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Human Need for Artificial Intelligence in Energy Storage

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ABSTRACT

It must be said that artificial intelligence has one of the richest histories, but in stories! High-understanding artificial machines and creatures were first introduced in ancient Greek mythology. Philosophers and mathematicians have long debated reasoning and logic, and today these arguments have been accepted in agreement. Such logics have become the basis of digital and programmable computers. One of the people who played a key role in this was Alan Turing. Turing's theory was that we could use mathematical symbols and numbers such as zero and one to perform any mathematical argument on a computer. Simultaneously with this theory, new discoveries were made in the field of neuroscience, information theory, and obedience. These developments have inspired a small group of researchers to seriously address the issue of creating an electronic brain. in 1950, Alan Turing published an article on artificial intelligence, which later became known as the Turing test. In this article, it was stated that if a person has a written conversation with a computer from behind a wall or anything else, and does not know that the other party is not human and does not realize this after the conversation, then the computer can be machine-made. He called it smart because he was able to use reason and logic well enough for a human being. The Turing test was able to justify some intelligence, but only (to some extent)! But since then, no machine has been invented that has successfully passed this test. Although the AIML language was invented, it never achieved this level of artificial intelligence.After these problems, in the 1990s and close to the 21st century, artificial intelligence achieved one of its greatest successes. Although things remained behind the scenes, artificial intelligence was used in important areas such as reasoning and logic, data processing, medical diagnoses, and a wide range of technology and industry. Soon, AI developers decided that they should use step-by-step problem solving in their algorithms. In fact, humans often use this method to solve cases such as making puzzles and so on. They were also able to come up with successful algorithms for understanding data and incomplete information after the 1980s and 1990s, which used probabilities to understand this information. But today we are witnessing the increasing progress of this technology in different parts of our lives. This technology is still emerging and growing, especially in terms of energy and storage, which can reduce the need for governments to use fossil fuels.

Keywords: Renewable energy, artificial machines, artificial intelligence, fossil fuels

1. INTRODUCTION

The development of new energy storage materials is playing a critical role in the transition to clean and renewable energy. However, improvements in performance and durability of batteries have been incremental due to a lack of understanding of both the materials and the complexities of the chemical dynamics occurring under operando conditions[1]. Generally, in order to test a chemical or physical property, parameter extensive experimental tests are performed. Unfortunately, these repetitive experimental and theoretical characterization studies are often time-consuming and inefficient because significant progress generally requires a combination of chemical intuition and serendipity. These approaches are therefore unable to characterise the millions of materials required to define even a small subclass of perfect crystalline materials, let alone more complex structures found within electrochemical cells [2]. This so-called `open` loop methodology of development results in the time frame for discovering new battery materials being remarkably long, often taking longer than a decade to bring a novel formulation to market.

In the recent decade, first-principle calculations, especially those based on more costeffective approximations such as density functional theory (DFT)[3,4] , are now reliably automated [5–7] for high-throughput property prediction across vast numbers of materials.

These methods have been used in successful materials design efforts such as alkali-ion batteries[8–10], to identifying promising solid-state Li-ion conductors for battery electrolyte applications[11], as well as other materials applications[12–15]. Building on these efforts, materials design guided by computation is expected to lead the discovery of new materials and greatly reduce materials development time and cost[16] via the expansion and development of machine learning (ML) techniques.

Machine learning is a branch of artificial intelligence which shows good applicability in classification, regression and other tasks related to high-dimensional data. Aimed at extracting knowledge and gaining insight from large databases, machine learning learns from previous computations to produce reliable, repeatable decisions and results [17,18]. With the rapid developmental pace in data-driven approaches that combine the wisdom of experts with powerful machine learning models, scientists are beginning to integrate human intuition in guiding scientific research. Scientists and engineers can now realistically simulate the properties and behaviours of materials in specific energy applications.

ML models have already shown their remarkable ability in the development of new crystalline solid materials with fast single-crystal Li-ion conductivity at room temperature[19].

