batteries

MDPI

Review

Machine-Learning Approaches for the Discovery of Electrolyte Materials for Solid-State Lithium Batteries

Shengyi Hu [1] and Chun Huang [1,2,3,*]

[1] Department of Materials, Imperial College London, London SW7 2AZ, UK
[2] The Faraday Institution, Quad One, Becquerel Ave., Harwell Campus, Didcot OX11 0RA, UK
[3] Research Complex at Harwell, Rutherford Appleton Laboratory, Didcot OX11 0FA, UK
* Correspondence: a.huang@imperial.ac.uk

Abstract: Solid-state lithium batteries have attracted considerable research attention for their potential advantages over conventional liquid electrolyte lithium batteries. The discovery of lithium solid-state electrolytes (SSEs) is still undergoing to solve the remaining challenges, and machine learning (ML) approaches could potentially accelerate the process significantly. This review introduces common ML techniques employed in materials discovery and an overview of ML applications in lithium SSE discovery, with perspectives on the key issues and future outlooks.

Keywords: solid-state batteries; machine learning; solid-state electrolyte; materials discovery

Citation: Hu, S.; Huang, C. Machine-Learning Approaches for the Discovery of Electrolyte Materials for Solid-State Lithium Batteries. *Batteries* **2023**, *9*, 228. https://doi.org/10.3390/batteries9040228

Academic Editors: Long Zhang and Kah Chun Lau

Received: 12 February 2023
Revised: 5 April 2023
Accepted: 13 April 2023
Published: 17 April 2023

1. Introduction

Lithium batteries are indispensable energy storage devices in the growth of electronic devices [1]. In addition, they are also expected to be the driving force for sustainability, powering energy plants and electric vehicles as energy storage units [2]. A typical commercial lithium battery contains electrodes with an electrolyte in liquid form, leading to safety issues being a significant concern due to the flammability and narrow stability domain of the liquid electrolyte [3,4].

Solid-state lithium batteries could be a potential solution due to the potential higher safety measurement and large energy densities using a lithium metal anode [5]. Flammable liquid electrolytes could be replaced by solid-state electrolytes (SSEs) with the advantage of longer device lifetime expectations due to lower reactivity of side reactions [6]. The SSE materials need to exhibit high lithium-ion conductivity, low electronic conductivity, and large electrochemical stability windows. In addition, they could also contribute to better stability thermally and mechanically in a wide range of operating temperatures, such as Li_2S-P_2S_5, which showed no sign of degradation up to 100 cycles at a high operating temperature of 170 °C and low temperature down to −40 °C [7,8]. The known good solid-state lithium-ion conductors could be characterised into different types depending on their compositions. For example, lithium thiophosphates (e.g., $Li_{10}GeP_2S_{12}$), garnet (e.g., $Li_7Li_3Zr_2O_{12}$), NASICON (e.g., $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$), perovskite (e.g., $Li_{0.5}La_{0.5}TiO_3$), and argyrodite (e.g., Li_6PS_5Cl) [9–13]. These conductors exhibit fast lithium-ion conduction properties, with relatively high ionic conductivities at room temperature (RT) compared with other lithium conductors. However, they are still far from large-scale production and application due to lacking well-rounded properties [14]. The early discovered lithium nitride (Li_3N) has a high ionic conductivity of 6×10^{-3} S cm^{-1} at RT, but it shows low electrochemical stabilities [15]. On the other hand, polymer electrolytes, such as polyethylene oxide, generally have significantly lower conductivities than common liquid electrolytes, which are unattractive for commercialisation [16,17]. Therefore, further research in discovering new solid-state lithium-ion conductors are needed.

There are more significant challenges for SSEs. For example, metallic lithium from anodes might still be able to penetrate the SEEs and could cause a similar dendrite growth and

short-circuit issue as in the liquid electrolytes [18,19]. The contact between solids also leads to the problem of contact maintenance, as the performance of batteries is dependent on ion diffusion, which is more influenced by any structural changes in solid-state batteries [20–22].

Therefore, there is an urgent need to research novel materials for solid-state lithium batteries such as SSEs. The machine-learning (ML) data-driven approach is a popular field that many research groups are currently exploring. Hence, this perspective paper will begin by briefly discussing a few ML techniques employed in materials discovery, followed by an emphasis on the discovery and screening methods of new materials for SSEs. Moreover, the recent progress in the materials discovery will be discussed with different ML approaches and results. Finally, this paper will offer a perspective on the ML screening results with a short outlook on challenges and future opportunities.

2. Discovery and Screening Methods of New Materials for SSEs

Computational methods have been developed over the years to accelerate material discovery progress. For solid-state lithium batteries, atomistic simulation techniques based on first-principles density functional theory (DFT) working with databases could perform various accurate calculations, including interface stability and new structure predictions, which overcome the labour-consuming and experimental limitations issues from laboratory approaches. Most importantly, as the methods are based on the fundamentals of quantum mechanics, ion transport mechanisms understanding could be obtained with little input required [23–30].

The modelling of ionic mobility mechanisms could be achieved by using ab initio molecular dynamics (AIMD) simulations, and the atoms in the system are driven by the atomic forces from the first principles [31,32]. The diffusivity could be evaluated at a constant temperature and volume. On the other hand, Kinetic Monte Carlo (kMC) simulation examines the hopping mechanism at a more microscopic level with the benefit of thermodynamic factors that could be considered in grand-canonical simulations [33–36]. There are more approaches available for different requirements. However, these computational methods are all physics-based and generally expensive and unsuitable for performing material screening for large databases, and there are already other reviews on these physics-based modelling methods for electrolyte materials of solid-state batteries [37–39].

3. Typical Machine Learning Techniques Used in Materials Discovery

Traditional approaches for materials discovery require trial-and-error methods, which usually employ DFT simulation and/or experiments that generally take months and years to obtain the desired properties [37]. On the other hand, ML techniques employ approximated features and data to recognise the pattern or provide predictions, usually taking a significantly shorter time combined with validations of the results [38–40]. Therefore, ML can be used to identify new materials, predict their properties, and gain insight into the electrochemical performance of novel battery chemistries, ML attracts attention in material discovery for possibilities to accelerate the process and reduce the cost [39–42]. Typically, ML methods can be categorised as supervised learning, unsupervised learning, reinforcement learning, and neural networks [43]. The ML techniques widely used in materials discovery are supervised learning and unsupervised learning. They could be selected based on the data quantity and data type, while the theoretical meaning of the properties in materials science is not understood by the ML models. Therefore, this opens opportunities for researchers to investigate a wide range of parameters in the battery design field. For example, Jalem et al. employed a partial least squares regression model to predict the activation energy barriers to lithium diffusion in olivine-type materials, which was a pioneer work of data-driven approaches used in battery research [41]. The partial least squares regression is a relatively robust model, even when the data contain significant noise, and the sample size is small. However, the model test statistics might be unreliable [42]. Moreover, Sendek et al. developed an ionic conductivity classification model with logistic regression to identify candidate lithium solids with desired fast ion conduction

properties, which was a relatively early form of research using the supervised learning ML model followed by further investigations using density functional theory molecular dynamics (DFT-MD) to validate the predictions [43]. Figure 1 shows commonly employed ML algorithms grouped in underlying mechanisms.

