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Machine learning for a sustainable energy future

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Abstract | Transitioning from fossil fuels to renewable energy sources is a critical global challenge; it demands advances — at the materials, devices and systems levels — for the efficient harvesting, storage, conversion and management of renewable energy. Energy researchers have begun to incorporate machine learning (ML) techniques to accelerate these advances. In this Perspective, we highlight recent advances in ML-driven energy research, outline current and future challenges, and describe what is required to make the best use of ML techniques. We introduce a set of key performance indicators with which to compare the benefits of different ML-accelerated workflows for energy research. We discuss and evaluate the latest advances in applying ML to the development of energy harvesting (photovoltaics), storage (batteries), conversion (electrocatalysis) and management (smart grids). Finally, we offer an overview of potential research areas in the energy field that stand to benefit further from the application of ML.

The combustion of fossil fuels, used to fulfill approximately 80% of the world's energy needs, is the largest single source of rising greenhouse gas emissions and global temperature[1]. The increased use of renewable sources of energy, notably solar and wind power, is an economically viable path towards meeting the climate goals of the Paris Agreement[2]. However, the rate at which renewable energy has grown has been outpaced by ever-growing energy demand, and as a result the fraction of total energy produced by renewable sources has remained constant since 2000 (REF.[3]). It is thus essential to accelerate the transition towards sustainable sources of energy[4]. Achieving this transition requires energy technologies, infrastructure and policies that enable and promote the harvest, storage, conversion and management of renewable energy.

In sustainable energy research, suitable material candidates (such as photovoltaic materials) must first be chosen from the combinatorial space of possible materials, then synthesized at a high enough yield and quality for use in devices (such as solar panels). The time frame of a representative materials discovery process is 15–20 years[5,6], leaving considerable room for improvement. Furthermore, the devices have to be optimized for robustness and reproducibility to be incorporated into energy systems (such as in solar farms)[7], where management of energy usage and generation patterns is needed to further guarantee commercial success.

Here we explore the extent to which machine learning (ML) techniques can help to address many of these challenges[8–10]. ML models can be used to predict specific properties of new materials without the need for costly characterization; they can generate new material structures with desired properties; they can understand patterns in renewable energy usage and generation; and they can help to inform energy policy by optimizing energy management at both device and grid levels.

In this Perspective, we introduce Acc(X)eleration Performance Indicators (XPIs), which can be used to measure the effectiveness of platforms developed for accelerated energy materials discovery. Next, we discuss closed-loop ML frameworks and evaluate the latest advances in applying ML to the development of energy harvesting, storage and conversion technologies, as well as the integration of ML into a smart power grid. Finally, we offer an overview of energy research areas that stand to benefit further from ML.

Performance indicators

Because many reports discuss ML-accelerated approaches for materials discovery and energy systems management, we posit that there should be a consistent baseline from which these reports can be compared. For energy systems management, performance indicators at the device, plant and grid levels have been reported[11,12], yet there are no equivalent counterparts for accelerated materials discovery.

The primary goal in materials discovery is to develop efficient materials that are ready for commercialization. The commercialization of a new material requires intensive research efforts that can span up to two decades: the goal of every accelerated approach should be to accomplish commercialization an order-of-magnitude faster. The materials science field can benefit from studying the case of vaccine development. Historically, new vaccines take 10 years from conception to market[13]. However, after the start of the COVID-19 pandemic, several companies were able to develop and begin releasing vaccines in less than a year. This achievement was in part due to an unprecedented global research intensity, but also to a shift in the technology: after a technological breakthrough in 2008, the cost of sequencing DNA began decreasing exponentially[14,15], enabling researchers to screen orders-of-magnitude more vaccines than was previously possible.

ML for energy technologies has much in common with ML for other fields like biomedicine, sharing the same methodology and principles. However, in practice, ML models for different technologies are exposed to additional unique requirements. For example, ML models for medical applications usually have complex structures that take into account regulatory oversight and ensure the safe development, use and

monitoring of systems, which usually does not happen in the energy field[16]. Moreover, data availability varies substantially from field to field; biomedical researchers can work with a relatively large amount of data that energy researchers usually lack. This limited data accessibility can constrain the usage of sophisticated ML models (such as deep learning models) in the energy field. However, adaptation has been quick in all energy subfields, with a rapidly increased number of groups recognizing the importance of statistical methods and starting to use them for various problems. We posit that the use of high-throughput experimentation and ML in materials discovery workflows can result in breakthroughs in accelerating development, but the field first needs a set of metrics with which ML models can be evaluated and compared.

