendrite formation is observed. The optimization process is iterative in that the input variables and optimization model are updated constantly to provide better electrochemical stability and longer cycle life.

2.2. Nanolayer-engineered interface model

A lithium metal anode, engineered nanolayer interface, solid-state electrolyte, and cathode are included in the configuration of batteries. The nanolayer has been designed to simulate an 'artificial interphase' and act as a medium to control the movement of lithium ions through the electrolyte and minimize large fluctuations in

local current density at the electrode/electrolyte boundary.

The lithium-ion mobility through the solid electrolyte interphase is described by the Nernst–Planck approach, where the diffusive transport of ions along with the effect of an electric field are taken into account. The described approach has been extensively used in modeling ion transport and electrochemical deposition in lithium batteries [23].

$$J_{Li} = -D_{eff}\nabla C_{Li} + \mu C_{Li}E \quad (1)$$

where J_{Li} denotes the lithium-ion flux, D_{eff} represents the effective diffusion coefficient, C_{Li} is the lithium-ion concentration, μ denotes the ionic mobility, and E represents the electric field intensity.

Equation (1) shows that while lithium ions are being moved, they are affected by concentration and electric fields acting on them. They are both responsible for lithium ions moving from point A to point B, and it is therefore critical to also look at how the electric field and lithium concentration are related to where dendritic growth occurs. Because of the changes to how the nanolayer interphase has been engineered, this allows for redistribution of ionic flux, allowing for more uniform deposition of lithium without increasing the chance that dendritic deposition happens. The current model focuses on diffusion and migration driven by the electric field because the non-uniform ionic flow and local current density play a crucial role in the formation of dendrites. However, other degradation factors such as mechanical stresses, interfacial reactions, cracks, and morphology changes cannot be included because their addition will lead to a more complex model. They will be taken into account in future model improvements.

An additional benefit to using an engineered nanolayer is that it serves to create an additional mechanical and electrochemical barrier between lithium metal and electrolyte, preventing them from making direct electrical contact, which prevents any parasitic interfacial reactions from occurring and reduces degradation at the interface.

2.3. Dendrite growth and interfacial resistance formulation

Dendrite growth is controlled by the non-homogeneous flow of Li-ions, local current density, and interfacial stability. Earlier researchers had demonstrated that interfacial resistance and the behavior of ionic conduction play important roles in the deposition of lithium and its dendrite growth [24]. On this basis, an empirical criterion called the dendrite growth index is proposed, which considers the effects of current density, interfacial resistance, and ionic conduction.

The dendrite growth index is defined as

$$D_g = \frac{J_{loc}R_{int}}{\sigma_{ion}} \quad (2)$$

where D_g represents the dendrite growth index, J_{loc} denotes the local current density, R_{int} is the interfacial resistance, and σion represents the i_{onic} conductivity of the electrolyte interface.

According to Equation (2), a greater current density at a given location has a significant effect on the potential for dendrite growth caused by a larger electric field due to higher resistance at the interfacial region. Therefore, the increase in ionic conductivity lowers the growth potential of dendrites and enhances the battery's electrochemical stability.

Nanostructured layers provide a more uniform conductive path for ions to travel through and fewer localized electric fields to develop. Therefore, over time and with repeated charge/discharge cycles, the polarisation effects at the interface and the

resistance at the interface are reduced. The probability of dendritic growth can be obtained by normalizing the proposed dendrite growth index that takes into account the effects of local current density, interfacial resistance, and ion transportation properties. The index is a relative one and cannot be interpreted as the experimental probability of dendrite growth. By using this model, the proposed nanolayer interface decreased the probability of dendrite growth from 31.8% to 11.2%.

2.4. AI-driven optimization mechanism

The optimization of nanolayer interface parameters involves multiple competing objectives, including enhancement of ionic conductivity, reduction of interfacial resistance, and suppression of dendrite growth. Thus, a multi-objective optimization function using weights is employed to derive the optimal nanolayer architecture. Such multi-objective optimization techniques have been extensively utilized in battery design applications in order to satisfy various electrochemical performance criteria [25]. In this research, an optimization technique based on reinforcement learning is employed to select the appropriate nanolayer design parameters adaptively. The states of the AI agent are constituted by the outputs from the electrochemical simulations, i.e., ionic conductivity, interface resistance, and dendrite formation index. The design parameters, such as nanolayer thickness and composition, are treated as the actions of optimization. The objective function defined in Equation (3) is used as the reward function.

$$F_{obj} = w_1\left(\frac{1}{\sigma_{ion}}\right) + w_2 R_{int} + w_3 D_g \tag{3}$$

where F_{obj} represents the objective function, w_1, w_2, and w_3 denote weighting coefficients, σ_{ion} represents ionic conductivity, R_{int} denotes interfacial resistance, and D_g is the dendrite growth index.