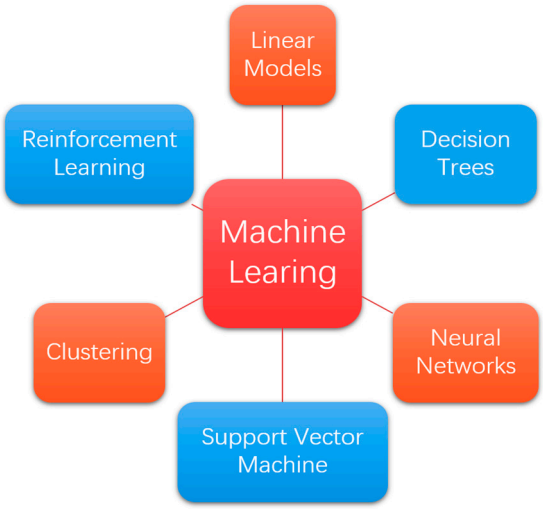

Figure 1. Commonly employed ML algorithms grouped in underlying mechanisms.

Supervised learning requires labelled data, and data is split into training data and testing data. Statistical regression is performed on training data to build the prediction model [44]. The model performance is examined by comparing the prediction and expected results using testing data [45]. The model then could be used to make predictions on new input when the model performance is satisfactory for specific applications [46,47]. In contrast, unsupervised learning could input data without labelled outputs and has been employed in material science for applications such as pattern recognition and clustering when the dataset is not well-labelled, with a limited quantity for training and relatively low quality [48–52]. The goals of using an unsupervised learning model in material discovery usually involve finding new suitable materials similar to the known good candidate materials with desired properties [53].

Reinforcement learning optimises the output by influencing the environment without labelled supervised samples and changes parameters based on feedback [54]. It may be considered a time-delayed version of supervised learning. On the other hand, neural networks are complex interconnected networks of many parameters, and theoretically, more parameters mean more model capacity and more complicated learning can be processed. Complex models are represented by deep learning, which uses neural networks with many layers [55,56]. It is worth noting that reinforcement learning and deep learning are advancing quickly in multiple research areas, showing promising potential for future materials discovery research. However, on the topic of lithium SSE materials discovery, these advanced ML techniques have not been used as much as other supervised and unsupervised learning approaches and more research focus in these areas are expected, and ML techniques and applications discussed later will focus on supervised and unsupervised learning. Figure 2 shows simplified framework for SSE materials discovery using ML data-driven approaches.

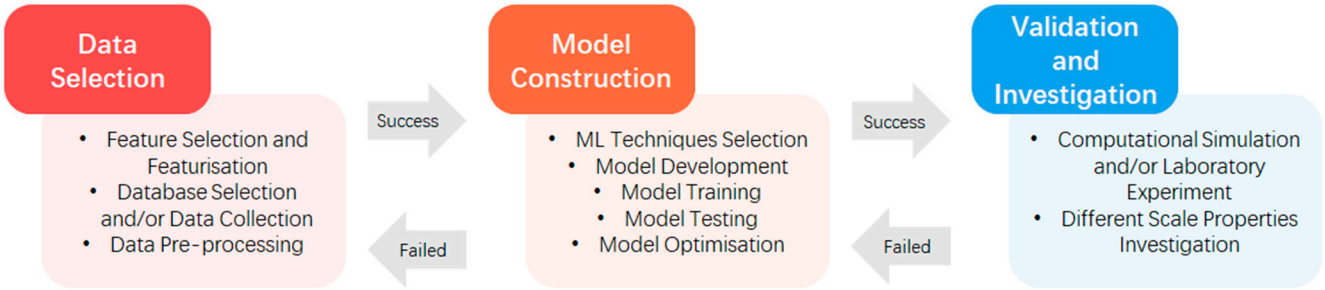

Figure 2. Simplified framework for SSE materials discovery using ML data-driven approaches.

3.1. Supervised Learning

Generally, frequently used supervised learning algorithms could be categorised into regression and classification. Regression is used to estimate the relationship between independent variables and a dependent variable using functions connecting data points and making predictions. On the other hand, classification is based on common characteristics and usually produces a label or probability as the output for the predictions [55–57].

Support vector machine (SVM) is a popular algorithm with capabilities in both regression and classification. It demonstrates effectiveness in high dimensional spaces even when the sample size is not sufficiently big compared to the feature size [58,59]. The mathematics theories are complex; however, in simple terms, the SVM mechanism divides space in order to group data points into different categories [60]. In the process, hyperplanes are generated in high dimensional space, and different Kernel functions could be employed to solve the problem by adding new dimensions [61]. Applying the technique requires careful consideration of Kernel functions and regularisation terms, as inappropriate choices might lead to unnecessary dimensions and overfitting [62]. Overfitting should be avoided as the model will perform poorly on testing data and application inputs despite having high-score performance on the training data [63–65]. To solve this problem, a trial-and-error method on standard functions and cross-validation may be needed, which is time-consuming [66]. Overall, it is an effective technique due to its versatility in function selections and strength in predictive power, with a relatively small number of samples required [67,68].

3.2. Unsupervised Learning

Clustering is an important concept in unsupervised learning, and the goal is grouping similar unlabelled input data points together in clusters based on selected methods [69,70]. Different clustering algorithms could be chosen carefully based on the application needs and sample size. K-means, spectral, and hierarchical clustering are some of the most common methods.

K-means clustering is general purpose, and the algorithm separates samples into clusters with equal variance, minimising the within-cluster sum-of-squares criterion [71]. It usually requires a very large sample size and a medium number of clusters input with advanced knowledge of the number of resultant clusters [69,72]. On the other hand, spectral clustering performs well for inputting a small number of clusters and medium size sample size. The mechanism is based on graph distance, employing eigenvalues of the similarity matrix [73–76]. These techniques are relatively straightforward to implement, giving the existing packages in multiple programming languages, such as Python, obtaining documentation and examples to follow. However, these clustering algorithms usually suffer from initialisations, and the cluster number is needed before running the codes [77]. There are papers in the computer science field suggesting methods, such as the global k-means algorithm from Likas et al. [78], using an incremental approach to dynamically add cluster centres. Nevertheless, it is difficult to find use cases in the material discovery that implement advanced methods in order to tackle this issue, and usually, extra steps to estimate the number of clusters is needed, which is not optimal [77].