DFT simulations guided by machine learning-based methods found that the ML-guided search was 2.7 times more likely to identify fast Li-ion conductors, with at least a 44 times improvement in the log-average of room temperature Li-ion conductivity and a 1000-fold increase in speed at which the candidates were discovered over trial and error methods (Fig.1). Methods such as these are for the first time allowing a means to move away from the traditional `open loop` methods of research to a far more efficient `closed-loop` method which is paving the way towards the inverse design of materials (Table 1). Inverse materials design effectively inverts the current design process by allowing the desired performance goals to define the composition and structure which best fulfils these targets without defining the starting material or structure beforehand[20–26]. Crucially, machine learning will play a pivotal role in battery development via aiding inverse design as their computational strategies will continue to automatically improve through

experience[27]. Cluster Expansion methods[28] are now widely employed to study the disorder in electrode materials, to neural networks which systematically improve the reliability of molecular dynamics simulations[29]. Probabilistic data-driven models are now able to narrow down likely candidates designed for specific applications from a chemical space of more than 1060 possible molecules. Generative models produce large numbers of candidate molecules which will require laboratory synthesis to validate the simulation results requiring synthesis automation also powered by ML and robotics. These forms of automation will allow research scientists to reduce the amount of time spent doing costly, intuitively driven, repetitive syntheses. Even with current databases derived from previous laboratory experiments there is already enough data for scientists to produced highly targeted molecules relative to an unguided, `open loop`, approach. The online state of charge and state of health of a battery can now be predicted via machine learning models each time a battery undergoes charge/discharge cycles and are crucial for durable and safe electric vehicles. Early detection of inadequate performance also facilitates timely maintenance of battery systems[30–33]. Deep generative learning models are able to map the underlying probability distribution of both structure and property and relate them in a nonlinear manner allowing these models to filter characteristic features inherent to certain molecules[34,35]. Machine learning methods have been recently applied to describing Li-ion battery architecture, properties, and performance[36].

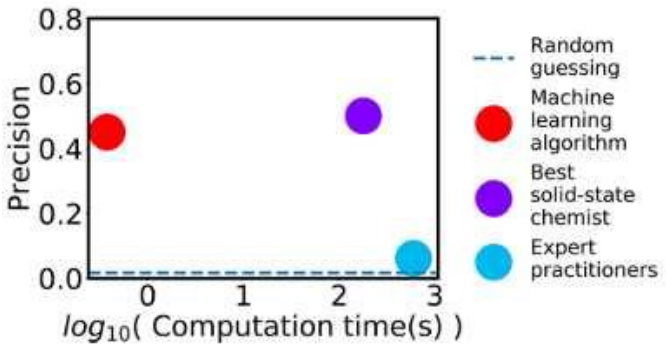

Fig.1 Comparison of computation time and precision for an ML algorithm, human experts, and random guessing. The algorithm performs as well as thebest humans but with higher speed, enabling the rapid screening of millions of candidate materials [2].

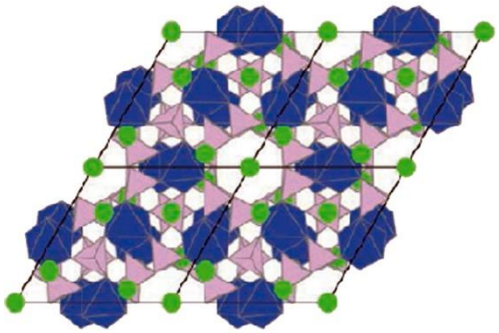

Fig.2 A simulated crystalline framework of a vanadium-containing cathode material for advanced batteries[37]. Lithium atoms shown in green are nestled into the framework. The formulation has since been synthesised and performed as the models predicted.

These results are due in part to the continually growing databases of atomic structural data necessary for DFT calculations as well as large improvements in compute resources which are paving the way for a step-change in research methods[38]. Meredig et al. showed their ML data-driven approach to materials screening was able to learn the rules of chemistry from DFT, make accurate energetic predictions for new compositions at six orders of magnitude lower computational expense, and further required no knowledge of the crystal structure[38]. These methods are now being applied to predict Li capacity in batteries. Ceder et al [37] showed how computational analysis can suggest new materials such as new vanadiumcontaining cathode material which was predicted to outperform the energy-storage capacity of conventional lithium iron phosphate cathodes by some 10% (Fig.2). The material was synthesised and behaved as the ML models predicted.