The weighting coefficients were selected based on the relative importance of the optimization objectives, where $w_1 = 0.4$ was assigned to ionic conductivity and $w_2 = w_3 = 0.3$ were assigned to interfacial resistance and dendrite suppression. A sensitivity analysis was performed by varying these coefficients, and the results confirmed that moderate changes affected the optimized parameters only marginally while maintaining the overall performance improvement trend. This demonstrates the robustness of the proposed optimization framework. Updates to each nanolayer's thickness and materials throughout the optimization are carried out until the objective function reaches its minimum value. The feedback mechanism illustrated in Figure 1 allows the interfacial design to adaptively refine based on the conditions it sees while in operation, including variations in temperature, charging rates, and current densities.

The AI-based strategy considerably diminishes the computational burden and therefore allows for the quick determination of optimal configurations for high-performance interfacing that would take an extensive number of experiments to develop otherwise.

2.5. AI model training and validation process

The training of the AI optimization model was done through the use of datasets created from simulation runs of multiphysics interface models. To generate a dataset with 2,000 samples, variables such as nanolayer thickness, material properties, temperature, and current density were used. The input variables were nanolayer thickness, ionic conductivity, interfacial resistance, temperature, and current density, while the output variable was the optimal interface configuration through the

objective function value.

Training of the AI model was done iteratively, with the objective function acting as the criterion for optimization. The loss function was the difference between the predicted and optimized objective values. Training was stopped when the error for objective function convergence was below 1 × 10−4. Optimal configurations were validated with other independent simulation cases.

2.6. Problem formulation

Lithium dendrite formation in solid-state Li metal batteries has become a major issue due to uncontrolled growth resulting from nonuniform ion transport and the unstable interface between electrodes and electrolytes. Existing interfacial engineering methods generally improve ionic conductivity or mechanical stability, but cannot be optimized concurrently. Interfacial engineering is currently limited by conventional optimization processes, which often do not effectively lead to the identification of the best nanolayer parameters due to their highly nonlinear relationship with electrochemical and interfacial phenomena.

Therefore, the research presented in this article has developed an optimization problem that minimizes interfacial resistance and dendrite growth probability while maximizing ionic conductivity and long-term cycling stability. The AI-modified nanolayering program aims to provide solutions to each of these requirements through the integration of intelligent complex interfacial modeling, intelligent routing optimization, and feedback control into a single structure to enhance the safety, reliability, and energy density of next-generation solid-state lithium-metal batteries.

3. Simulation setup and experimental design

3.1. Simulation environment

A multiphysics simulation framework, which includes an AI-based optimization module, was utilized to assess the proposed nanolayer-engineered solid-state electrolyte interface. The multiphysics environment allows for an accurate representation of the interdependent processes of lithium-ion movement, interfacial resistance, and dendrite growth in realistic working environments. The multiphysics model was combined with an artificial intelligence (AI) module that can perform an optimization process iteratively to improve ionic conductivity and electrochemical stability through tuning of the nanolayer thickness and interfacial parameters. Simulations were run on the proposed interface under a variety of current densities and temperatures in order to evaluate the responsiveness of the interface design to next-generation, high-energy-density battery applications. The designed interface of a nanolayer-engineered solid-state electrolyte was characterized by developing a multiphysics simulation model that was accompanied by an AI-based optimization tool. The simulation model was created to characterize lithium-ion transport behavior, electric field distribution, interfacial resistance changes, and dendrite formation behavior under varying conditions. The computational process of optimizing the interface was based on the feedback from simulation results.

Multiphysics modeling was carried out using COMSOL multiphysics software along with electrochemical transport modules. In the computational model, the lithium electrode, nanolayer interface, solid-state electrolyte, and cathode regions were included. Lithium-ion transport was simulated based on the Nernst–Planck

equation, and the electric potential was solved through charge conservation equations. Appropriate boundary conditions were included for lithium-ion concentration and flux at the time of the plating/stripping process. Mesh refinement was carried out close to the nanolayer interface, and the mesh independence was checked using various mesh densities. The simulation result converged with a residual error of < 10−4.