Hierarchical clustering does not require pre-specifying the number of clusters, and the mechanism could be stopped at any number of clusters [79]. The algorithm merges or splits clusters successively, and the result could be visualised as a dendrogram [80]. It does not require a very large sample size to perform well, and a range of pairwise distance metrics could be selected as a criterion for clustering results. For the parameters, Euclidean is a typical distance metric used to measure the distance between [81] clusters and is simply the straight-line distance between two points. Additionally, the standard linkage criterion parameter 'ward' minimises the variance of the clusters being merged as a cluster dissimilarity measurement [53,82].

4. Machine Learning Applications for Materials Discovery of SSEs

ML algorithms offer a wide range of options for SSEs research, as the models themselves input data points without understanding the underlying physical meanings as humans do. Any properties, in theory, could be featured, and this, indeed, could be reflected in the diversity of ML applications. Typically, SSEs could be categorised into organic and inorganic materials, as well as, more specifically, into groups based on their compositions, such as oxides, halides, etc. As this perspective emphasises ML techniques, the following section will cover recent advances in applications considered with their ML methods.

Fujimura et al. employed an ML technique combined with DFT data to estimate the lithium-ion conductivity values at 373 K [83]. The datasets contain both theoretical and experimental data, and the support vector regression (SVR) was applied with a Gaussian kernel, along with bootstrapping method error optimisation. Input features included the diffusivity at 1600 K, the average volume of disordered structures, transition temperatures from simulations and experimental temperatures. The predicted ionic conductivity was obtained for 72 compositions, and γ-Li_4GeO_4 had the highest predictive conductivity at 373 K, which was reported as approximately 5.5 $\times$ 10^{-4} S cm^{-1} from the ML model. It could potentially exceed the conductivity of LISICON ($Li_{3.5}Zn_{0.25}GeO_4$) by a significant amount. However, primarily due to the difficulties in synthesising γ-Li_4GeO_4, further experiments are expected for the prediction validations to evaluate this candidate as one of the next-generation SSE materials. Guo et al. mapped the lithium thiophosphate (LPS) phase diagram by combining first-principles and artificial intelligence (AI) methods, integrating DFT, artificial neural network potentials, genetic algorithm sampling, and ab initio molecular dynamics simulations [84]. Based on the discovered trends in the LPS phase diagram, Guo et al. propose a candidate solid-state electrolyte composition, $(Li_2S)_x(P_2S_5)_{1-x}$ (x~0.725), that exhibits high ionic conductivity of >10^{-2} S cm^{-1}, demonstrating a design strategy for amorphous or glassy/ceramic solid electrolytes [84].

For the case of unsupervised ML applications, Zhang et al. utilised data entries from Inorganic Crystal Structure Database (ICSD) and processed 528 modified X-ray diffraction (mXRD) quantitative representations as the training dataset [53,85]. An agglomerative hierarchical clustering model was first trained, and the clustering results showed good differentiations between the clusters. Then, an additional spectral clustering model and a third model with limited information were employed to confirm the results. All methods showed that the most already-known fast-conducting examples in the input data were aggregated into two clusters out of seven, which means the clustering models were highly likely to successfully draw boundaries between the promising and bad candidates for SSEs. The materials in these two clusters were further investigated using AIMD simulations. Three structures, Li_8N_2Se, Li_6KBiO_6 and $Li_5P_2N_5$, had conductivities exceeding the best-known lithium fast-conductors, which showed the effectiveness of the clustering techniques. However, some materials did not exhibit high conductivity values in the simulation, and the clustering results might be improved by further research in the featurisation of the clustering input. In addition, experimental validations are required to investigate the fast-conducting SSE candidates from the AIMD simulation.

While ICSD is the most extensive database for completely identified inorganic crystal structures, the Materials Project provides data on diverse properties of inorganic materials with an easy-to-use interface, which is also a popular choice for solid-state battery research [86]. Sendek et al. employed an ML model with DFT-MD simulations to perform material discovery for SSEs based on ionic conductivity [87]. A logistic regression model was used to predict the possibility of an input material exhibiting superionic behaviour at RT based on its atomic and electronic structure data with a 0.1 mS cm^{-1} boundary of ionic conductivity. The model predicted 317 fast-ion lithium-conducting materials from over 12,000 inputs, and 21 crystalline compounds were identified as promising candidates with desired structural and electrochemical stability. Only one false positive material prediction was reported as LiCl obtains poor conduction properties from the literature. DFT-MD was then performed for identified candidates with unknown conductivity at 900 K to evaluate the performance of the ML model. With scaling to RT based on the Arrhenius relationship, eight candidates exhibit high ionic conductivity at RT. In particular, $Li_5B_7S_{13}$ exhibited a conductivity of 74 mS cm^{-1}, which is many times higher than the best-known lithium conductors. In addition, the ML-based approach showed a much higher efficiency and accuracy for predicting superionic materials compared with a random selection from 317 materials and Ph.D. student screening [87]. With further experimental research, these eight candidates could be promising materials for SSEs.

Due to the limited availability of a large volume of data in the materials design field, Cubuk et al. demonstrated that it is difficult to apply standard learning methodologies using genetic descriptors on small data [88]. A linear SVM model was initially trained with 40 data points and 30 elemental descriptors using the leave-one-out cross-validation. Then, a model with physically motivated descriptors using structural information was compared using validation error. The performance showed a trade-off between the model accuracy and the potential for screening previously uncharacterised materials. A novel transfer learning approach was suggested, and an accurate ML model was trained with structural information descriptors on the lithium-ion conductivity measurements from the experimental literature. Predictions were made on the Materials Project database, and these predictions were used as labels to train a new model referred to as esML with elemental descriptors. An accurate esML model could screen all possible element combinations for novel materials with only composition information, approaching nearly 90% validation accuracy. The model was able to provide a screening for 20 billion ternary and quaternary lithium-containing compounds at an extremely fast speed compared with DFT calculations. Overall, the methods allow for training models on available datasets and provide predictions about other tasks with unavailable datasets. A number of promising lithium-ion conductors were suggested after screening 20 billion materials, including $LiPO_3$ and Li_2MgO_2. While some compounds were studied before, further investigations are required for other candidate materials. Table 1 summarises the algorithms and approaches used in the literature and compares their advantages and disadvantages.

Table 1. Algorithms and approaches used in the literature and their comparisons.

Approaches	Advantages	Disadvantages
Support vector regression (SVR) [89,90]	Effective models for small quantities of data, multiple Kernel functions available based on applications, and relatively high predictive power in supervised learning models.	Require careful research for function selections to avoid overfitting.
Agglomerative hierarchical clustering [91,92]	No prior knowledge of the number of clusters is required; the approach does not require very large sample sizes to perform well.	Relatively large computational costs are required.
Spectral clustering [93]	Perform well on small numbers of clusters and medium sample sizes.	Require prior knowledge of the number of clusters.
Logistic regression [94]	The approach can be employed relatively easily in classification.	Non-linear problems are not applicable, but linear boundary data is relatively rare.

