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LEVERAGING MACHINE LEARNING TO DISCOVER NEW SOLID-STATE MATERIALS: TOPOLOGICAL INSULATORS, SEMICONDUCTORS, AND SOLID ELECTROLYTES APPLICATIONS (REVIEW ARTICLE)

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Abstract
Machine learning is used to rapidly predict, screen, and design materials functioning in solid-state for use in a growing range of chemical spaces that are too large for traditional trial and error approaches. This article reviews how machine learning accelerates the discovery of novel solid-state materials with emphasis on three technologically important classes: topological insulators, semiconductors, and solid electrolytes. The conversation highlights data infrastructures, chemical and structural representations, graph neural networks, foundation models, high-throughput screening and generative design, and closed-loop validation. Machine learning is used in topological materials to classify the topology and to generate a potential insulator or semimetal inverse. It is used in semiconductors to predict band gaps, phase stability and optoelectronic properties in an efficient manner. It can be used to solve multi-property optimization issues such as ionic conductivity, electrochemical stability, interfacial compatibility, and synthesizability in solid electrolytes. The authors suggest that the most successful methods for discovery are based on a combination of data-driven models, density-functional theory, atomistic simulation, uncertainty quantification, and experimental feedback. Despite recent progress, there are significant challenges in data quality, transferability, interpretability, synthesis prediction, and laboratory validation. The future will rely on the ability to embed physics-driven machine learning, self-driving laboratories and foundation models in clear and reproducible materials discovery pipelines that are supported by experimental data.

1. Introduction

Solid-state materials are the basis of today's technologies including microelectronics, photovoltaics, quantum devices, and electrochemical energy storage. However, identifying materials with appropriate properties is still challenging due to the huge, and highly constrained, search space resulting from the combination of designed materials, crystal structure, defects, synthesis routes, and operating conditions. Traditional discovery has been based on intuition, step-by-step chemical substitutions and trial and error experiments. These methods are still essential but too time consuming and not fast enough to meet the needs and speed of modern technology. Machine learning is thus now an important instrument to help fast-track the discovery, ranking and validation of potential materials candidates. There are several recent reviews with a focus on inverse design, generative modeling, active learning, and autonomous experimentation by AI (Cheng et al., 2026), which are now activities that are no longer just limited to predicting the future.

Machine learning's role in materials science is that it can learn from relationships between composition, structure, processing history and properties. The discovery logic is now reversed from the traditional method of synthesizing a material and then measuring its properties, to instead screening millions of hypothetical materials computationally, narrowing down to the most promising materials, and then validating these materials by either atomistic simulation or density-functional theory or by synthesizing them. Broad studies on materials-property prediction indicate that the

quality of the representation and training data can often influence the model's scientific usefulness or just its ability to mimic the bias of the data set (Chibani & Coudert, 2020).

This article explores three areas of application that exemplify how machine learning is being used to identify new solid state materials. Topological insulators are chosen because there is a linkage between symmetry, electronic band structure, and quantum topology. Because of the importance of accurately predicting electronic and optical properties, such as band gaps and stability, semiconductors are chosen. The choice of solid electrolyte is based on the fact that it must be optimised in terms of ionic conductivity, electrochemical stability, mechanical strength and interfacial compatibility.

2. Machine Learning Workflow for Discovery of Solid-State Materials

2.1 Data Infrastructure and Data Representations

The data is the starting point of the machine-learning model for materials discovery. The data can be extracted from high throughput density functional theory calculations, experimental databases, crystallographic repositories, literature mining, or taken from isolated laboratory measurements. The simplest is to represent it by its chemical composition. The benefit of the use of composition-based models is that they can make predictions in the absence of crystal structure, which is useful at early screening stages. In the case of useful predictions of materials properties, deep learning from the stoichiometry has been demonstrated to provide such predictions without any explicit crystal structure information, but naturally this approach is limited if properties are strongly dependent on local bonding geometry (Goodall & Lee, 2020).

For instance, CrabNet is a compositionally restricted attention-based network that can predict the properties of materials from their formulae, and also can learn complex chemical trends without needing a complete crystal graph (Wang et al., 2021). Although this type of model is suitable for fast pre-screening, it is not completely feasible for applications like topology, phonon stability and ionic transport. In many Solid State applications the structure is not a detail; it is the property determining object.

The limitation is overcome by using a graph neural network, as atoms are represented by nodes and bonds or neighbour relationships by edges. From this perspective, message passing enables a model to learn about the local chemical environments and to convey information between crystal regions. Benchmarking of graph neural networks for materials chemistry has shown that the architecture, representation, size of the materials datasets, and the target property are all key to performance (Fung et al., 2021). Line-graph architectures include bond-angle information and can also enhance the prediction of materials properties as many properties are dependent on both pair-distance (Choudhary & DeCost, 2021) and bond-angle information.