Modelling of the structures and properties of specific electrode materials, understanding the charge/discharge mechanisms at the atomic scale, and delivering rational, `closed` loop design strategies for electrode materials as well as electrolytes are well underway. A comprehensive review of modelling and theoretical design studies on sulphur cathodes, oxygen cathodes, lithium metal anodes, and solid-state electrolytes of lithium metal batteries can be found here[39].

The big data era has already arrived with experiments from large scale facilities such as synchrotrons generating enormous data rates. Combining big data with machine learning is already a crucial research priority. Questions relating to storage, management and analysis of high-volume data are challenging problems that need to be solved. Data management platforms are vital as supervised ML models generally require large amounts of reliable training data to construct reliable models[40,41] as existing experimental data and that of future experimental efforts still only cover a fraction of the stable chemical combinations possibly found in nature.

The development of generic data management and sharing platforms is required to provide impetus to accelerate materials discovery and design. Advanced materials characterization techniques, with their ever-growing rates of data acquisition and storage capabilities, represent a challenge in modern materials science, and new procedures for quickly assessing and analysing the collected data are needed to bring new energy solutions to market in less time[42]. Currently, large, high-quality open databases of computed materials properties such as the Materials Project[15], Open Quantum Materials Database[43] and the AFLOW repository are growing at a rapid pace and helping to map the vast regions of chemical space. Databases and libraries for battery electrolytes[44] are also being built which will be used in the future to rapidly formulate next-generation electrolytes. The European Large Scale Research Initiative `Battery 2030+` has recently identified establishing the `Battery Interface Genome (BIG)` and a `Materials Acceleration Platform (MAP)` as essential milestones towards the accelerated discovery of ultra-high performance batteries[45]. In one of the largest collections of molecules, the chemical space project[46] has mapped 166.4 billion molecules that contain at most 17 heavy atoms.

In the near future, we can expect to see huge growth in these new databases and libraries which will, in turn, increase the predictive power of machine learning. An important development to note is work from a Stanford, Google Brain collaboration where researchers show a novel approach to transfer physical insights onto more general descriptors derived from physical equations allowing

them to screen billions of unknown compositions for Li-ion conductivity using an accurate model trained with physical insights to generate a large database from small data[47]. Central to machine learning methodologies applied to chemical sciences is the representation of molecules. These representations that act to encode the relevant physics and chemistry will tend to generalize better as research progresses allowing for even faster materials screening. Despite considerable progress, much work remains.

Graph and hierarchical representations of molecules are an area requiring further study[48]. Finally, access to compute infrastructure in order to undertake these simulations is required. Around the world, new AI centres are under development or already operating to provide comprehensive assistance to scientists and institutions looking to combine ML methods to their research. The combination of large research institutions and powerful ML infrastructure will accelerate materials design dramatically in the coming years and allow for close participation of leading tech companies to play a part in the development of fundamental scientific research as well as spur on new economic development.

2. SUSTAINABILITY AND TECHNOLOGY

The impacts of Climate change on cities have been greatly covered in literature, and urban leaders, policy makers, and other stakeholders are driven to strategize on to mitigate those impacts (49).Cutter, Emrich, Gall, and Reeves (2018) [50] highlights that one the most prevalent impact of climate change is that of flooding, that tend to occur in cities that were previously relatively deemed as safe. Besides flooding, there are increased incidences of bushfires which are impacting on the liveability of cities as shelters are at risk, and even rendering entire urban areas as uninhabitable [51,52], thus forcing people to leave their homes. In certain instances, further accentuates the sad phenomenon of 'climate refugees'. For cities in developing countries where the local governments are financially constrained; hence unable to offer alternative lands, infrastructure repairs, or housing subsidies, a portion of the population ultimately ends up homeless and this leads to the creation of an informal economy; which are even more vulnerable to the impacts of climate change[53]. Emilsson and Sang (2017)[54] further shares how cities are seen to experience higher temperatures, especially in form of heat waves which result to loss of lives,