It is worth noting that there are other challenges for solid-state lithium batteries developing into high-performance large-scale production applications. For example, the interface electrochemical stabilisation [95], interfacial physical contact maintenance during cycling [96], and cathode materials performance improvement [97]. ML applications for these issues were also explored by researchers. Eckhoff et al. constructed a DFT-based high-dimensional neural network potential which could predict a range of properties, including lattice parameters, volume changes, phase transition, lithium diffusion barriers, and phonon frequencies for electrode material lithium manganese oxide spinels [98]. Furthermore, Gao et al. utilised an AI scheme via the swarm-intelligence-based crystal structure analysis with particle swarm optimisation method to predict heterogeneous interface structures and investigate the lithium-ion transport mechanism at the cathode/SSE interface [99]. ML data-driven approach could potentially accelerate the research process for tackling these problems and aid the commercialisation of solid-state lithium batteries. Promising cathode materials need to have a high voltage against lithium, a high capacity, and high energy density while keeping the cathode volume as stable as possible without excessive expansion, which may cause mechanical stress to the SSE. Hence, putting the battery pieces together, cathode and SSE, is needed to make sure they are compatible with each other and use ML to predict the time and extent of degradation that occurs.

5. Conclusions and Future Directions

In this perspective, brief introductions about screening techniques for materials discovery are presented with emphasis on ML approaches and their applications on SSE materials discovery. Employing ML techniques significantly accelerates the screening process compared with experimental and DFT-based methods and provides a promising future for design acceleration with new lithium fast-conductors.

However, substantial research effort is required for follow-up validations of the ML prediction results, including more computational simulations and experimental investigations. The newly discovered SSE candidates must go through a long research period before reaching applications. A range of properties should be evaluated, including interfacial and electrochemical stability when in contact with electrodes. These parameters are critical for feasibility in large-scale production beyond the lab and will likely take a lot more research efforts than the initial electrolyte discovery stages. Although the overall development process is usually accelerated by ML, the new potential electrolyte materials candidates from the discovery results would not be meaningful if lacking in practical validations. As mentioned in the previous section, some recent ML applications of material discovery of SSEs gave promising candidates that have high possibilities of performance exceeding current SSEs and also potentially provide well-rounded properties for a wide range of applications. Unfortunately, in most cases, necessary follow-up research has not been carried out to the experimental investigation stage yet or struggles to synthesise the specific composition of the candidate materials from the modelling results.

Moreover, the ML models do not understand the physical meaning of the features but investigate the correlations and patterns of the input data. Obtaining a pattern from the results is difficult and requires significant research effort to find the optimal models for the specific data sets. Nevertheless, understanding the physical reasons behind the results is even more challenging. After arriving at the results from the ML discovery stages, the questions of why the candidate materials are standing out arise. Why does this specific composition obtain high ionic conductivity? Which is the crystallographic structure at what temperature? Are the physical reasons related to lithium-ion diffusion channels? At what conditions will the desired ionic conductivity and stability no longer exist? Therefore, ML techniques should be used with caution, and the output quality hugely relies on the data quantity, which makes data pre-processing and model selection critical. Extensive research training on ML models and their mechanisms is required before implementing ML data-driven approaches and a robust understanding of the fundamental principles of

electrolyte applications needs to be obtained to ensure the results are relatively reliable for inspiring further research.

Applying ML models to lithium SSE materials discovery is still a niche research area. For future outlooks, attention to both materials databases and ML models is suggested. More established databases are great sources for ML training, e.g., PubChem [100], NIST [101], Open Quantum Materials Database (OQMD) [102,103], also ICSD and the Materials Project, as mentioned in the previous section, as these datasets usually provide good quality and quantity data. At the same time, web interfaces are often more user-friendly and can be connected to the programming environment. Therefore, more exploration of these databases is suggested. In general, no matter what databases are chosen, the most important step is the featurisation of the data. The representation of the properties needs to be effective in order to summarise the specific properties of the molecules with the lowest dimensions possible.

Finally, advanced ML models, including reinforcement learning, can be employed to aid the discovery. ML is a very popular research topic constantly developing in the computer science field, with more advanced concepts and models becoming available for more accurate and higher predictive power applications. These complex models generally require more understanding before implementation. Utilising these advanced ML techniques with an improved understanding of their effectiveness on materials science databases would be a potential solution to accelerate further the design process. Therefore, collaboration with experts in the ML field might be a new trend for materials discovery in order to drive the development of next-generation SSEs.

Author Contributions: Conceptualization, C.H. and S.H.; writing—original draft preparation, C.H. and S.H.; writing—review and editing, C.H. and S.H.; supervision, C.H.; funding acquisition, C.H. All authors have read and agreed to the published version of the manuscript.

Funding: This work was carried out with the support of the EPSRC UKRI Innovation Fellowship (EP/S001239/1, EP/S001239/2), the Faraday Institution Industry Fellowship (FIIF015), the Faraday Institution Training Grant (FITG034), and the Imperial College London UKRI Impact Acceleration Account (EP/X52556X/1). This work was supported by the Faraday Institution (FIRG060).

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

SSE	Solid-State Electrolyte
ML	Machine Learning
DFT	Density Functional Theory
AIMD	Ab Initio Molecular Dynamics
kMC	Kinetic Monte Carlo
SVM	Support Vector Machine
SVR	Support Vector Regression
ICSD	Inorganic Crystal Structure Database
mXRD	Modified X-ray Diffraction
DFT-MD	Density Functional Theory Molecular Dynamics
RT	Room Temperature

References

1. Assad, M.; Rosen, M.A.A. (Eds.) *Design and Performance Optimization of Renewable Energy Systems*; Elsevier: Amsterdam, The Netherlands, 2021. [CrossRef]
2. Yang, Z.; Huang, H.; Lin, F.; Yang, Z.; Lin, F.; Huang, H. Sustainable Electric Vehicle Batteries for a Sustainable World: Perspectives on Battery Cathodes, Environment, Supply Chain, Manufacturing, Life Cycle, and Policy. *Adv. Energy Mater.* **2022**, *12*, 2200383. [CrossRef]
3. Wen, J.; Yu, Y.; Chen, C. A Review on Lithium-Ion Batteries Safety Issues: Existing Problems and Possible Solutions. *Mater. Express* **2012**, *2*, 197–212. [CrossRef]