Another approach to the encoding of crystalline compounds is through topological representation. They present mathematically systematic descriptions of connectivity, shape and multiscale structure rather than just using the conventional descriptors. These representations have been used to predict material properties, such as modeling crystalline compounds via topology-based descriptors (Jiang et al., 2021). Scientific assumptions become the question of representation in discovery problems where local geometry, coordination and connectivity play a key role in the problem.

2.2 Education Models and Transmission Logic

There are four types of machine-learning models for materials discovery: forward predictors, generative models, interatomic potentials, and closed-loop decision systems. Forward predictors can predict properties like band gap, formation energy, elastic constants, ionic conductivity or topological class etc. Generative models generate new candidate structures/compositions. Interatomic potentials are an approximation to quantum mechanical energy surfaces, enabling larger-scale atomistic simulation. Closed loop systems make use of experimental or computational feedback to determine the next candidate to test.

Interatomic potentials, in particular, are of key importance, as they link atomistic simulations with data-driven modeling methods, and are universal machine-learned potentials. A universal graph deep-learning interatomic potential for the periodic table was found to be able to approximate energies and forces of chemically diverse systems (Chen & Ong, 2022). Another strategy focused on the development of a universal neural-network potential applicable to arbitrary combinations of 45

elements, towards the development of scalable, transferable atomistic potentials (Takamoto et al., 2022). These models are applicable to problems of temperature dependency, defects, diffusion barriers, static and dynamic descriptors of solid electrolyte, and metastability, which are hard to represent with static descriptors. Large-scale deep-learning approaches have also proven to be useful for recognizing significant number of previously unknown stable inorganic crystals, which also increases the range of candidate crystals for downstream screening (Merchant et al., 2023).

Deeper Graph Neural Networks (GNNs) have also been designed to enhance the performance of materials-property prediction tasks. To address these oversmoothing and computation issues, scalable architectures try to address the deep message passing and the complexity of the coordination networks within crystals (Omee et al., 2022). MatGL is an open source graph deep-learning library for materials science and chemistry, for property prediction and machine-learned interatomic potentials (Ko et al., 2025).

2.3 Closed-Loop Detection and Autonomous Corroboration

A good discovery process isn't complete until it produces a ranked list of candidates. Autonomous laboratories are a significant advancement in this direction as they integrate literature information, computational predictions, active learning, robotic synthesis and experimental characterization. Machine learning has been shown to inform real synthesis decisions not just by providing computational rankings of materials (Szymanski et al., 2023).

However, if you are going to use closed loop discovery you need the right performance metrics. While accuracy is not enough, a self-driving laboratory should be evaluated by efficiency, novelty, reproducibility, and the utilization of resources, as well as successful experimental results. In a recent discussion of the metrics of self-driving labs, the authors state that there is a need for the field to have standardized methods of assessing autonomous discovery systems in chemistry and materials science (Volk & Abolhasani, 2024). The point is very important for the three applications discussed here; a predicted topological material must have a structure that can be realized, a predicted semiconductor must be stable and processable, and a predicted solid electrolyte must be operational in a real electrochemical cell.

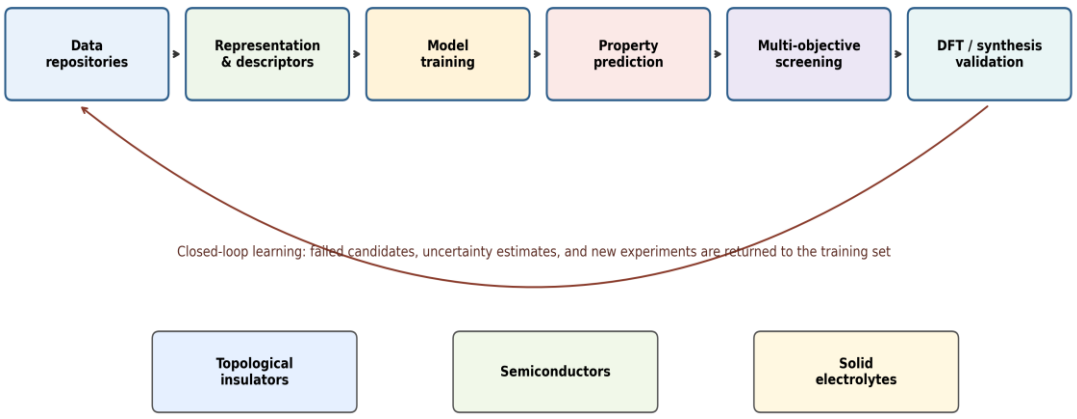

Figure 1: Machine-learning pipeline for accelerated discovery of solid-state materials.