Accelerated materials discovery methods should be judged based on the time it takes for a new material to be commercialized. We recognize that this is not a useful metric for new platforms, nor is it one that can be used to decide quickly which platform is best suited for a particular scenario. We therefore propose here XPIs that new materials discovery platforms should report.

Acceleration factor of new materials, XPI-1

This XPI is evaluated by dividing the number of new materials that are synthesized and characterized per unit time with the accelerated platform by the number of materials that are synthesized and characterized with traditional methods. For example, an acceleration factor of ten means that for a given time period, the accelerated platform can evaluate ten times more materials than a traditional platform. For materials with multiple target properties, researchers should report the rate-limiting acceleration factor.

Number of new materials with threshold performance, XPI-2

This XPI tracks the number of new materials discovered with an accelerated platform that have a performance greater than the baseline value. The selection of this baseline value is critical: it should be something that fairly captures the standard to which new materials need to be compared. As an example, an accelerated platform that seeks to discover new perovskite solar cell materials should track the number of devices made with new materials that have a better performance than the best existing solar cell[17].

Performance of best material over time, XPI-3

This XPI tracks the absolute performance — whether it is Faradaic efficiency, power conversion efficiency or other — of the best material as a function of time. For the accelerated framework, the evolution of the performance should increase faster than the performance obtained by traditional methods[18].

Repeatability and reproducibility of new materials, XPI-4

This XPI seeks to ensure that the new materials discovered are consistent and repeatable: this is a key consideration to screen out materials that would fail at the commercialization stage. The performance of a new material should not vary by more than x% of its mean value (where x is the standard error): if it does, this material should not be included in either XPI-2 (number of new materials with threshold performance) or XPI-3 (performance of best material over time).

Human cost of the accelerated platform, XPI-5

This XPI reports the total costs of the accelerated platform. This should include the total number of researcher hours needed to design and order the components for the accelerated system, develop the programming and robotic infrastructure, develop and maintain databases used in the system and maintain and run the accelerated platform. This metric would provide researchers with a realistic estimate of the resources required to adapt an accelerated platform for their own research.

Use of the XPIs

Each of these XPIs can be measured for computational, experimental or integrated accelerated systems. Consistently reporting each of these XPIs as new accelerated platforms are developed will allow researchers to evaluate the growth of these platforms and will provide a consistent metric by which different platforms can be compared. As a demonstration, we applied the XPIs to evaluate the acceleration performance of several typical platforms: Edisonian-like trial-test, robotic photocatalysis development[19] and design of a DNA-encoded-library-based kinase inhibitor[20] (TABLE 1). To obtain a comprehensive performance estimate, we define one overall acceleration score S adhering to the following rules. The dependent acceleration factors (XPI-1 and XPI-2), which function in a synergetic way, are added together to reflect their contribution as a whole. The independent acceleration factors (XPI-3, XPI-4 and XPI-5), which may function in a reduplicated way, are multiplied together to value their contributions respectively. As a result, the overall acceleration score can be calculated as $S = (\text{XPI-1} + \text{XPI-2}) \times \text{XPI-3} \times \text{XPI-4} \div \text{XPI-5}$. As the reference, the Edisonian-like approach has a calculated overall XPIs score of around 1, whereas the most advanced method, the DNA-encoded-library-based drug design, exhibits an overall XPIs score of 10^7. For the sustainability field, the robotic photocatalysis platform has an overall XPIs score of 10^5.

For energy systems, the most frequently reported XPI is the acceleration factor, in part because it is deterministic, but also

Table 1 | **Demonstration of the use of the XPIs in evaluating the acceleration performance of typical materials development platforms**

	Edisonian-like trial-test	Robotic photocatalysis development[19]	DNA-encoded-library-based kinase inhibitor design[20]
Acceleration factor of new materials, XPI-1 (candidates examined per week)	0–1	~10^3	~10^5
Number of new materials with threshold performance, XPI-2	0–1	~10^2	~10^1
Performance of best material over time, XPI-3 (times of increment)	~1×	~5×	~10^1×
Repeatability and reproducibility of new materials, XPI-4 (percentage of success)	≤100%	100%	100%
Human cost of the accelerated platform, XPI-5 (percentage of the amount demanded by the trial-test method)	100%	~6%[a]	10%[b]
Overall acceleration score, S	~1	~10^5	~10^7

XPIs, Acc(X)eleration Performance Indicators. [a]Required half a day of initiation for 8 days of unattended running[19]. [b]Value is a rough estimate.