3.2. Experimental parameters

It has been found that the best choice for nanolayer formation with the optimal thickness of 80 nm is Li_3PO_4. This is justified by the high ionic transport and interfacial stability of such a nanolayer and the right balance between mechanical protection and lithium-ion transport. Thus, it ensures uniform ion distribution, low interfacial resistance, and efficient dendrite suppression. The chosen Li_3PO_4 nanolayer can be regarded as an artificial interphase due to its lithium-ion conductivity, chemical compatibility with lithium metal, and electrochemical stability. Its thickness was optimized in the range of 20–200 nm, as thinner nanolayers ensure insufficient interfacial protection and thicker layers increase ion transport resistance. Such a deposition method can be regarded as compatible with the ALD-based fabrication approach.

The simulation dataset was obtained by changing the values of the most important parameters of the interface and operation, including the thickness, ionic conductivity, temperature, and current density of the nanolayer. These parameters were chosen according to the characteristics of solid-state lithium batteries. In total, configurations have been generated for simulations.

The study's material type and operational parameters are provided in **Table 1** below. The range of values selected in each case corresponds to previous experimental work done using solid-state Li-on batteries, thereby allowing for a broad evaluation of the performance of the interfaces with respect to both charge and discharge conditions.

Table 1. Simulation parameters and experimental settings.

Parameter	Symbol	Value
Solid electrolyte thickness	t_{SE}	40 μm
Nanolayer thickness range	t_{NL}	20–200 nm
Initial ionic conductivity	σ_{ion}	9.0×10^{-4} S cm^{-1}
Operating temperature	T	25–80 °C
Current density range	J	0.2–2.5 mA cm^{-2}
Initial interfacial resistance	R_{int}	82 Ω cm^2
Charge–discharge cycles	N_c	500 cycles
AI optimization iterations	N_{iter}	200
Learning rate	η	0.001
Weight coefficients	w_1, w_2,w_3	0.4, 0.3, 0.3
Cell operating voltage	V	3.7 V
Simulation time step	Δt	1 s

3.3. Performance evaluation strategy

To test the effectiveness of the framework, four major parameters were considered: ionic conductivity, interfacial resistance, critical current density, and cycle stability in terms of capacity retention. The optimized nanolayer structure achieved by the framework was then compared to a regular solid-state electrolyte interface in order to assess any advancements in terms of suppressing dendrites and electrochemical performance. Also, simulations of charge-discharge operations were carried out under various conditions in order to analyze the stability of the proposed interface for future solid-state lithium batteries.

3.4. Validation strategy and reliability assessment

The predictions by the model were further confirmed by comparing the values to those reported experimentally for solid-state lithium metal batteries. The optimized interface provided an ionic conductivity of 1.21 × 10−3 S cm−1, interfacial resistance of 46 Ω cm^2, and critical current density of 2.1 mA cm−2, which are within the experimental range reported for solid-state electrolyte interfaces. Moreover, capacity retention of 93.4% after 500 cycles shows enhanced cycling stability similar to that reported in nanolayer-engineered lithium metal battery interfaces. This confirms the physical viability of the simulation framework. Further experimental fabrication and testing of the optimized nanolayer interface are planned for future validation.

This is a computational simulation and optimization study. While the performance predictions are within the range reported experimentally, experimental fabrication and testing are required for full validation.

3.5. Uncertainty analysis

The stability of the simulation outcomes was investigated via uncertainty analysis conducted by conducting simulation runs at various operating temperatures and current densities. The performance data was analyzed through mean variation intervals to determine the stability of the proposed model. The optimized interface showed stable performance with minimal variations, thus validating the robustness of the predicted outcomes.

4. Results and discussion

4.1. Influence of nanolayer engineering on ionic transport

To investigate the proposed nanolayer-engineered interface to determine if it could improve lithium-ion migration within the solid-state electrolyte, the ionic transport characteristics were examined. **Figure 2** shows the change in ionic conductivity with the number of cycles for both the conventional and proposed interfaces. At the beginning of the operation, the conductivity of the proposed system was approximately 9.5×10−4 S cm−1, which gradually increased due to the stabilization of the engineered interface and the formation of continuous ion-conduction pathways. After 500 cycles, the conductivity reached 1.21×10−3 S cm−1, whereas the conventional interface exhibited a maximum conductivity of only 8.98×10−4 S cm−1.