3. Discussion

3.1 Applications in Topological Insulators

Topological insulators are a class of materials which are insulators in bulk and have conducting surface/edge states protected by topology. Their discovery is not as straightforward as a conventional band-gap prediction, but analysis of the electronic wave functions, their symmetry indicators, spin-orbit coupling and band inversions are required. In this regard, machine learning can be used to assist classification in topological character, prioritization of promising compounds and to generate new candidate structures.

Topological materials were first studied using machine-learning techniques, which demonstrated that the machine-learning classifiers could find topological candidates from materials descriptors efficiently. Machine learning has been applied in a study to detect topological materials where statistical models learn topological signals and can help in screening of large materials spaces (Claussen et al., 2020). This sort of model can be useful, as a full topological analysis can be quite computationally intensive, particularly when a large library of candidates is used.

Topological band structures have also been explored rapidly by using deep learning. A deep learning based study of rapid exploration of topological band structures found that the search in parameter spaces can be accelerated and nontrivial phases can be identified (Peano et al., 2021). These are not just quick alternatives to theory; they alter the nature of the exploratory process as they enable the researcher to "map" large areas and then perform detailed calculations on the most interesting areas.

A second path is also chemical-rule learning. Topogivity is a machine-learned chemical rule for the discovery of topological materials that demonstrates that data-driven approaches can capture chemically interpretable patterns linked to nontrivial topology (Ma et al., 2023). It is especially useful for topological materials, where a black-box classification is not sufficient, and the understanding of which structural and chemical motifs make topological behavior likely is needed.

New works are beginning to integrate machine learning with topology-specific descriptors more and more. A classifier for topological quantum materials using persistent homology and graph neural networks demonstrated that topological data analysis can be linked with the current machine learning techniques for topology prediction (Rasul et al., 2024). Machine learning has been employed to look for two-dimensional magnetic topological insulators, which are hard to find due to the simultaneous constraints that topology and magnetism place on the electronic structure (Xu et al., 2024).

The field is also trending towards Inverse Design. From screening known structures, to proposing new candidates, deep generative models have been employed to structure the discovery of new topological insulators and semimetals (Hong et al., 2025). Another prediction of 3-D magnetic topological insulators and semimetals indicates that machine learning can aid in targeted search of complex quantum materials in which symmetry, magnetism, and band topology are interacting (Boulton & Kim, 2025).

3.2 Applications in Semiconductors

The application of semiconductors is one of the most critical application fields for machine-learning materials discovery since properties including band gap, carrier transport, stability, abundance, defect tolerance, optical absorption, and processability are all key. While for topological materials the key issue is perhaps classification of nontrivial electronic topology, for semiconductors, it is usually a quantitative regression target, like direct or indirect band gap. However, a useful semiconductor material requires to meet several conditions.

As is well known, the discovery is crucial in semiconductor design, particularly when it is interpretable. Another example was evolutionary search used with machine-learning surrogate to find semiconductors and derive design rules for direct band gaps and optoelectronic applications (Choubisa et al., 2023). The interpretability component is important because discovery of semiconductors is not just a ranker's issue, it also relies on rules that facilitate chemical intuition and future synthesis.

Direct band-gap materials that are relevant to light emission and photovoltaics have also been modeled with machine learning. The study was recently targeted to search for direct band-gap materials and highlighted the need for the ability to differentiate between optoelectronic suitability and generic stability of the models (Dinic et al., 2024). This separation is key, as a material might have a stable crystal structure, a poor absorption capacity, a small band gap, or an indirect band gap and thus be technically uninteresting.

Perovskite and low symmetry materials show the need of flexible models. The machine-learning assisted band-gap prediction of low-symmetry double and layered perovskites revealed that ensemble methods and boosted models can be used to aid the prediction of the band gap in chemically complex families (Sabagh Moeini et al., 2024). The work is essential because of the need

for low symmetry materials may have distortions, layered motifs, and complexity of composition that makes simple descriptors inadequate.

The band gap model works well for many compounds but not some less common or chemically unusual. The safest workflow is machine learning for prioritization, followed by density-functional theory, if available, and methods of higher electronic-structure level, and experimental synthesis. In this context, machine learning is not a definitive assessment of material performance, but rather a filter which narrows the search space.