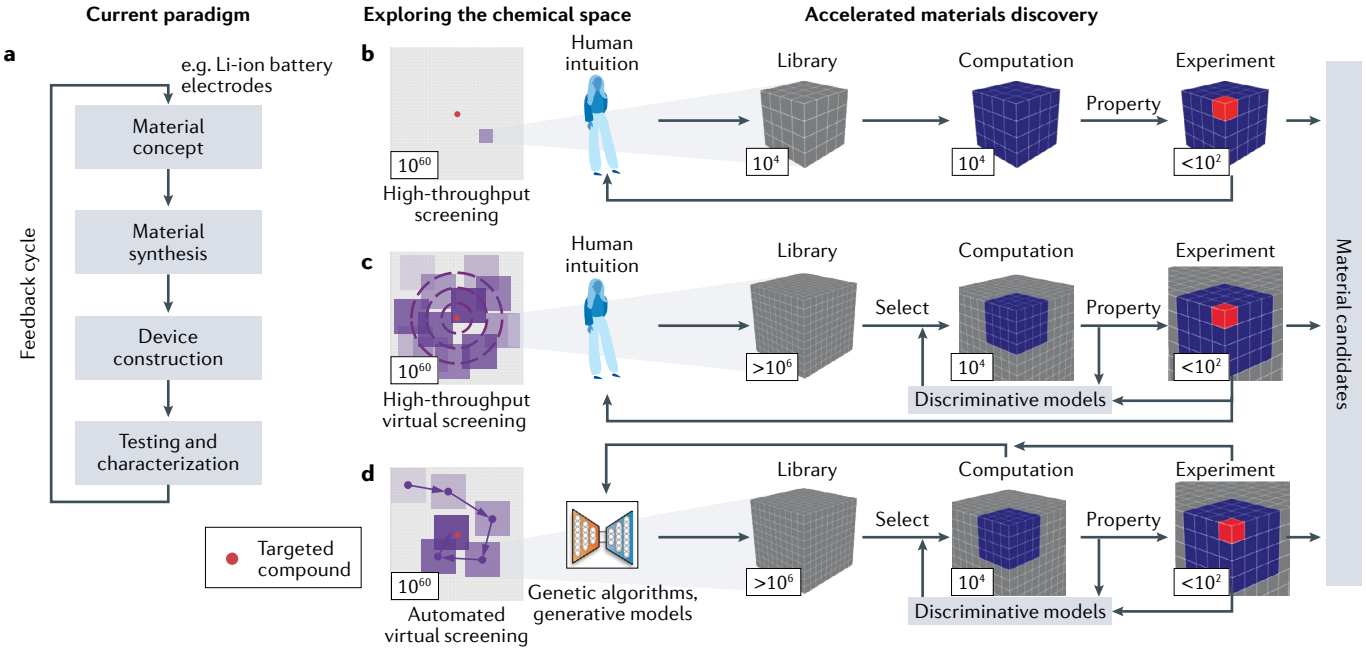

Fig. 1 | **Traditional and accelerated approaches to materials discovery. a** | Traditional Edisonian-like approach, which involves experimental trial and error. **b** | High-throughput screening approach involving a combination of theory and experiment. **c** | Machine learning (ML)-driven approach whereby theoretical and experimental results are used to train a ML model for predicting structure–property relationships. **d** | ML-driven approach for property-directed and automatic exploration of the chemical space using optimization ML (such as genetic algorithms or generative models) that solve the 'inverse' design problem.

because it is easy to calculate at the end of the development of a workflow. In most cases, we expect that authors report the acceleration factor only after completing the development of the platform. Reporting the other suggested XPIs will provide researchers with a better sense of both the time and human resources required to develop the platform until it is ready for publication. Moving forward, we hope that other researchers adopt the XPIs — or other similar metrics — to allow for fair and consistent comparison between the different methods and algorithms that are used to accelerate materials discovery.