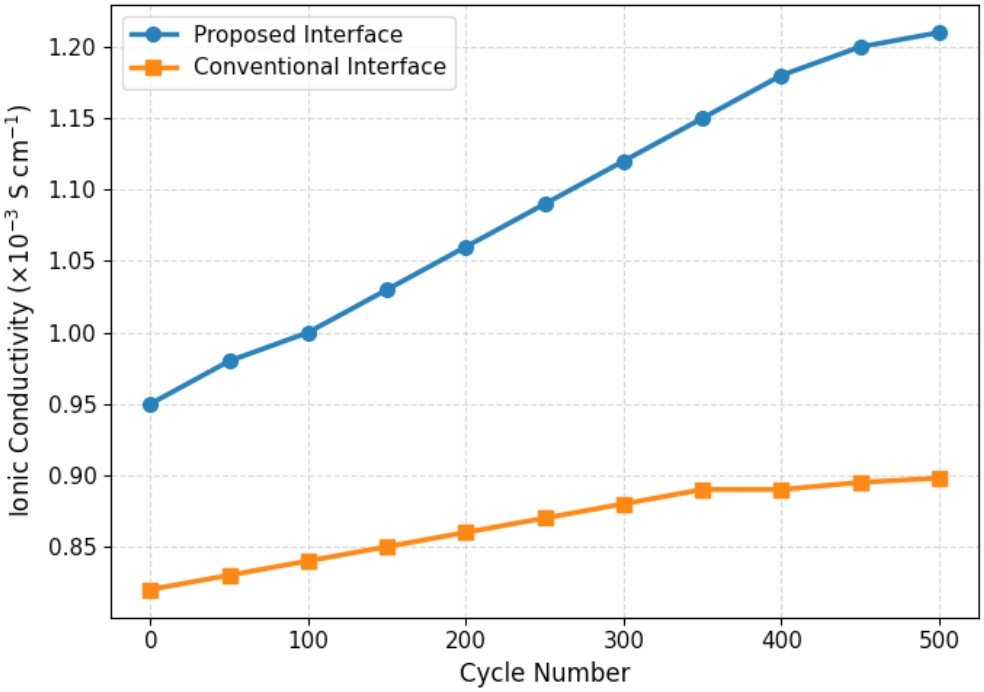


Figure 2. Comparison of ionic conductivity between the conventional and proposed nanolayer-engineered interfaces.

This demonstration of about 34.8% improvement in performance was due to improved ion transport resistance and improved uniformity of lithium-ion diffusion at the electrode-electrolyte interface through the application of nanolayer structures. Three main factors caused the improvement in conductivity: the architecture of the nanolayers decreases local concentration polarization by more uniformly distributing the electric field, optimizing the engineered interphase reduces the presence of interfacial defects, which create barriers to ion transport, and finally, the AI-based optimization procedure has determined the optimum thickness for the nanolayers, which maximizes ionic mobility while minimizing the loss of transport.

An increase in ionic conductivity directly enhances overall battery performance through decreased overpotential and improved charge-transfer kinetics; results suggest that it is possible to significantly enhance the electrochemical performance of solid-state lithium cells through nanolayer engineering without any degradation of interfacial stability.

4.2. Interfacial resistance and AI optimization performance

The resistance at the electrode-electrolyte interface is an essential thing to look at when figuring out cycling stability and energy efficiency for all-solid-state batteries. As shown in **Figure 3**, the interfacial resistance changed over time during the AI optimization. The interfacial resistance of the conventional interface was about 82 Ω cm^2; this high value was caused by poor interface contact and uneven ionic transport paths. As more iterations were completed during the optimization, the interfacial resistance value kept decreasing until it reached a stable value of about 46 Ω cm^2.