4. Pigłowska, M.; Kurc, B.; Galiński, M.; Fuć, P.; Kamińska, M.; Szymlet, N.; Daszkiewicz, P. Challenges for Safe Electrolytes Applied in Lithium-Ion Cells—A Review. *Materials* **2021**, *14*, 6783. [CrossRef] [PubMed]
5. Lin, D.; Liu, Y.; Cui, Y. Reviving the Lithium Metal Anode for High-Energy Batteries. *Nat. Nanotechnol.* **2017**, *12*, 194–206. [CrossRef]
6. Xu, L.; Tang, S.; Cheng, Y.; Wang, K.; Liang, J.; Liu, C.; Cao, Y.C.; Wei, F.; Mai, L. Interfaces in Solid-State Lithium Batteries. *Joule* **2018**, *2*, 1991–2015. [CrossRef]
7. Ogawa, M.; Yoshida, K.; Harada, K. All-Solid-State Lithium Batteries with Wide Operating Temperature Range. *SEI Tech. Rev.* **2012**, *74*, 88–90.
8. Zheng, F.; Kotobuki, M.; Song, S.; Lai, M.O.; Lu, L. Review on Solid Electrolytes for All-Solid-State Lithium-Ion Batteries. *J. Power Sources* **2018**, *389*, 198–213. [CrossRef]
9. Kamaya, N.; Homma, K.; Yamakawa, Y.; Hirayama, M.; Kanno, R.; Yonemura, M.; Kamiyama, T.; Kato, Y.; Hama, S.; Kawamoto, K.; et al. A Lithium Superionic Conductor. *Nat. Mater.* **2011**, *10*, 682–686. [CrossRef]
10. Kumazaki, S.; Iriyama, Y.; Kim, K.H.; Murugan, R.; Tanabe, K.; Yamamoto, K.; Hirayama, T.; Ogumi, Z. High Lithium Ion Conductive $Li_7La_3Zr_2O_{12}$ by Inclusion of Both Al and Si. *Electrochem. Commun.* **2011**, *13*, 509–512. [CrossRef]
11. Aono, H.; Sugimoto, E.; Sadaoka, Y.; Imanaka, N.; Adachi, G. Ionic Conductivity and Sinterability of Lithium Titanium Phosphate System. *Solid State Ion.* **1990**, *40–41*, 38–42. [CrossRef]
12. Ibarra, J.; Várez, A.; León, C.; Santamaría, J.; Torres-Martínez, L.M.; Sanz, J. Influence of Composition on the Structure and Conductivity of the Fast Ionic Conductors $La_{2/3-x}Li_{3x}TiO_3$ ($0.03 \leq x \leq 0.167$). *Solid State Ion.* **2000**, *134*, 219–228. [CrossRef]
13. Boulineau, S.; Courty, M.; Tarascon, J.M.; Viallet, V. Mechanochemical Synthesis of Li-Argyrodite Li6PS5X (X = Cl, Br, I) as Sulfur-Based Solid Electrolytes for All Solid State Batteries Application. *Solid State Ion.* **2012**, *221*, 1–5. [CrossRef]
14. Zhu, Y.; He, X.; Mo, Y. Origin of Outstanding Stability in the Lithium Solid Electrolyte Materials: Insights from Thermodynamic Analyses Based on First-Principles Calculations. *ACS Appl. Mater. Interfaces* **2015**, *7*, 23685–23693. [CrossRef]
15. Lapp, T.; Skaarup, S.; Hooper, A. Ionic Conductivity of Pure and Doped Li3N. *Solid State Ion.* **1983**, *11*, 97–103. [CrossRef]
16. Edman, L.; Ferry, A.; Doeff, M.M. Slow Recrystallization in the Polymer Electrolyte System Poly(Ethylene Oxide)$_n$-LiN(CF^3SO^2)$_2$. *J. Mater. Res.* **2000**, *15*, 1950–1954. [CrossRef]
17. Croce, F.; Appetecchi, G.B.; Persi, L.; Scrosati, B. Nanocomposite Polymer Electrolytes for Lithium Batteries. *Nature* **1998**, *394*, 456–458. [CrossRef]
18. Porz, L.; Swamy, T.; Sheldon, B.W.; Rettenwander, D.; Frömling, T.; Thaman, H.L.; Berendts, S.; Uecker, R.; Carter, W.C.; Chiang, Y.M. Mechanism of Lithium Metal Penetration through Inorganic Solid Electrolytes. *Adv. Energy Mater.* **2017**, *7*, 1701003. [CrossRef]
19. Bai, P.; Li, J.; Brushett, F.R.; Bazant, M.Z. Transition of Lithium Growth Mechanisms in Liquid Electrolytes. *Energy Environ. Sci.* **2016**, *9*, 3221–3229. [CrossRef]
20. Koerver, R.; Zhang, W.; de Biasi, L.; Schweidler, S.; Kondrakov, A.O.; Kolling, S.; Brezesinski, T.; Hartmann, P.; Zeier, W.G.; Janek, J. Chemo-Mechanical Expansion of Lithium Electrode Materials—On the Route to Mechanically Optimized All-Solid-State Batteries. *Energy Environ. Sci.* **2018**, *11*, 2142–2158. [CrossRef]
21. Koerver, R.; Aygün, I.; Leichtweiß, T.; Dietrich, C.; Zhang, W.; Binder, J.O.; Hartmann, P.; Zeier, W.G.; Janek, J. Capacity Fade in Solid-State Batteries: Interphase Formation and Chemomechanical Processes in Nickel-Rich Layered Oxide Cathodes and Lithium Thiophosphate Solid Electrolytes. *Chem. Mater.* **2017**, *29*, 5574–5582. [CrossRef]
22. Bucci, G.; Talamini, B.; Renuka Balakrishna, A.; Chiang, Y.M.; Carter, W.C. Mechanical Instability of Electrode-Electrolyte Interfaces in Solid-State Batteries. *Phys. Rev. Mater.* **2018**, *2*, 105407. [CrossRef]
23. De Pablo, J.J.; Jackson, N.E.; Webb, M.A.; Chen, L.-Q.; Moore, J.E.; Morgan, D.; Jacobs, R.; Pollock, T.; Schlom, D.G.; Toberer, E.S. New Frontiers for the Materials Genome Initiative. *Npj Comput. Mater.* **2019**, *5*, 41. [CrossRef]
24. Yang, K.; Setyawan, W.; Wang, S.; Buongiorno Nardelli, M.; Curtarolo, S. A Search Model for Topological Insulators with High-Throughput Robustness Descriptors. *Nat. Mater.* **2012**, *11*, 614–619. [CrossRef] [PubMed]
25. Wang, S.; Wang, Z.; Setyawan, W.; Mingo, N.; Curtarolo, S. Assessing the Thermoelectric Properties of Sintered Compounds via High-Throughput Ab-Initio Calculations. *Phys. Rev.* **2011**, *1*, 021012. [CrossRef]
26. Curtarolo, S.; Hart, G.L.W.; Nardelli, M.B.; Mingo, N.; Sanvito, S.; Levy, O. The High-Throughput Highway to Computational Materials Design. *Nat. Mater.* **2013**, *12*, 191–201. [CrossRef]
27. Yu, L.; Zunger, A. Identification of Potential Photovoltaic Absorbers Based on First-Principles Spectroscopic Screening of Materials. *Phys. Rev. Lett.* **2012**, *108*, 068701. [CrossRef]
28. Greeley, J.; Jaramillo, T.F.; Bonde, J.; Chorkendorff, I.; Nørskov, J.K. Computational High-Throughput Screening of Electrocatalytic Materials for Hydrogen Evolution. *Nat. Mater.* **2006**, *5*, 909–913. [CrossRef]
29. Nørskov, J.K.; Bligaard, T.; Rossmeisl, J.; Christensen, C.H. Towards the Computational Design of Solid Catalysts. *Nat. Chem.* **2009**, *1*, 37–46. [CrossRef]
30. Jain, A.; Shin, Y.; Persson, K.A. Computational Predictions of Energy Materials Using Density Functional Theory. *Nat. Rev. Mater.* **2016**, *1*, 15004. [CrossRef]
31. Frenkel, D.; Smit, B. *Understanding Molecular Simulation: From Algorithms to Applications*; Elsveier: Amsterdam, The Netherlands, 2001; ISBN 9780080519982.

