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Research on the Application of Machine Learning in the R&D of Automotive Solid-State Electrolyte Materials

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Abstract. With the rapid development of the new energy vehicle industry, solid-state electrolytes, as key materials to improve the safety and energy density of lithium-ion batteries, have attracted extensive attention. The traditional research and development (R&D) of solid-state electrolyte materials relies on the "trial-and-error" model, which features long cycles and high costs, making it difficult to meet the demand for efficient screening of excellent materials. This paper systematically sorts out the key performance indicators of solid-state electrolytes, including stability, electronic conductivity and ionic conductivity, and focuses on the application progress of machine learning technology in the property prediction and inverse design of solid-state electrolyte materials. By analyzing the development overview and application examples of generative models (such as variational autoencoders, generative adversarial networks, recurrent neural networks, reinforcement learning) and predictive models (such as artificial neural networks, graph neural networks) in material design, this paper summarizes the challenges faced by current methods in data dependence, model interpretability, generation stability and other aspects. Research shows that the machine learning-based material R&D paradigm is expected to break through the limitations of traditional methods, accelerate the discovery and optimization of high-performance solid-state electrolyte materials, and provide strong support for the development of solid-state batteries for electric vehicles.

Keywords: Solid-state electrolyte, Machine learning, Ionic conductivity

1. Background

Driven by global energy shortage and low-carbon development, new energy vehicles have become an important direction for the future automotive industry. At present, power batteries, as the core component of new energy vehicles, have received high attention. With the national "dual carbon" policy proposed, the replacement with advanced energy storage devices has become an urgent task. Automotive power batteries represented by lithium-ion batteries are widely used due to their reasonable cost and mature technology, but problems such as short cruising range and poor safety have seriously hindered the further development of the new energy vehicle industry. An effective way to improve energy density is to increase the cut-off voltage, but this will cause problems such as high-voltage side reactions of liquid electrolytes. An effective solution to such problems is to replace flammable liquid electrolytes with solid-state electrolytes, which significantly reduces the risks of

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leakage, evaporation and decomposition, ensuring higher safety. At present, one of the key challenges in this research is how to construct stable solid-state electrolyte materials with high ionic conductivity. Ideal electrolytes for solid-state lithium-ion power batteries should possess excellent properties such as high ionic conductivity [1], low migration energy barrier [2], wide electrochemical window [3], strong electrochemical stability and high mechanical stiffness. However, it is not easy to rapidly develop solid-state electrolyte materials [4] that simultaneously meet these commercial requirements and performance standards. Traditional material discovery often adopts the "trial-and-error" model, that is, putting forward hypotheses based on existing expert experience and understanding of the physicochemical properties of solid-state electrolyte materials, and conducting experimental verification to find target materials. This process needs to be repeated and requires a lot of time and resources to achieve the goal. This method seriously relies on the scientific experience of researchers, with high experimental costs and long time consumption, which seriously hinders the research process. Therefore, to improve R&D efficiency and save R&D costs, physics, materials science and computer science are integrated. The accuracy and reliability of computational simulation methods have been improved through the vigorous development of multi-scale computational simulation methods at micro, meso and macro levels.

Among them, Density Functional Theory (DFT), classical Molecular Dynamics (MD) simulation and Ab Initio Molecular Dynamics (AIMD) simulation are gradually becoming useful tools to solve the challenges in the R&D of solid-state electrolyte materials. Using computational materials science simulation, materials scientists can study many properties of solid-state electrolyte materials, such as ion transport mechanism, current density of charging and discharging, mechanical properties of materials, and chemical stability at the atomic scale, accelerating the R&D process. However, these simulation methods rely on high-performance large-scale computing equipment and the microstructure of solid-state electrolyte materials, and there are still challenges in computational accuracy and speed. The biggest problem is that this simulation method can only optimize and study a single performance of solid-state electrolyte materials at a time, so it is difficult to simultaneously design and screen solid-state electrolyte materials with excellent multiple properties. Artificial intelligence technology has been applied to the design and R&D of new battery materials. Existing studies show that AI has great potential in finding new high-quality solid-state electrolyte materials. This facilitates data-driven material mining and design research, and materials science has subsequently entered the fourth scientific paradigm. In June 2011, the United States proposed a new material R&D model—the Materials Genome Initiative, which closely integrates experiments, theories and computational results to make full use of the achievements in computational materials simulation, high-throughput experiments and data mining, establish connections between various fields, reduce the R&D cycle and cost of new materials, and accelerate the speed of material discovery, design and deployment. With the attention and investment of countries around the world in the Materials Genome Initiative, China also launched major scientific research projects related to the Materials Genome Initiative in December 2012, opening a new era of material R&D. In this stage, the database accumulated through physicochemical theories, experiments and computational simulation methods is used as the input of artificial intelligence methods, and then modeling and analysis are carried out for target properties, so as to realize the efficient R&D of solid-state electrolyte materials. At present, one of the most common applications of machine learning technology in the R&D of solid-state electrolytes is the screening of materials with high ionic conductivity, which highly relies on the extensive search ability and precise classification of machine learning algorithms. In addition, the accurate prediction of solid-state electrolyte performance using machine learning models has gradually attracted attention. The predicted