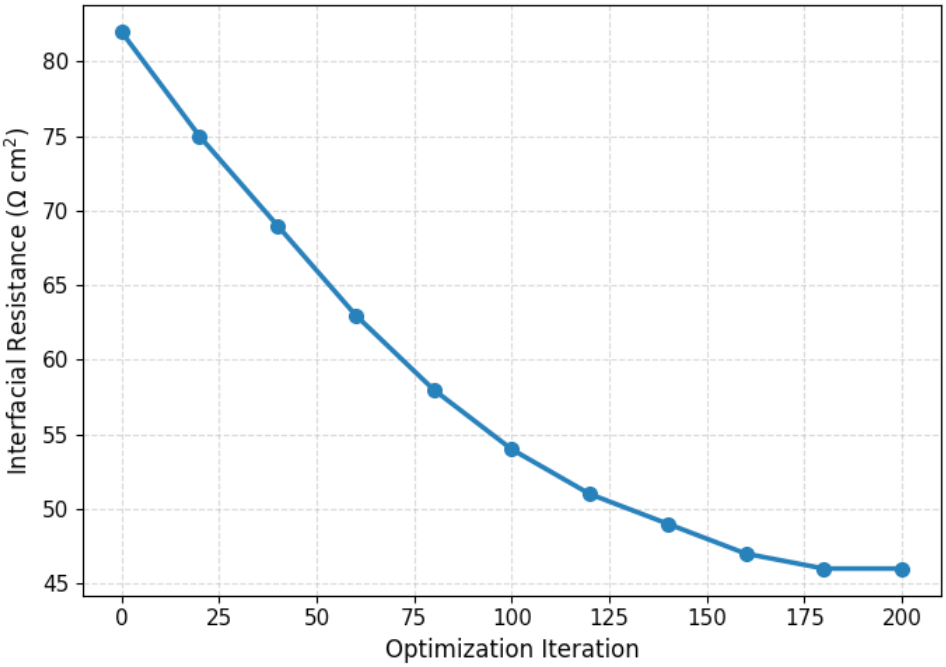


Figure 3. Variation of interfacial resistance during AI-driven optimization.

The decrease of nearly 43.9% demonstrates that this proposed optimization framework has successfully determined nanolayer configurations that can be optimally designed for reducing the overall interfacial impedance. The significant amount of resistance that was reduced in the initial 100 iterations of this algorithm indicates that it has been able to eliminate many states of highly resistive interfaces and has created stable ionic conduction pathways within the nanolayers. After approximately 150 iterations, there are very minimal reductions in the resistance as the system has been optimally converged.

By lowering the interfacial resistance of the battery, the electrochemical reaction kinetics improve significantly by lowering the polarization losses during the charge-discharge cycles. As a result, a battery can be operated at higher current densities with stable electrochemical performance. Furthermore, the reduction in the total impedance of a battery also creates less localized heat generation, which is one of the primary ways to improve the safety and extend the lifetime of high-energy-density batteries.

Results of this optimization show that nanolayer thickness has a significant effect on the measurement of the interface. Layers that are excessively thin do not provide adequate mechanical protection to prevent dendrite growth, while layers that are too thick have additional resistance to the movement of ions through them. The use of the AI-based platform thus allows a systematic and objective means of determining an appropriate balance between ionic conductivity and interfacial stability.

4.3. Electrochemical stability and dendrite suppression

To reduce lithium dendrite formation during periodic cycling for the proposed design. **Figure 4** compares retention capacity for both the conventional and proposed interfaces over 500 charge-discharge cycle tests. The conventional system's retention decreases steadily throughout the full cycle test and is only able to retain 79.6% of its original retention capacity at the conclusion of the test. Conversely, the proposed interface (created by a modified, nano-engineered coating material) retained 93.4% of its original retention capacity under identical testing conditions.

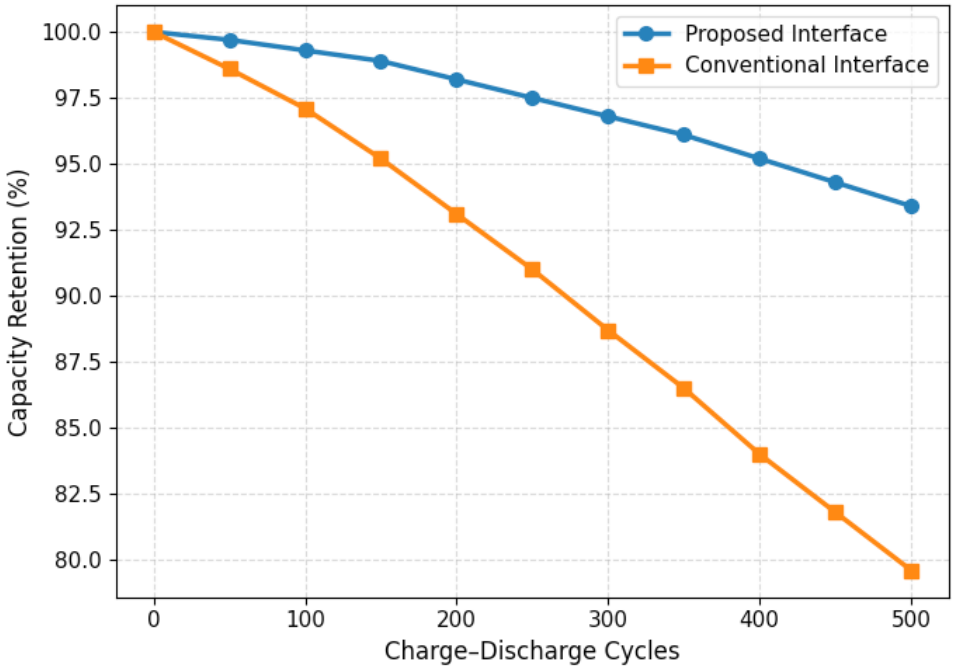


Figure 4. Capacity retention comparison between the conventional and proposed interfaces over 500 charge-discharge cycles.