32. Marx, D.; Hutter, J. *Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods*; Cambridge University Press: Cambridge, UK, 2009; ISBN 9780521898638.
33. van der Ven, A.; Ceder, G.; Asta, M.; Tepesch, P.D. First-Principles Theory of Ionic Diffusion with Nondilute Carriers. *Phys. Rev. B* **2001**, *64*, 184307. [CrossRef]
34. van der Ven, A.; Thomas, J.C.; Xu, Q.; Swoboda, B.; Morgan, D. Nondilute Diffusion from First Principles: Li Diffusion in Lix TiS2. *Phys. Rev. B-Condens. Matter Mater. Phys.* **2008**, *78*, 104306. [CrossRef]
35. Bulnes, F.M.; Pereyra, V.D.; Riccardo, J.L. Collective Surface Diffusion: N-Fold Way Kinetic Monte Carlo Simulation. *Phys. Rev E* **1998**, *58*, 86. [CrossRef]
36. Voter, A.F. Introduction to the Kinetic Monte Carlo Method. *Radiat. Eff. Solids* **2007**, *235*, 1–23. [CrossRef]
37. Chen, W.; Li, Y.; Feng, D.; Lv, C.; Li, H.; Zhou, S.; Jiang, Q.; Yang, J.; Gao, Z.; He, Y.; et al. Recent Progress of Theoretical Research on Inorganic Solid State Electrolytes for Li Metal Batteries. *J. Power Sources* **2023**, *561*, 232720. [CrossRef]
38. Baktash, A.; Reid, J.C.; Yuan, Q.; Roman, T.; Searles, D.J.; Baktash, A.; Reid, J.C.; Yuan, Q.; Roman, T.; Searles, D.J. Shaping the Future of Solid-State Electrolytes through Computational Modeling. *Adv. Mater.* **2020**, *32*, 1908041. [CrossRef]
39. Hao, F.; Mukherjee, P.P. Mesoscale Analysis of the Electrolyte-Electrode Interface in All-Solid-State Li-Ion Batteries. *J. Electrochem. Soc.* **2018**, *165*, A1857–A1864. [CrossRef]
40. Bo, Z.; Li, H.; Yang, H.; Li, C.; Wu, S.; Xu, C.; Xiong, G.; Mariotti, D.; Yan, J.; Cen, K.; et al. Combinatorial Atomistic-to-AI Prediction and Experimental Validation of Heating Effects in 350 F Supercapacitor Modules. *Int. J. Heat Mass Transf.* **2021**, *171*, 121075. [CrossRef]
41. Jalem, R.; Aoyama, T.; Nakayama, M.; Nogami, M. Multivariate Method-Assisted Ab Initio Study of Olivine-Type $LiMXO_4$ (Main Group M^{2+}-X^{5+} and M^{3+}-X^{4+}) Compositions as Potential Solid Electrolytes. *Chem. Mater.* **2012**, *24*, 1357–1364. [CrossRef]
42. Pirouz, D.M.; Student, D. *An Overview of Partial Least Squares*; University of California: Los Angeles, CA, USA, 2006.
43. Sendek, A.D.; Yang, Q.; Cubuk, E.D.; Duerloo, K.A.N.; Cui, Y.; Reed, E.J. Holistic Computational Structure Screening of More than 12000 Candidates for Solid Lithium-Ion Conductor Materials. *Energy Environ. Sci.* **2017**, *10*, 306–320. [CrossRef]
44. Sendek, A.D.; Ransom, B.; Cubuk, E.D.; Pellouchoud, L.A.; Nanda, J.; Reed, E.J. Machine Learning Modeling for Accelerated Battery Materials Design in the Small Data Regime. *Adv. Energy Mater.* **2022**, *12*, 2200553. [CrossRef]
45. Regonia, P.R.; Pelicano, C.M.; Tani, R.; Ishizumi, A.; Yanagi, H.; Ikeda, K. Predicting the Band Gap of ZnO Quantum Dots via Supervised Machine Learning Models. *Optik* **2020**, *207*, 164469. [CrossRef]
46. Pei, J.-F.; Cai, C.-Z.; Zhu, Y.-M.; Yan, B. Modeling and Predicting the Glass Transition Temperature of Polymethacrylates Based on Quantum Chemical Descriptors by Using Hybrid PSO-SVR. *Macromol. Theory Simul.* **2013**, *22*, 52–60. [CrossRef]
47. Fang, S.F.; Wang, M.P.; Qi, W.H.; Zheng, F. Hybrid Genetic Algorithms and Support Vector Regression in Forecasting Atmospheric Corrosion of Metallic Materials. *Comput. Mater. Sci.* **2008**, *44*, 647–655. [CrossRef]
48. Balachandran, P.V.; Theiler, J.; Rondinelli, J.M.; Lookman, T. Materials Prediction via Classification Learning. *Sci. Rep.* **2015**, *5*, 13285. [CrossRef] [PubMed]
49. Isayev, O.; Fourches, D.; Muratov, E.N.; Oses, C.; Rasch, K.; Tropsha, A.; Curtarolo, S. Materials Cartography: Representing and Mining Materials Space Using Structural and Electronic Fingerprints. *Chem. Mater.* **2015**, *27*, 735–743. [CrossRef]
50. Zhou, Q.; Tang, P.; Liu, S.; Pan, J.; Yan, Q.; Zhang, S.C. Learning Atoms for Materials Discovery. *Proc. Natl. Acad. Sci. USA* **2018**, *115*, E6411–E6417. [CrossRef]
51. Long, C.J.; Hattrick-Simpers, J.; Murakami, M.; Srivastava, R.C.; Takeuchi, I.; Karen, V.L.; Li, X. Rapid Structural Mapping of Ternary Metallic Alloy Systems Using the Combinatorial Approach and Cluster Analysis. *Rev. Sci. Instrum.* **2007**, *78*, 072217. [CrossRef]
52. Kireeva, N.; Baskin, I.I.; Gaspar, H.A.; Horvath, D.; Marcou, G.; Varnek, A. Generative Topographic Mapping (GTM): Universal Tool for Data Visualization, Structure-Activity Modeling and Dataset Comparison. *Mol. Inform.* **2012**, *31*, 301–312. [CrossRef]
53. Zhang, Y.; He, X.; Chen, Z.; Bai, Q.; Nolan, A.M.; Roberts, C.A.; Banerjee, D.; Matsunaga, T.; Mo, Y.; Ling, C. Unsupervised Discovery of Solid-State Lithium Ion Conductors. *Nat. Commun.* **2019**, *10*, 5260. [CrossRef]
54. Alharin, A.; Doan, T.N.; Sartipi, M. Reinforcement Learning Interpretation Methods: A Survey. *IEEE Access* **2020**, *8*, 171058–171077. [CrossRef]
55. Zhou, Z.-H. *Machine Learning*; Springer Singapore: Singapore, 2021; ISBN 978-981-15-1966-6.
56. Bell, J. *Machine Learning*; John Wiley & Sons, Inc.: Indianapolis, IN, USA, 2014; ISBN 9781119183464.
57. Matloff, N. *From Linear Models to Machine Learning Regression and Classification, with R Examples*; University of California: Los Angeles, CA, USA, 2017.
58. Utkin, L. An Imprecise Extension of SVM-Based Machine Learning Models. *Neurocomputing* **2019**, *331*, 18–32. [CrossRef]
59. Battineni, G.; Chintalapudi, N.; Amenta, F. Machine Learning in Medicine: Performance Calculation of Dementia Prediction by Support Vector Machines (SVM). *Inform. Med. Unlocked* **2019**, *16*, 100200. [CrossRef]
60. Vapnik, V.N. *The Nature of Statistical Learning Theory*; Springer: Berlin/Heidelberg, Germany, 2000. [CrossRef]
61. Noble, W.S. What Is a Support Vector Machine? *Nat. Biotechnol.* **2006**, *24*, 1565–1567. [CrossRef]
62. Gavriilidis, A.; Velten, J.; Tilgner, S.; Kummert, A. Machine Learning for People Detection in Guidance Functionality of Enabling Health Applications by Means of Cascaded SVM Classifiers. *J. Frankl. Inst.* **2018**, *355*, 2009–2021. [CrossRef]
63. Kotenko, I.; Saenko, I.; Branitskiy, A. Improving the Performance of Manufacturing Technologies for Advanced Material Processing Using a Big Data and Machine Learning Framework. *Mater. Today Proc.* **2019**, *11*, 380–385. [CrossRef]