Closed-loop ML for materials discovery

The traditional approach to materials discovery is often Edisonian-like, relying on trial and error to develop materials with specific properties. First, a target application is identified, and a starting pool of possible candidates is selected (FIG. 1a). The materials are then synthesized and incorporated into a device or system to measure their properties. These results are then used to establish empirical structure–property relationships, which guide the next round of synthesis and testing. This slow process goes through as many iterations as required and each cycle can take several years to complete.

A computation-driven, high-throughput screening strategy (FIG. 1b) offers a faster turnaround. To explore the overall vast chemical space (~10^{60} possibilities), human intuition and expertise can be used to create a library with a substantial number of materials of interest (~10^4). Theoretical calculations are carried out on these candidates and the top performers (~10^2 candidates) are then experimentally verified. With luck, the material with the desired functionality is 'discovered'. Otherwise, this process is repeated in another region of the chemical space. This approach can still be very time-consuming and computationally expensive and can only sample a small region of the chemical space.

ML can substantially increase the chemical space sampled, without costing extra time and effort. ML is data-driven, screening datasets to detect patterns, which are the physical laws that govern the system. In this case, these laws correspond to materials structure–property relationships. This workflow involves high-throughput virtual screening (FIG. 1c) and begins by selecting a larger region (~10^6) of the chemical space of possibilities using human intuition and expertise. Theoretical calculations are carried out on a representative subset (~10^4 candidates) and the results are used for training a discriminative ML model. The model can then be used to make predictions on the other candidates in the overall selected chemical space[9]. The top ~10^2 candidates are experimentally verified, and the results are used to improve the predictive capabilities of the model in an iterative loop. If the desired material is not 'discovered', the process is repeated on another region of the chemical space.

An improvement on the previous approaches is a framework that requires limited human intuition or expertise to direct the chemical space search: the automated virtual screening approach (FIG. 1d). To begin with, a region of the chemical space is picked at random to initiate the process. Thereafter, this process is similar to the previous approach, except that the computational and experimental data is also used to train a generative learning model. This generative model solves the 'inverse' problem: given a required property, the goal is to predict an ideal structure and composition in the chemical space. This enables a directed, automated search of the chemical space, towards the goal of 'discovering' the ideal material[8].

ML for energy

ML has so far been used to accelerate the development of materials and devices for energy harvesting (photovoltaics), storage (batteries) and conversion (electrocatalysis), as well as to optimize power grids. Besides

Box 1 | **Essential concepts in ML**

With the availability of large datasets[122,125] and increased computing power, various machine learning (ML) algorithms have been developed to solve diverse problems in energy. Below, we provide a brief overview of the types of problem that ML can solve in energy technology, and we then summarize the status of ML-driven energy research. More detailed information about the nuts and bolts of ML techniques can be found in previous reviews[173–175].

Property prediction
Supervised learning models are predictive (or discriminative) models that are given a datapoint *x*, and seek to predict a property *y* (for example, the bandgap[27]) after being trained on a labelled dataset. The property *y* can be either continuous or discrete. These models have been used to aid or even replace physical simulations or measurements under certain circumstances[176,177].

Generative materials design
Unsupervised learning models are generative models that can generate or output new examples *x*′ (such as new molecules[104]) after being trained on an unlabelled dataset. This generation of new examples can be further enhanced with additional information (physical properties) to condition or bias the generative process, allowing the models to generate examples with improved properties and leading to the property-to-structure approach called inverse design[52,178].

Self-driving laboratories
Self-driving or autonomous laboratories[19] use ML models to plan and perform experiments, including the automation of retrosynthesis analysis (such as in reinforcement-learning-aided synthesis planning[124,179]), prediction of reaction products (such as in convolutional neural networks (CNNs) for reaction prediction[137,138]) and reaction condition optimization (such as in robotic workflows optimized by active learning[19,160,180–183]). Self-driving laboratories, which use active learning for iterating through rounds of synthesis and measurements, are a key component in the closed-loop inverse design[52].

Aiding characterization
ML models have been used to aid the quantitative or qualitative analysis of experimental observations and measurements, including assisting in the determination of crystal structure from transmission electron microscopy images[184], identifying coordination environment[81] and structural transition[83] from X-ray absorption spectroscopy and inferring crystal symmetry from electron diffraction[176].

Accelerating theoretical computations
ML models can enable otherwise intractable simulations by reducing the computational cost (processor core amount and time) for systems with increased length and timescales[69,70] and providing potentials and functionals for complex interactions[68].