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information can not only reveal the characteristics of the tested materials, but also provide effective guidance for the next round of experiments. Therefore, the effective use of machine learning technology can effectively mine the structure-activity relationship between the target properties and structures of automotive solid-state electrolyte materials and their performance change rules from experimental or computational data, and complete the accurate prediction of ionic conductivity of screened materials.

2. Application of machine learning in the properties of solid-state electrolyte materials

2.1. Performance indicators of solid-state electrolytes

The key of the current work is to change the original method of material development, starting from the target properties of materials, exploring the "structure-activity relationship" between material composition and structure and the key indicators of solid-state electrolytes, and finally achieving the inverse generation effect from properties to structures, and providing possible material composition and structure as guidance. For target properties, the main focus is on stability, electronic conductivity and ionic conductivity. Stability is the first key parameter to be considered. If the material is unstable, the subsequent performance analysis will be meaningless due to the lack of practical basis. There are a large number of non-conductive ions in the solid electrolyte crystal, which can form a rigid framework to ensure that the available ion positions are more than the migrating ions, and can be connected to form channels for ion migration. If the structure of the electrolyte material collapses under external force, it will cause blockage of ion migration channels. Therefore, the stability of the material must be ensured to guarantee the normal use of lithium-ion solid-state electrolytes. When judging the stability of a material by energy, it may be more practical to choose formation energy. This is because materials are generally synthesized from their constituent elements in experiments, and under normal circumstances, stable materials should preferably have negative formation energy at the same time. Another core problem in the development of lithium-ion solid-state electrolytes is the harmful intrinsic electronic conductivity, which will lead to the growth of lithium dendrites and, in the worst case, short circuit of the battery. Electronic conductivity changes with the band gap value. Band gap refers to the energy difference between the conduction band and the valence band in a material. In a crystal, electrons in the valence band are in a bound state, while electrons in the conduction band can move freely. The larger the band gap, the more difficult it is for the material to conduct electricity; conversely, the smaller the band gap, the easier it is for the material to conduct electricity. For example, metals have a very small band gap, so they can conduct electrons freely; insulators have the largest band gap, so they cannot conduct electrons under any circumstances. Ideal lithium-ion solid-state electrolyte materials should be ion-conductive rather than electronically conductive. Therefore, this paper needs to set the upper limit of electronic conductivity according to the design requirements of solid-state electrolytes and find the minimum value of the corresponding band gap. Finally, high ionic conductivity greater than 310 −4 S/cm is considered a key requirement for solid-state electrolytes. However, the ionic conductivity of most solid-state electrolytes at room temperature has not yet met the requirements of traditional liquid electrolytes. The crystal structure of solid-state electrolytes is usually composed of a rigid lattice (composed of framework ions) and a sublattice (composed of migrating ions). A high defect concentration in the sublattice will result in the number of migrating ion positions being greater than that of the migrating ions themselves, thus causing a high degree of disorder. This sublattice disorder state allows all ions to migrate, that is, increases the carrier concentration, and at the same time promotes the cooperative movement of ions. The conductance

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activation energy will be greatly reduced, and the ionic conductivity will be correspondingly increased. From the above discussion, it can be seen that the factor affecting ionic conductivity is activation energy. The lower the activation energy, the stronger the ability of ions to move in the electrolyte, and the higher the ionic conductivity. Therefore, predicting the activation energy of lithium-ion solid-state electrolytes can provide scientists with more comprehensive information for in-depth understanding of the ion transport properties of electrolytes. In summary, ideal lithium-ion solid-state electrolytes should possess stability, high ionic conductivity and low electronic conductivity at the same time, and researchers have sufficient space to discover or find new solid-state electrolyte materials with excellent properties.