64. Zhao, H.; Ezeh, C.I.; Ren, W.; Li, W.; Pang, C.H.; Zheng, C.; Gao, X.; Wu, T. Integration of Machine Learning Approaches for Accelerated Discovery of Transition-Metal Dichalcogenides as Hg0 Sensing Materials. *Appl. Energy* **2019**, *254*, 113651. [CrossRef]
65. Chen, W.; Pourghasemi, H.R.; Kornejady, A.; Zhang, N. Landslide Spatial Modeling: Introducing New Ensembles of ANN, MaxEnt, and SVM Machine Learning Techniques. *Geoderma* **2017**, *305*, 314–327. [CrossRef]
66. Chang, C.-C.; Lin, C.-J. LIBSVM: A Library for Support Vector Machines. *ACM Trans. Intell. Syst. Technol. (TIST)* **2001**, *2*, 1–27. [CrossRef]
67. Anusha, K.S.; Ramanathan, R.; Jayakumar, M. Link Distance-Support Vector Regression (LD-SVR) Based Device Free Localization Technique in Indoor Environment. *Eng. Sci. Technol. Int. J.* **2020**, *23*, 483–493. [CrossRef]
68. Yu, C.; Fan, W.; Yu, H.; Si, F. A Machine Learning NOxemission Model for SCR System Considering Mechanism Knowledge and Catalyst Deactivation. *E3S Web Conf.* **2020**, *194*, 04064. [CrossRef]
69. Jain, A.K.; Dubes, R.C. *Algorithms for Clustering Data*; Prentice Hall: Hoboken, NJ, USA, 1988; ISBN 978-0-13-022278-7.
70. Kaufman, L.; Rousseeuw, P.J. *Finding Groups in Data: An Introduction to Cluster Analysis*; Kaufman, L., Rousseeuw, P.J., Eds.; Wiley Series in Probability and Statistics; John Wiley & Sons, Inc.: Hoboken, NJ, USA, 1990; ISBN 9780470316801.
71. Jain, A.K. Data Clustering: 50 Years Beyond K-Means. *Mach. Learn. Knowl. Discov. Databases* **2008**, *1 Pt 19*, 3–4. [CrossRef]
72. Alhawarat, M.; Hegazi, M. Revisiting K-Means and Topic Modeling, a Comparison Study to Cluster Arabic Documents. *IEEE Access* **2018**, *6*, 42740–42749. [CrossRef]
73. von Luxburg, U. A Tutorial on Spectral Clustering. *Stat. Comput.* **2007**, *17*, 395–416. [CrossRef]
74. Zhao, J.; Li, X.; Yu, D.; Zhang, J.; Zhang, W. Lithium-Ion Battery State of Health Estimation Using Meta-heuristic Optimization and Gaussian Process Regression. *J. Energy Storag.* **2023**, *58*, 106319. [CrossRef]
75. Zhuzhunashvili, D.; Knyazev, A. Preconditioned Spectral Clustering for Stochastic Block Partition Streaming Graph Challenge. In Proceedings of the 2017 IEEE High Performance Extreme Computing Conference, Waltham, MA, USA, 12–14 September 2017. [CrossRef]
76. Bolla, M. *Spectral Clustering and Biclustering: Learning Large Graphs and Contingency Tables*; John Wiley & Sons, Ltd.: Hoboken, NJ, USA, 2013; pp. 1–268. [CrossRef]
77. Sinaga, K.P.; Yang, M.S. Unsupervised K-Means Clustering Algorithm. *IEEE Access* **2020**, *8*, 80716–80727. [CrossRef]
78. Likas, A.; Vlassis, N.J.; Verbeek, J. The Global K-Means Clustering Algorithm. *Pattern Recognit.* **2003**, *36*, 451–461. [CrossRef]
79. Murtagh, F.; Contreras, P. Algorithms for Hierarchical Clustering: An Overview. *Wiley Interdiscip. Rev. Data Min. Knowl. Discov.* **2012**, *2*, 86–97. [CrossRef]
80. Espinoza, F.A.; Oliver, J.M.; Wilson, B.S.; Steinberg, S.L. Using Hierarchical Clustering and Dendrograms to Quantify the Clustering of Membrane Proteins. *Bull. Math. Biol.* **2012**, *74*, 190. [CrossRef]
81. Sasirekha, K.; Baby, P. Agglomerative Hierarchical Clustering Algorithm-A Review. *Int. J. Sci. Res. Publ.* **2013**, *83*, 83.
82. Murtagh, F.; Legendre, P. Ward's Hierarchical Agglomerative Clustering Method: Which Algorithms Implement Ward's Criterion? *J. Classif.* **2014**, *31*, 274–295. [CrossRef]
83. Fujimura, K.; Seko, A.; Koyama, Y.; Kuwabara, A.; Kishida, I.; Shitara, K.; Fisher, C.A.J.; Moriwake, H.; Tanaka, I. Accelerated Materials Design of Lithium Superionic Conductors Based on First-Principles Calculations and Machine Learning Algorithms. *Adv. Energy Mater.* **2013**, *3*, 980–985. [CrossRef]
84. Guo, H.; Wang, Q.; Urban, A.; Artrith, N. Artificial Intelligence-Aided Mapping of the Structure-Composition-Conductivity Relationships of Glass-Ceramic Lithium Thiophosphate Electrolytes. *Chem. Mater.* **2022**, *34*, 6702–6712. [CrossRef]
85. Bergerhoff, G.; Hundt, R.; Sievers, R.; Brown, I.D. The Inorganic Crystal Structure Data Base. *J. Chem. Inf. Model.* **1983**, *23*, 66–69. [CrossRef]
86. Jain, A.; Ong, S.P.; Hautier, G.; Chen, W.; Richards, W.D.; Dacek, S.; Cholia, S.; Gunter, D.; Skinner, D.; Ceder, G.; et al. Commentary: The Materials Project: A Materials Genome Approach to Accelerating Materials Innovation. *APL Mater.* **2013**, *1*, 011002. [CrossRef]
87. Sendek, A.D.; Cubuk, E.D.; Antoniuk, E.R.; Cheon, G.; Cui, Y.; Reed, E.J. Machine Learning-Assisted Discovery of Solid Li-Ion Conducting Materials. *Chem. Mater.* **2019**, *31*, 342–352. [CrossRef]
88. Cubuk, E.D.; Sendek, A.D.; Reed, E.J. Screening Billions of Candidates for Solid Lithium-Ion Conductors: A Transfer Learning Approach for Small Data. *J Chem. Phys.* **2019**, *150*, 214701. [CrossRef]
89. Ma, Y.; Guo, G. *Support Vector Machines Applications*; Springer: Berlin/Heidelberg, Germany, 2014; ISBN 9783319022994.
90. Cristianini, N.; Shawe-Taylor, J. *An Introduction to Support Vector Machines and Other Kernel-Based Learning Methods*; Cambridge University Press: Cambridge, UK, 2000; ISBN 9780521780193.
91. Miyamoto, S. *Theory of Agglomerative Hierarchical Clustering*; Behaviormetrics: Quantitative Approaches to Human Behavior; Springer Singapore: Singapore, 2022; Volume 15, ISBN 978-981-19-0419-6.
92. Erbacher, M. *Cluster Analysis*; Atkinson, P., Delamont, S., Cernat, A., Sakshaug, J.W., Williams, R.A., Eds.; SAGE Publications Ltd.: New York, NY, USA, 2020; ISBN 9781529748222.
93. Liu, J.; Han, J. Spectral Clustering. In *Data Clustering*; Chapman and Hall/CRC: Boca Raton, FL, USA, 2018; pp. 177–200. ISBN 9781315373515.
94. Hosmer, D.W.; Lemeshow, S.; Sturdivant, R.X. *Applied Logistic Regression*, 3rd ed.; Wiley: New York, NY, USA, 2013; ISBN 9781118548387.
95. Richards, W.D.; Miara, L.J.; Wang, Y.; Kim, J.C.; Ceder, G. Interface Stability in Solid-State Batteries. *Chem. Mater.* **2016**, *28*, 266–273. [CrossRef]