3.3 Applications in Solid Electrolytes

Solid electrolytes are key for the development of safer, higher energy density solid-state batteries. The difficulty in discovering their existence lies in the fact that a good electrolyte has to meet a set of requirements: to be ionic conductor, electronic conductor, and have a wide electrochemical stability window; to be chemically compatible with the electrodes; to be mechanically stable; and above all, it has to be easily synthesised. The requirements make up a multi-objective optimization problem which is ideally suited to machine-learning-guided screening, but is challenging in purely data-driven models due to the limited and heterogeneous nature of experimental data.

A combination of data-driven models and computational screening has been applied to discover solid-state electrolytes for lithium-ion batteries using high throughput machine learning workflows. In a study of machine-learning-assisted high-throughput discovery of solid-state electrolytes, candidate materials were efficiently screened for battery-relevant criteria (Guo et al., 2024). The scientific significance of this approach is that it allows prioritization of materials that meet several criteria instead of optimizing one of the properties alone.

Ionic conductivity is still crucial and is dependent on migration path, activation barrier, lattice softness, defects and temperature, an atomistic modeling is still necessary. In terms of understanding fast-ion conduction and interfacial effects and chemical stability in crystalline electrolytes, a review on solid-state battery electrolytes highlighted the role of atomistic modelling and machine learning (Dutra et al., 2025). Such a view is important because a high bulk level predicted conductivity is not sufficient to ensure good battery performance if interfacial reactions or mechanical failure is present.

In addition to that, the AI is also used in the assessment of solid-state batteries in general, such as material screening, battery performance prediction, and the design of battery components. A recent review proposed that AI can assist in the solid-state battery research by linking materials selection and performance evaluation of the battery system (Wang et al., 2025). The battery context is significant because the discovery of the electrolyte depends on the compatibility of the electrodes, processing and cell architecture.

The latest literature presents the discovery of a solid electrolyte as a pipeline problem. The key challenges in designing machine learning pipelines for solid-state electrolyte design are data curation, selection of descriptors, algorithm selection, multi-objective optimization, and experimental validation (Jain et al., 2026). A pipeline view is better than isolated model reporting since it is not only the prediction accuracy that is the bottleneck, it is also the reliable movement from prediction to synthesis and device testing.

Table 1: Application map showing property targets and validation requirements across three material classes.

Material Class	Target Properties	Typical ML Task	High-Value Output	Validation Need
Topological Insulators	Band topology, symmetry, gap	Classification / inverse design	New TIs and semimetals	DFT topology + synthesis
Semiconductors	Band gap, stability, mobility	Regression + screening	Emitters, PV absorbers	DFT + optical tests
Solid Electrolytes	Ionic conductivity, stability	Multi-objective ranking	Battery-safe conductors	MD/DFT + cell tests

3.4 Cross-Cutting Challenges

3.4.1 Data Quality and Bias and 7.2 Benchmarking

One of the worst drawbacks of machine-learning materials discovery is not necessarily model architecture, it's often the data. Computational databases are skewed toward materials that have low complexity in terms of calculation, are known in experiment or are structurally more conventional. Your experimental data may be incomplete and/or contain some noise and/or different experimental parameters for different measurements. A model fitted to these data may look good on one set of data and be wrong on novel chemical spaces. Standardized benchmarks are one way to solve this problem, but benchmarks need to be continuously updated as the targets for discovery become increasingly elusive.

Data leakage and improper splitting can also boost performance. More stringent testing is needed for extrapolation to new chemistries, structures or functional classes. This is particularly relevant for topological materials, as such symmetry and/or spin-orbit coupling changes could affect the classification, and for solid electrolytes, different transport mechanisms could exist in different families of structures.

3.4.2 Interpretability and Physical Consistency.7.2 Interpretability and Physical Consistency.

Interpretability is a must-have in materials discovery. To determine if a model has learnt meaningful chemical principles or spurious correlations in the dataset, researchers should determine this. Discovering semiconductors, an interpretable example, demonstrates the ability of machine learning to give design rules, not just a number prediction. (Choubisa et al., 2023) Likewise, chemical-rule extraction in topological materials can be used to look for motifs that are expected to produce nontrivial electronic phases (Ma et al., 2023).

Even consistency is important when it comes to physical factors. The properties of a predicted material should be charge balance, structural plausibility, thermodynamic stability and synthesizability. The power of generative models can lead to proposals of mathematically valid, but chemically unrealistic, structures when not used in conjunction with physical filtering.