Optimizing system management
ML models can aid the management of energy systems at the device or grid power level by predicting lifetimes (such as battery life[43,44]), adapting to new loads (such as in long short-term memory for building load prediction[95]) and optimizing performance (such as in reinforcement learning for smart grid control[94]).

all the examples discussed here, we summarize the essential concepts in ML (BOX 1), the grand challenges in sustainable materials research (BOX 2) and the details of key studies (TABLE 2).

Photovoltaics

ML is accelerating the discovery of new optoelectronic materials and devices for photovoltaics, but major challenges are still associated with each step.

Photovoltaics materials discovery. One materials class for which ML has proved particularly effective is perovskites, because these materials have a vast chemical space from which the constituents may be chosen. Early representations of perovskite materials for ML were atomic-feature representations, in which each structure is encoded as a fixed-length vector comprised of an average of certain atomic properties of the atoms in the crystal structure[21,22]. A similar technique was used to predict new lead-free perovskite materials with the proper bandgap for solar cells[23] (FIG. 2a). These representations allowed for high accuracy but did not account for any spatial relation between atoms[24,25]. Materials systems can also be represented as images[26] or as graphs[27], enabling the treatment of systems with diverse number of atoms. The latter representation is particularly compelling, as perovskites, particularly organic–inorganic perovskites, have crystal structures that incorporate a varying number of atoms, and the organic molecules can vary in size.

Although bandgap prediction is an important first step, this parameter alone is not sufficient to indicate a useful optoelectronic material; other parameters, including electronic defect density and stability, are equally important. Defect energies are addressable with computational methods, but the calculation of defects in structures is extremely computationally expensive, which inhibits the generation of a dataset of defect energies from which an ML model can be trained. To expedite the high-throughput calculation of defect energies, a Python toolkit has been developed[28] that will be pivotal in building a database of defect energies in semiconductors. Researchers can then use ML to predict both the formation energy of defects and the energy levels of these defects. This knowledge will ensure that the materials selected from high-throughput screening will not only have the correct bandgap but will also either be defect-tolerant or defect-resistant, finding use in commercial optoelectronic devices.

Even without access to a large dataset of experimental results, ML can accelerate the discovery of optoelectronic materials. Using a self-driving laboratory approach, the number of experiments required to optimize an organic solar cell can be reduced from 500 to just 60 (REF.[29]). This robotic synthesis method accelerates the learning rate of the ML models and drastically reduces the cost of the chemicals needed to run the optimization.

Solar device structure and fabrication. Photovoltaic devices require optimization of layers other than the active layer to maximize performance. One component is the top transparent conductive layer, which needs to have both high optical transparency and high electronic conductivity[30,31]. A genetic algorithm that optimized the topology of a light-trapping structure enabled a broadband absorption efficiency of 48.1%, which represents a more than threefold increase over the Yablonovitch limit, the $4n^2$ factor (where n is the refractive index of the material) theoretical limit for light trapping in photovoltaics[32].

A universal standard irradiance spectrum is usually used by researchers to determine optimal bandgaps for solar cell operation[33]. However, actual solar irradiance fluctuates based on factors such as the position of the Sun, atmospheric phenomena and the season. ML can reduce yearly spectral sets into a few characteristic spectra[33], allowing for the calculation of optimal bandgaps for real-world conditions.

To optimize device fabrication, a CNN was used to predict the current–voltage characteristics of as-cut Si wafers based on their photoluminescence images[34]. Additionally, an artificial neural network was used to predict the contact resistance

of metallic front contacts for Si solar cells, which is critical for the manufacturing process[35].

Although successful, these studies appear to be limited to optimizing structures and processes that are already well established. We suggest that, in future work, ML could be used to augment simulations, such as the multiphysics models for solar cells. Design of device architecture could begin from such simulation models, coupled with ML in an iterative process to quickly optimize design and reduce computational time and cost. In addition, optimal conditions for the scaling-up of device area and fabrication processes are likely to be very different from those for laboratory-scale demonstrations. However, determining these optimal conditions could be expensive in terms of materials cost and time, owing to the need to construct much larger devices. In this regard, ML, together with the strategic design of experiments, could greatly accelerate the optimization of process conditions (such as the annealing temperatures and solvent choice).