and in some cities it drives a higher energy demand for mechanical cooling [55]. Furthermore, unlike before, cities are now experiencing shortage of food supplies as climate change has also affected the agricultural sector due to the unpredictability of climate from conventional farming techniques [56]. Doherty, Klima, and Hellman (2016)[57] and Allam (2012)[58] support that finding solutions to these impacts will be key to the survival of cities and that mitigation strategies, potent with sustainability consciousness in mind, must be sought at various levels of policy making. They peg their argument on results from other researchers [59,60] that established that cities contribute greatly in aggravating climate change. On the same line, many city managements have started to fashion policies in such a way so as to have as little as negative impacts as possible to prevent the compromise of the environment and available resources [61,62]. In this front, many cities have managed to leverage on the available advanced technologies such as AI, Big data, IoT, Blockchain, amongst others to render sustainable solutions to both city planning and management [63,64,65,66,67].

Barns et al. (2016)[68] highlights that one such area where technology has been helpful is the implementation of the Smart Cities concept, which can be key in helping cities achieve resilience and sustainability. Koenig et al. (2017)[69] and Beatley (2011)[70], amongst others, argue that analysis, through AI enabled devices and systems, of data from IoT; that Smart Cities prone, have allowed the customization of different urban fabrics such that they optimize on the available resources. For instance, Smart Cities have catalyzed the introduction of autonomous vehicles, and even encouraged sustainability passive methods through the creation of bicycle lanes and walking paths; hence, contributing to the reduction in fossil fuel consumption [71]. These technologies have encouraged the adoption of construction tools in the building sector that can possibly integrate low power and water consumption, allow for green spaces and also accommodate green walls and roofs and have smart waste management systems [72,73]. These types of constructions also allow for increased conservation of land as there is reduced sprawl; hence, the land can be used for other purposes like agriculture, open space and forest reserve, amongst other uses that can benefit the local population and users of the urban fabric [74].

Dengel (2013)[75] succinctly shares how, through AI and big data, the agricultural sector is enhanced since information on issues like weather patterns, soil types and the best crops to plant at particular areas are readily available and this provides informed decisions as to crop management; which leads to higher yields and related proportional economic growth. The same approach in other sectors, especially in developing countries, through domains such as health, business, transport, services, amongst others, can render economic benefits while catering for sustainability outcomes by saving resources from these sectors[76,77]. The same can be used for climate change mitigation projects, and benefit cities, countries and regions that need it the most; like Small Island Developing States and Low-Income Economies that are on the front line of the impacts of Climate Change.

3. CONCLUSIONS

In the development of the next generation of batteries, we can expect that an increasing role will be played by modern multiscale computation approaches. In combination with machine learning[78,79]. ML inverse design [80,81] can enable a model that adapts as it explores chemical space, which allows for expanding a model in regions of high uncertainty and enabling the discovery of regions of molecular space with desirable properties as a function of composition53. Notably, even data from failed experiments is proving useful in training ML models. In recent years, machine learning techniques51 and big data methods[82] have successfully resolved the difficulties of modelling the relationships between materials properties and complex physical factors. ML models can already significantly outperform humans in terms of both speed and accuracy in the interpretation of materials spectra and images (X-ray, neutron, electron)[19]. These types of approaches will complement continued advances in instrumentation, especially under *operando* studies and artificial intelligence guided design of experiments.

Active learning in the space of objective functions could lead to a better understanding of the best rewards to seek while carrying out machine learning. In the near future researchers

may simultaneously conceive, create, and characterise with each data point transmitting and receiving data to constantly improve
the accuracy of the models[1,34,83]. With the continuous development of theories and methods, the topics to which machine learning can be applied in materials science will become broader and have an ever increasing effect on the efficacy of research.