96. Luntz, A.C.; Voss, J.; Reuter, K. Interfacial Challenges in Solid-State Li Ion Batteries. *J. Phys. Chem. Lett.* **2015**, *6*, 4599–4604. [CrossRef]
97. Huo, S.; Sheng, L.; Xue, W.; Wang, L.; Xu, H.; Zhang, H.; Su, B.; Lyu, M.; He, X. Challenges of Stable Ion Pathways in Cathode Electrode for All-Solid-State Lithium Batteries: A Review. *Adv. Energy Mater.* **2023**, 2204343. [CrossRef]
98. Eckhoff, M.; Schönewald, F.; Risch, M.; Volkert, C.A.; Blöchl, P.E.; Behler, J. Closing the Gap between Theory and Experiment for Lithium Manganese Oxide Spinels Using a High-Dimensional Neural Network Potential. *Phys. Rev. B* **2020**, *102*, 174102. [CrossRef]
99. Gao, B.; Jalem, R.; Ma, Y.; Tateyama, Y. Li+ Transport Mechanism at the Heterogeneous Cathode/Solid Electrolyte Interface in an All-Solid-State Battery via the First-Principles Structure Prediction Scheme. *Chem. Mater.* **2020**, *32*, 85–96. [CrossRef]
100. Kim, S.; Chen, J.; Cheng, T.; Gindulyte, A.; He, J.; He, S.; Li, Q.; Shoemaker, B.A.; Thiessen, P.A.; Yu, B.; et al. PubChem in 2021: New Data Content and Improved Web Interfaces. *Nucleic Acids Res.* **2021**, *49*, D1388–D1395. [CrossRef] [PubMed]
101. Materials Data Repository Home. Available online: https://materialsdata.nist.gov/ (accessed on 7 March 2023).
102. Kirklin, S.; Saal, J.E.; Meredig, B.; Thompson, A.; Doak, J.W.; Aykol, M.; Rühl, S.; Wolverton, C. The Open Quantum Materials Database (OQMD): Assessing the Accuracy of DFT Formation Energies. *Npj Comput. Mater.* **2015**, *1*, 15010. [CrossRef]
103. Saal, J.E.; Kirklin, S.; Aykol, M.; Meredig, B.; Wolverton, C. Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). *JOM* **2013**, *65*, 1501–1509. [CrossRef]