Electrochemical energy storage

Electrochemical energy storage is an essential component in applications such as electric vehicles, consumer electronics and stationary power stations. State-of-the-art electrochemical energy storage solutions have varying efficacy in different applications: for example, lithium-ion batteries exhibit excellent energy density and are widely used in electronics and electric vehicles, whereas redox flow batteries have drawn substantial attention for use in stationary power storage. ML approaches have been widely employed in the field of batteries, including for the discovery of new materials such as solid-state ion conductors[36–38] (FIG. 2b) and redox active electrolytes for redox flow batteries[39]. ML has also aided battery management, for example, through state-of-charge determination[40], state-of-health evaluation[41,42] and remaining-life prediction[43,44].

Electrode and electrolyte materials design. Layered oxide materials, such as $LiCoO_2$ or $LiNi_xMn_yCo_{1-x-y}O_2$, have been used extensively as cathode materials for alkali metal-ion (Li/Na/K) batteries. However, developing new Li-ion battery materials with higher operating voltages, enhanced energy densities and longer lifetimes is of paramount interest. So far, universal design principles for new battery materials remain undefined, and hence different approaches have been explored. Data from the Materials Project have been used to model the electrode voltage profile diagrams for different materials in alkali metal-ion batteries (Na and K)[45], leading to the proposition of 5,000 different electrode materials with appropriate moderate voltages. ML was also employed to screen 12,000 candidates for solid Li-ion batteries, resulting in the discovery of ten new Li-ion conducting materials[46,47].

Flow batteries consist of active materials dissolved in electrolytes that flow into a cell with electrodes that facilitate redox reactions. Organic flow batteries are of particular interest. In flow batteries, the solubility of the active material in the electrolyte and the charge/discharge stability dictate performance. ML methods have explored the chemical space to find suitable electrolytes for organic redox flow batteries[48,49]. Furthermore, a multi-kernel-ridge regression method accelerated the discovery of active organic molecules using multiple feature training[48]. This method also helped in predicting the solubility dependence of anthraquinone molecules with different numbers and combinations of sulfonic and hydroxyl groups on pH. Future opportunities lie in the exploration of large combinatorial spaces for the inverse design of high-entropy electrodes[50] and high-voltage electrolytes[51]. To this end, deep generative models can assist the discovery of new materials based on the simplified molecular input line entry system (SMILES) representation of molecules[52].

Battery device and stack management. A combination of mechanistic and semi-empirical models is currently used to estimate capacity and power loss in lithium-ion batteries. However, the models are applicable only to specific failure mechanisms or situations and cannot predict the lifetimes of batteries at the early stages of usage. By contrast, mechanism-agnostic models based on ML can accurately predict battery cycle life, even at an early stage of a

Box 2 | **Grand challenges in energy materials research**

Photovoltaics

Materials

- Discover non-toxic (Pd- and Cd-free) materials with good optoelectronic properties
- Identify and minimize materials defects in light-absorbing materials
- Design effective recombination-layer materials for tandem solar cells
- Develop materials design strategies for long-term operational stability[125]
- Develop (hole/electron) transport materials with high carrier mobility[125]

Devices

- Optimize cell structure for maximum light absorption and minimum use of active materials
- Tune materials bandgaps for optimal solar-harvesting performance under complex operation conditions[21,22]

Batteries

Materials

- Develop Earth-abundant cathode materials (Co-free) with high reversibility and charge capacity[4]
- Design electrolytes with wider electrochemical windows and high conductivity[4]
- Identify electrolyte systems to boost battery performance and lifetime[4]
- Discover new molecules for redox flow batteries with suitable voltage[4]

Devices

- Understand correlation between defect growth in battery materials and overall degradation process of battery components
- Tune operando (dis)charging protocol for minimized capacity loss, (dis)charging rate and optimal battery life under diversified conditions[7,53]

Electrocatalysis

Materials

- Design materials with optimal adsorption energy for maximized catalytic activity[60,61]
- Identify and study active sites on catalytic materials[58]
- Engineer catalytic materials for extended durability[58,60,61]
- Identify a fuller set of materials descriptors that relate to catalytic activity[60,61]
- Engineer multiple catalytic functionalities into the same material[60,61]

Devices

- Design multiscale electrode structures for optimized catalytic activity
- Correlate atomistic contamination and growth of catalyst particles with electrode degradation process
- Tune operando (dis)charging protocol for minimized capacity loss and optimal cell life

Table 2 | **Summary of advances in applying ML to energy harvesting, storage and conversion**