Table 1. Summary of machine learning techniques applied to energy storage materials

Materials	Prediction	Method	Key findings	References
NaNi1/3Mn1/3Co1/3O2 cathode material for Na-ion batteries	Modelling and optimization of the fabrication process of the positive electrode material for sodium-ion batteries	Support vector regression synchronized crossvalidation simplex algorithm cluster	Obtained optimized value of capacity is 176 mAhg-1 for 99 cycles, which is better than those of conventional batteries used for commercial storage purposes	84
Ni-rich cathode materials: LiNixCo1 xyMn1- x-y-zO2 (NCM) for electric vehicle applications.	**1**. To construct a predictive model to propose optimized experimental parameters that satisfy the target specifications. **2**. Search for an ideal synthesis process of Ni-rich cathode materials, leading to accelerated development of lithium-ion batteries with higher capacity and longer cycle	1. ML regression models: Support vector machine (SVM), Decision tree (DT), Ridge regression (RR), Random forest (RF), Extremely randomized tree (ERT), and Neural network (NN) with multi-layer perceptron. ML model (ERT + AdaBoost) 2. The pythonbased	1. Optimized synthetic parameters for Ni-rich cathode materials, LiNixCo1-x-yMn1-x-y-zO2 (NCM) with x> 0.85 for improve the electrochemical performance 2. Showed that the calcination temperature and the particle size are determining factors for achieving a long cycle life. 3. Confirmed that structures with higher calcination temperatures, higher Ni content,	85

	life for electric vehicles 3. Design, predict and improve the electrochemical performance of Nirich cathode materials: LiNixCo1-xyMn1- x-y-zO2 (NCM) for electric vehicle applications	ML package Scikitlearn	and a larger primary particle size result in poorer cycle life performance 4. ML model (ERT + AdaBoost) exhibited the best performance for predicting the initial capacity, residual Li, and the cycle life. 5. Reverse engineering scheme was successfully used to propose ideal experimental parameters to fulfil the target specifications.	

Li5B7S13, Li2B2S5, Li3ErCl6, LiSO3F, Li3InCl6, Li2HIO, LiMgB3(H9N)2, and CsLi2BS3. Li5B7S13	Develop a machine learning (ML)-based model to predict superionic Li-ion conduction	Machine learning (ML)-based prediction model for material selection and density functional theory molecular dynamics (DFT-MD) simulations for calculating ionic conductivity	1. Discovery many new solid materials with predicted superionic Li-ion conduction (≥10−4 S/cm) at room temperature: Li5B7S13, Li2B2S5, Li3ErCl6, LiSO3F, Li3InCl6, Li2HIO, LiMgB3(H9N)2, and CsLi2BS3. 2. Li5B7S13, has a DFT-MD predicted RT Li conductivity (74mScm-1) many times larger than the fastest known Li-ion conductors	19
LiPF6 electrolyte for lithium-ion batteries	Determine unknown concentrations of major components in typical lithium-ion battery electrolytes.	Fourier Transform Infrared Spectroscopy and machine learning	Confirmed that the concentration of LiPF6 was depleted by 10–20% when the cells ran 200 cycles at 55◦C. Cell failure due to a large amount of salt loss	86
Carbon-based molecular electrode materials	To identify promising positive electrode materials with high performance	DFT-machine learning framework	1. Design carbon-based molecular electrode materials 2. Found that the electron affinity has the highest contribution to redox potential, followed by the number of oxygen atoms, the HOMO–LUMO gap, the number of lithium atoms, LUMO, and HOMO in order respectively	87

Layered structure cathode materials for lithium-ion batteries	Predicting the electrochemical properties: discharge energy density and capacity fading	Artificial neural network algorithm	Proposed 3D-QANN model: a quantitative structure−property relaKonship model for predicting the physical properties of inorganic crystalline solids and the design new materials	88
LiFePO4	The cycle life of lithium-ion batteries	Bayesian LS-SVR and wavelet neural network	Predicted the cycle life of the battery within a very short prediction time (within 1.41s) with the average error is only about one-third of that of the traditional algorithm	89
Lithium-ion batteries	The battery capacity	Gaussian process regression	In situ capacity estimation over short periods of galvanostatic operation	90

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