2.2. Development overview

In recent years, machine learning technology has made great progress in the inverse design of lithium-ion battery materials. Machine learning technology can mine useful information from a large amount of historical data and explore the relationship between chemical structure and battery performance. For example, machine learning methods based on deep neural networks can infer the optimal composition of solid-state electrolytes according to the chemical structure characteristics in the experimental data of battery performance, which are generally called generative models. Common representative methods include Auto-Encoders (AE) and Variational Autoencoders (VAE), Recurrent Neural Networks (RNN), and Generative Adversarial Networks (GAN), which have been successfully applied to the inverse design of organic polymer battery materials. These algorithms mainly use the sequential or graphical representation of materials to learn the rules of constructing materials, so as to generate effective and novel hypothetical battery materials. It solves the inverse design problem by learning to model the distribution of the data set. At this time, the data set is a set of materials and properties, and the generative model extracts new compositions and structures from the learned distribution. Generative models are mainly divided into four types: The first type is the approximate distribution of solving the likelihood function through variational encoders. The representative method is VAE, which contains two neural networks: an encoder and a decoder. Both networks are trained to deconstruct (encoder) and reconstruct (decoder) data, learning to compress and decompress data through meaningful intermediate representations. Kan developed a heuristic material exploration system combining supervised and unsupervised learning using the VAE model, and designed and synthesized a new solid polymer lithium-ion battery electrolyte with room temperature conductivity of 10^{-5} S/cm, as well as reasonable thermal, chemical and mechanical properties. However, their system works on a quantum annealing system and can only process binary information at present. Ren proposed a framework capable of general inverse design (not limited to a given set of elements or crystal structures), which is characterized by adopting a generalized reversible representation method and using the attribute structure latent space of autoencoders to encode crystals in real space and reciprocal space. Compared with previous methods, this research method expands the applicable scope of crystals. Court proposed a deep representation learning model based on autoencoders for geometric optimization of three-dimensional crystal structures, while predicting the values of eight target properties. However, it is still an extremely challenging task to thoroughly and effectively sample the entire design space in a computable way. To solve this problem, Fung proposed an inverse design framework, using reversible neural networks to map the forward and reverse processes between the design space and target properties. However, these methods are limited to generating new structures of given material systems and tend to generate molecules with unstable physical properties. The second type is the implicit method that can avoid solving the maximum likelihood process, and the representative

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method is GAN. Dan proposed a GAN-based machine learning generative model MatGAN for the efficient generation of new inorganic materials. However, it requires a large amount of training data to learn rules, posing challenges to data collection and computing resources. Kim constructed a generative adversarial network for crystal structures and generated 23 new crystal structures with reasonable stability and band gap. Although GAN has shown strong performance in material generation tasks, it also has the disadvantage of model collapse due to the complex training process. Therefore, changing the training method of GAN is also the current research focus. The third type is the RNN sequence formed by VAE and GAN on the basis of retaining previous character information. This method adapts the distribution function according to the acquired data distribution rules, trains the model according to the data distribution in the generation process, and finally samples to generate new molecules. However, due to the characteristics of RNN, gradient disappearance or gradient explosion is prone to occur in the later sequence processing with the increase of network layers. Josep studied molecular examples with few required properties in the training generation data based on RNN. However, due to the sequence-based attribute of RNN, its application in the field of inverse molecular design is not extensive. The fourth type is the generation of new molecules through reinforcement learning. The principle of the reinforcement learning method is to maximize the cumulative reward through the interaction between actions and the environment, so as to meet the requirements of specific target properties. Steven used dual-loop reinforcement learning and Simplified Molecular Input Line Entry System (SMILES) to effectively calculate target property scores and obtain molecules with good scores faster. Zhou proposed a molecular deep Q-network framework for molecular optimization by combining chemical domain knowledge and state-of-the-art reinforcement learning techniques (double Q-learning and stochastic value functions). This study directly defines modifications on molecules, thus ensuring 100% chemical validity. However, this method only uses one chemical data set in the experiment, which may have insufficient representativeness, and the universality of the results needs to be further verified. All the above models map from input (e.g., composition) to output, and only utilize the superficial content in the molecular input representation without involving the implicit knowledge of the underlying structure of the molecular chemical space. However, unlike polymer molecules, the application of generative models in inorganic solid materials has been challenging due to the limited available data of inorganic solid materials, the huge chemical breadth provided by the periodic table, and the lack of effective reversible representations. In this regard, Jorgensen combined image recognition and reinforcement learning to determine the atomic structure of the reconstructed crystal surface. A deep neural network represents a reinforcement learning agent that obtains training rewards through interaction with the environment. The environment contains a quantum mechanical potential energy evaluator in the form of a density function theory program. The agent processes the three-dimensional atomic structure as a series of stacked two-dimensional images and outputs the next type of atom to be placed and the atomic position to be occupied. However, this method relies on the quality and diversity of the data set for feature extraction and representation of surface structures, and the quality and quantity of the data set will seriously affect its prediction ability. In addition, it requires a lot of computing resources and time for training and prediction, with high costs. SUI used deep reinforcement learning to automate the composite material design process without the prior knowledge of designers. Based on the reward signal of the change of structural mechanical properties, the deep reinforcement learning algorithm can initiate new design modes in the self-updating process. However, this method may be inapplicable or perform poorly in the design of some special materials. Therefore, reinforcement learning methods are often used in the design of organic materials, especially in drug research and development, and there are few