The improved retention of capacity indicates that the engineered interface can alleviate dendrite-mediated degradation mechanisms. The increase in stability can be attributed to a more uniform distribution of lithium-ion flux at the engineered interface. As a result of large peaks in current density being dramatically reduced, lithium deposition occurs more uniformly and avoids the formation of needle-like dendritic structures.

After 250 cycles of testing, there is a discernible difference between the two systems. For the traditional system, accelerated deterioration occurs at this point as a result of duplicate dendrite growth and interface fracture. Conversely, because of the nanolayer interface's ability to regulate ion transport and maintain structural integrity, the proposed architecture exhibits stable electrochemical behavior even after many more cycles.

The experimental results support the conclusion that the designed interface has the ability to prevent dendrite creation and mechanical degradation between interfaces over extended periods of time, thus greatly increasing the long-term reliability of a solid-state lithium-ion battery.

4.4. Uncertainty analysis

The validity of the proposed system was investigated through uncertainty analysis by running the simulation at various operating temperatures and current density values. The outcomes of the analysis showed minor changes in the performance criteria of the system. For the optimized interface, the ionic conductivity was 1.21 × 10−3 S cm−1 ± 0.04 × 10−3, the interfacial resistance was 46 ± 3 Ω cm^2, and the capacity retention was 93.4% ± 1.8% after 500 cycles.

4.5. Comparative performance analysis

The optimized interface was benchmarked against exemplary solid-state electrolytes to ensure physical significance. $Li_7La_3Zr_2O_{12}$ (LLZO) shows an ionic conductivity range from 104 to 103 S cm−1, whereas sulfide, Na Super-ionic CONductor (NASICON), and halide electrolytes provide high transport properties

with interface issues. The attained values of ionic conductivity and critical current density (1.21 × 10−3 S cm−1 and 2.1 mA cm−2, respectively) fall within the range of solid-state battery interfaces.

To quantitatively evaluate the effectiveness of the proposed methodology, the key performance metrics are summarized in **Table 2**.

Table 2. Performance comparison between conventional and proposed interfaces.

Performance metric	Conventional interface	Proposed interface	Improvement
Ionic conductivity (Scm^{-1})	8.98×10^{-4}	1.21×10^{-3}	34.8%
Interfacial resistance ($\Omega\ cm^2$)	82	46	43.9% reduction
Critical current density ($mA\ cm^{-2}$)	1.3	2.1	61.5%
Capacity retention after 500 cycles (%)	79.6	93.4	17.3%
Estimated dendrite growth probability (%)	31.8	11.2	64.8% reduction

Optimizing the ionic transport and interfacial stability of solid-state lithium batteries greatly improves their overall electrochemical performance. The increase in critical current density demonstrates a significant improvement in the tolerance of dendrite penetration and supports high power levels of operation.

The presented approach is aimed at serving as a transferable approach for optimization through adjusting interface-related parameters, including ionic conductivity, resistance, and suppression of dendrites for various types of solid-state electrolytes. While sulfide, oxide, and hybrid electrolytes have distinctive physical and electrochemical features, the suggested AI-powered approach does not depend on the type of electrolyte and is able to optimize nanolayer features based on the properties of particular materials. Nevertheless, additional experimentation is needed to test the performance of the optimized interface for specific electrolyte systems.

4.6. Ablation analysis of framework components

The ablation study is carried out to find the effect of each component of the proposed system. There are four variants under study: traditional solid-state electrolyte interface, engineered nanolayered interface, nanolayered interface with multiphysics modeling, and the entire AI optimization system.

Table 3 ablation study shows that all three elements contribute progressively to improving the performance. Nanolayer engineering increases interface stability, multiphysics modeling increases parameter understanding, while AI optimization helps in finding the optimal configuration, resulting in the highest ionic conductivity, minimum interfacial resistance, improved critical current density, and improved cycling stability.

Table 3. Ablation analysis of individual framework components.