3.4.3 Transferability, Indecision, and Justification

The reliability of a model transferred to a domain different from where it was learned is its transferability. This is hard to do with solid-state materials, however, since the chemical diversity is huge, and many technologically interesting materials lie in un-sampled areas of data space. Uncertainty quantification can be used to determine when the model is extrapolating and when more computations and/or experiments are required. Closed-loop: If there is uncertainty, it can be utilized proactively; the system can select candidates that are both promising and informative.

While DFT can be used to demonstrate stability and electronic properties, it can be inappropriate for finite-temperature effects, defects, surfaces, and synthesis kinetics. Experiments can be used to confirm synthesis and performance but are slower and more expensive.

3.5 Future Perspectives

It is likely that three trends will dominate the next step of machine learning in materials discovery: autonomous laboratories, physics-informed learning, and foundation models. Many tasks could benefit from having a representation that can be transferred from a foundation model trained on data from disparate materials, without the need to train a new model from scratch for each property. In a recent review, Pyzer-Knapp et al. (2025) have proposed that foundation models could change the landscape of materials data, prediction, and design in the materials community.

There will be an increased importance of physics-informed learning. Models that are based on symmetry, equivariance, conservation principles, thermodynamic constraints, or uncertainty will be more likely to generalize than a black box for which there is no such restriction. Particularly, for topological insulators, symmetry plays a key role, and for solid electrolytes, pathways for transport and the stability of the interfaces have to be physically relevant.

The most important transformative long-term solution can be offered by autonomous laboratories, which have the capability to close the loop between prediction and synthesis. Ideally, the model suggests candidates; a robotic platform generates and characterizes them, the results are

fed back into the model and the next experiment is automatically picked. These are emerging systems which could indicate a future where materials discovery is more rapid, more adaptable and more quantitatively measurable.

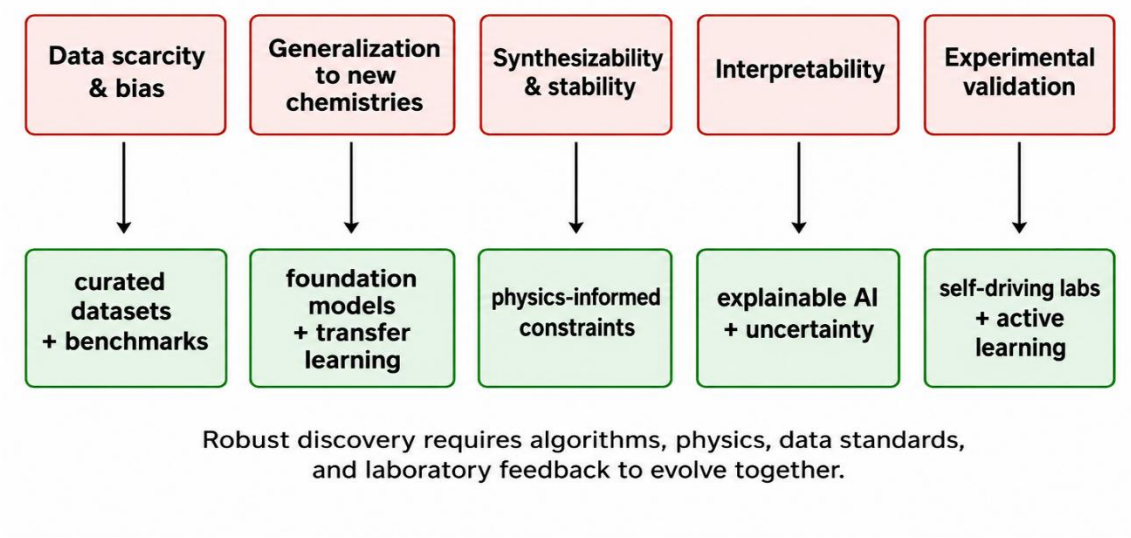

Figure 2. Roadmap linking current limitations with practical AI-enabled solutions for reliable discovery.

4. Conclusion

The ability to link large datasets, chemical representations, predictive modeling, generative design and validation workflows within machine learning has made it an effective engine for the discovery of solid-state materials. It speeds up the classification and inverse design of nontrivial quantum materials in topological insulators. In solid electrolytes it enables multi-objective optimization of ionic transport, stability and matchability to batteries. In any of these areas, the best workflows don't think of ML as a standalone solution to replace experiments or theory. Today the field is shifting from prediction to discovery in a closed loop, autonomous fashion. However, it will be built on clear data and reproducible benchmarks, understandable models, and strict validation. The challenge related to predicting materials that work can be addressed through machine learning, but the true power of machine learning is helping to direct human and experimental effort toward finding materials that can not only be predicted to work, but also synthesized, characterized, and used.

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