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applications for solid-state electrolytes. Obviously, the current generative models for the inverse design of new battery materials are very powerful, but still face many challenges. For example, GAN-based models are prone to collapse; VAE-based models cannot avoid likelihood function analysis errors; reinforcement learning methods are mostly used in the field of organic and drug generation, lacking applications in solid-state electrolyte materials. In summary, given the complex and non-differentiable characteristics of the target properties to be optimized, it is still a challenging task to directly generate effective molecules that meet the requirements. Therefore, the current dilemma is that an efficient and highly intelligent generative model that does not overly rely on the manual guidance of scientists is needed. This model should have the dual capabilities of in-depth exploration of chemical space and learning prior knowledge from the existing data distribution. Because the distribution of molecules with target properties may not match the distribution of molecules in the training set used for learning, but they have some same characteristics at the same time, which is also the key to designing new solid-state electrolyte materials, that is, learning to explore new material structures on the basis of correct basic public knowledge.

2.3. Application

Machine learning is a powerful tool for discovering and predicting new material properties in high-dimensional data, which is divided into three parts: input, model and output. ML models can be trained through training data using optimization algorithms, and then automatically establish the relationship between input and output without any physical conditions. In recent years, ML has been successfully applied in crystal structure prediction, electronic properties, material performance search, new material discovery and other fields. Numerous researchers have developed many ML methods to discover new electrolyte materials and predict their properties [5].

In 2014, Jalem combined Artificial Neural Network (ANN) and Partial Least Squares (PLS) algorithm with DFT to predict the diffusion barrier and formation energy of olivine-type $LiMXO_4$ electrolytes, and finally screened 15 promising solid electrolyte materials for lithium-ion batteries. However, this method requires a large number of parameters, the output results are difficult to interpret, and the learning time is too long. Nakayama combined PLS, ANN and Bayesian optimization with DFT, extracted 400 lithium and zinc-containing oxides from the material project data set, calculated the lithium ion mobility and material stability through simulation, and applied Bayesian optimization to determine the material with the highest ionic conductivity, promoting the discovery of new inorganic solid electrolytes. Compared with the former, this method not only narrows the search space, but also significantly shortens the calculation time and improves the calculation efficiency. In 2017, Sendek of Stanford University proposed a guided search method based on machine learning predictive models. He screened 317 candidate electrolyte materials from 12,831 lithium-containing crystal solids. Then, a data-driven ionic conductivity classification model was established through logistic regression, and finally 21 crystal compounds were predicted to be ideal solid-state electrolyte materials. However, even if the above methods can perform accurate simulations, they are limited by the search strategies used to explore the chemical space. Kan constructed the largest database of lithium-ion conductive solid polymers and accurately predicted their lithium-ion conductivity using transfer learning graph neural networks. Unfortunately, this study only focused on aromatic polymer electrolytes, with a relatively single type. Xu proposed a machine learning-based method to predict the ionic conductivity of sodium-based and lithium-based compounds, and used theoretical element feature descriptors to distinguish inferior and high-quality superionic conductors on a limited data set of 70 NASICON examples, with a verification accuracy of over 84%. However, this method relies on a large number of feature screenings. In summary,

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machine learning methods have become an important approach for the property prediction of solid-state electrolyte materials, breaking the limitations of the traditional "trial-and-error" method, being able to quickly identify potential relationships in complex data, and revealing the relationship between the structure and properties of solid-state electrolyte materials. However, the inherent black-box characteristics of machine learning models hinder materials experts unrelated to computers from understanding these predictive models, and it is inevitable for materials scientists to face certain challenges in understanding the models without the help of other auxiliary materials.

3. Conclusion

In solid-state lithium-ion batteries, solid-state electrolyte is a crucial component, which plays a decisive role in ion transport performance. This paper classifies solid-state electrolytes, introduces their ion transport mechanisms and key indicators in detail, and through in-depth analysis of these contents, provides a strong theoretical basis for the design of electrolyte materials for solid-state lithium-ion batteries, enabling researchers to better understand their performance characteristics and application scenarios, so as to optimize and improve their performance. On the premise of understanding the basic knowledge of solid-state electrolytes, a structure-activity model mapping structures to target properties is established combined with graph neural networks to predict material properties quickly and accurately, accelerating the design and screening process of lithium-ion solid-state electrolyte materials. Reinforcement learning makes the inverse design from target properties to structures possible, which will discover more new materials with excellent properties, accelerate the development of solid-state electrolytes, and inject impetus into the popularization of electric vehicles. Machine learning-based methods provide researchers with a new way to solve problems, especially creating a new paradigm for solving current obstacles under the condition of limited data and computing power.

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