Configuration	Ionic conductivity ($S\ cm^{-1}$)	Interfacial resistance ($\Omega\ cm^2$)	Capacity retention (%)
Conventional interface	0.90×10^{-3}	82	79.6
Nanolayer engineering	1.05×10^{-3}	61	85.7

Continuation Table:

Configuration	Ionic conductivity (S cm^{-1})	Interfacial resistance (Ω cm^2)	Capacity retention (%)
Nanolayer + multiphysics modeling	1.13×10^{-3}	53	89.8
Proposed AI-assisted framework	1.21×10^{-3}	46	93.4

4.7. Discussion on practical implications

These results suggest that the combination of nanotechnology and AI can be used as a means of overcoming the primary obstacle to implementing lithium metal batteries into practical use; hence, by improving the electrolyte properties in terms of higher ionic conductivity and lower interfacial resistance, this architecture design leads to higher energy efficiency and shorter charging time. Moreover, the cycle stability of this design and the dendrite suppression ability also mean that this architecture design greatly increases battery safety and lifetime.

Practical applications show that the optimized interface is feasible for incorporation into sulfide-, oxide-, or composite-based solid-state batteries without extensive changes to the current production methods. The AI-enabled optimization methodology also allows for the rapid identification of the best interfacial configurations for many different electrolyte materials and operational settings, providing scalability. In terms of manufacturing, the new nanolayer structure can be fabricated using scalable thin-film deposition techniques, like atomic layer deposition and solution-assisted coating processes. While ALD enables precise control over the film thickness and good uniformity of the interface, the problem associated with the process is the comparatively low deposition speed and the cost of equipment required for this approach. Further research should address high-throughput coating techniques and cost reductions.

The data collected supports the conclusion that the proposed nanolayer-engineered interface is a viable route for producing safe, long-lasting, high-performance solid-state lithium-ion batteries to be used in electric vehicles and large energy storage systems.

5. Conclusion

The key results of this study can be highlighted as follows:

An AI-enabled framework for a nanolayer-engineered solid-state electrolyte interface was proposed to improve lithium-ion mobility, stabilize the interface, and hinder lithium dendrite formation in high-energy lithium metal batteries.

The improved interface showed an ionic conductivity value of 1.21 × 10−3 S cm−1, which is 34.8% better than the conventional interface.

The proposed approach decreased the interfacial resistance value from 82 Ω cm^2 to 46 Ω cm^2, which means a reduction in the value by 43.9%.

The critical current density was raised from 1.3 mA cm−2 to 2.1 mA cm−2, meaning increased tolerance to dendrite formation.

The optimized interface retained 93.4% capacity after 500 charge-discharge cycles, while the conventional one maintained 79.6%, showing improved cycling stability.

The ablation analysis revealed that the combination of nanolayer engineering, multiphysics modeling, and AI optimization improved the performance of the battery.

In summary, the proposed framework provides possible application areas like

electric cars, energy storage devices for renewable sources, and high-end portable electronic systems. More efforts should be made towards experiments, incorporation into battery management systems, electrochemistry-mechanics modeling, and scalability in the manufacturing process.

Author contributions: All authors contributed equally to the conception, design, data collection, analysis, and writing of this study. All authors have read and agreed to the published version of the manuscript.

Institutional review board statement: Not applicable.

Informed consent statement: Not applicable.

Data availability statement: The data used in this study are available from the corresponding author upon reasonable request.

Conflict of interest: The authors declare no conflict of interest.

AI use statement: In the process of preparing this manuscript, the authors have relied only on AI technology to enhance the linguistic quality and readability of the manuscript. No AI technology has been used in the process of analyzing and interpreting data and generating scientific results. The results were critically reviewed and edited by the authors.

Abbreviation

LMB	Lithium Metal Battery
SSE	Solid-State Electrolyte
AI	Artificial Intelligence
ALD	Atomic Layer Deposition
σ	Ionic conductivity
R_{int}	Interfacial resistance
J	Lithium-ion flux/current density
C	Lithium-ion concentration
D	Diffusion coefficient
μ	Ionic mobility
E	Electric field intensity
T	Operating temperature
δ	Nanolayer thickness
η	Optimization objective function
w_1, w_2, w_3	Weight coefficients
C_r	Capacity retention
CCD	Critical Current Density
GI	Dendrite Growth Index
ML	Machine Learning
FEM	Finite Element Method

References

1. Taghavi M, Lee CJ. Development of a novel hydrogen liquefaction structure based on liquefied natural gas regasification operations and solid oxide fuel cell: Exergy and economic analyses. Fuel. 2025; 384: 133826.
2. Taghavi M, Colpan CO, Dincer I. Development of an integrated production and liquefaction system of hydrogen and green natural gas: energy, exergy, economic and sensitivity assessments. Energy. 2026; 360: 141476.
3. Janek J, Zeier WG. A solid future for battery development. Nature Energy. 2016; 1(9): 16141.
4. Mwangi S. Solid-State Battery Integration Strategies for Next-Generation Renewable Energy Storage Networks. National Journal of Renewable Energy Systems and Innovation. 2026; 2(4): 38–50.
5. Lin D, Liu Y, Cui Y. Reviving the lithium metal anode for high-energy batteries. Nature Nanotechnology. 2017; 12(3): 194–206.
6. Lemeon M, Noria F. Advanced Battery Management and Control Algorithms for Sustainable Lithium-Ion and Solid-State Energy Storage Systems. Transactions on Energy Storage Systems and Innovation. 2025; 1(3): 19–25.
7. Shen J, Cui C, Zhao J, et al. Advancing NASICON solid-state electrolytes for lithium metal batteries: Interfacial challenges, engineering strategies, and future directions. Energy Storage Materials. 2025; 81: 104471.
8. Manthiram A, Yu X, Wang S. Lithium battery chemistries enabled by solid-state electrolytes. Nature Reviews Materials. 2017; 2(4): 16103.
9. Han F, Westover AS, Yue J, et al. High electronic conductivity is the origin of lithium dendrite formation within solid electrolytes. Nature Energy. 2019; 4(3): 187–196.
10. Hashim IM. Mechanical Analysis of Stress and Deformation in Lithium Battery Electrodes During Charge–Discharge Cycles. Archives for Technical Sciences. 2026; 1(35): 598–609.
11. Porz L, Swamy T, Sheldon BW, et al. Mechanism of lithium metal penetration through inorganic solid electrolytes. Advanced Energy Materials. 2017; 7(20): 1701003.
12. Zhang Z, Shao Y, Lotsch B, et al. New horizons for inorganic solid-state ion conductors. Energy & Environmental Science. 2018; 11(8): 1945–1976.
13. Yang X, Wang Y, Guo Y, et al. Interfacial engineering of suppressing Li dendrite growth in all-solid-state Li-metal batteries. Journal of Materials Chemistry A. 2024; 12(25): 14848–14865.
14. Cheng XB, Zhao CZ, Yao YX, et al. Recent advances in energy chemistry between solid-state electrolyte and safe lithium-metal anodes. Chem. 2019; 5(1): 74–96.
15. Xu R, Cheng XB, Yan C, et al. Artificial interphases for highly stable lithium metal anode. Matter. 2019; 1(2): 317–344.
16. Zhao Q, Stalin S, Zhao CZ, et al. Designing solid-state electrolytes for safe, energy-dense batteries. Nature Reviews Materials. 2020; 5(3): 229–252.
17. Krauskopf T, Richter FH, Zeier WG, et al. Physicochemical concepts of the lithium metal anode in solid-state batteries. Chemical Reviews. 2020; 120(15): 7745–7794.
18. Yang C, Fu K, Zhang Y, et al. Protected lithium-metal anodes in batteries: From liquid to solid. Advanced Materials. 2017; 29(36): 1701169.
19. Sun C, Ruan Y, Zha W, et al. Recent advances in anodic interface engineering for solid-state lithium-metal batteries. Materials Horizons. 2020; 7(7): 1667–1696.
20. Chen C, Zuo Y, Ye W, et al. A critical review of machine learning of energy materials. Advanced Energy Materials. 2020; 10(8): 1903242
21. Li W, Li M, Ren H, et al. Nitride solid-state electrolytes for all-solid-state lithium metal batteries. Energy & Environmental Science. 2025; 18(10): 4521–4554.
22. Esmizadeh S, Cabras L, Serpelloni M, et al. A review on modeling of nucleation and growth of Li dendrites in solid electrolytes. Journal of Energy Storage. 2024; 97: 112897.
23. Wang H, Yan X, Zhang R, et al. Application-driven design of non-aqueous electrolyte solutions through quantification of interfacial reactions in lithium metal batteries. Nature Nanotechnology. 2025; 20(8): 1034–1042.
24. Chen XR, Zhao BC, Yan C, et al. Review on Li deposition in working batteries: From nucleation to early growth. Advanced Materials. 2021; 33(8): 2004128.
25. Ng MF, Zhao J, Yan Q, et al. Predicting the state of charge and health of batteries using data-driven machine learning. Nature Machine Intelligence. 2020; 2(3): 161–170.