ML approach	Main research outcome
Photovoltaics	
Bayesian optimization	By sampling just 1.8% of the compositional space, the perovskites identified showed a >17-fold stability improvement over the original methylammonium lead iodide ($MAPbI_3$) without compromising conversion efficiency[160]
Random forest classifier	Approach reliability was verified by screening ten newly designed donor materials, with good consistency between model predictions and experimental outcomes[161]
ML regression algorithms	Six lead-free hybrid perovskites that are stable at room temperature and have suitable bandgaps for solar cells were successfully screened out of 5,158 candidates[23]
Gaussian process regression	The ML model was able to make bandgap predictions of elpasolite compounds with similar accuracy to that of high-cost computational calculations[21]
KRR	Starting from a set of 1.2 million features, two of them were identified as the most important factors that influence the bandgap of double perovskites[22]
Random forest regressor	Compared with the brute-force method, an acceleration factor of 700 was achieved with an experimentally validated new perovskite[24]
DNN-based classifier	The ML model could classify compounds ten times faster than human analysis with 90% accuracy, and four lead-free layered perovskites were realized experimentally[162]
CNN-based classifier and random forest regressor	CNN-based crystal recognition enabled autonomous characterization of the outcomes of the robotic experiments. The regressor predicted the optimal conditions for the synthesis of a new perovskite single crystal[163]
Bayesian optimization	Using an automated experimentation platform with a Bayesian optimization, a four-dimensional parameter space of organic photovoltaics blends was mapped and optimized for photostability[164]
Random forest regressor	Essential features were identified and used to screen the most promising thin low-dimensional perovskite capping layer, which then led to a many-fold increase in the stability of the state-of-the-art perovskite cell[165]
Random forest regressor	Major patterns regarding materials selection/device structure were captured, which could be used to predict perovskite solar cell efficiencies[166]
Genetic algorithm	Experimental samples processed under conditions suggested by the model showed substantial improvements in performance[167]
Batteries	
DNNs, KRR and support vector machine	The model enabled a reduction in the amount of density functional theory calculations required to explore the chemical space. Up to 5,000 candidate materials for Na-ion and K-ion electrodes were identified[45]
Artificial neural network	The model demonstrated accurate estimation of the redox potentials of molecular electrode materials in Li-ion batteries, with contribution analysis confirming that electron affinity has the highest contribution to the redox potential[168]
Gaussian KRR and GBR	The method predicted the redox potentials well. The redox potentials could be explained by a small number of features, improving the interpretability of the results[169]
Logistic regression	The screening reduced the list of candidate materials from 12,831 down to 21 structures that showed promise as electrolytes[36]
Linear regression and support vector machine	The method transferred physical insights onto more generic descriptors, allowing the screening of billions of unknown compositions for Li-ion conductivity[46]
Logistic regression	The ML-guided search was 2.7 times more likely to identify fast Li ion conductors, with at least a 44-fold improvement of room-temperature Li ion conductivity[47]
Hierarchical and spectral clustering	Ab initio molecular dynamics simulations were used to validate the clustering in Li-containing compounds and identify top candidates for high ionic conduction, with 16 new Li-ion conductors discovered[38]
Artificial neural network	Predicted electrode specific resistances were found to agree well with simulated values[170]
Crystal graph CNN, KRR and GBR	The ML model was used to screen over 12,000 inorganic solids for their use as solid electrolytes. Four of these solid electrolytes could be used to suppress Li dendrite growth[37]
Model-free reinforcement learning	This method was used to explore trade-offs in the power–performance design space and converge to a better power management policy. Experimental results obtained with this technique exhibited a remarkable power reduction compared with the existing expert-based power management[171]
Bagged decision tree	The model led to a policy for battery usage optimization that substantially outperformed the leading algorithms. The policy was capable of improving and adapting as new data were collected over time[172]
Electrocatalysis	
Random forest regressor and extra trees regressor	The framework was able to identify 131 intermetallic surfaces across 54 alloys as promising candidates for CO_2 reduction. Specifically, a Cu–Al alloy catalyst was identified and experimentally verified to selectively convert CO_2 into ethylene with record performance[75,76]
Neural networks	The model reduced the number of intermediate ab initio calculations needed to locate saddle points on the potential-energy surface using a nudged elastic band simulation[69]
Gaussian process regressor	The model predicted the most important reaction step that needed to be calculated with the computationally demanding electronic structure theory. Using this method, the most likely reaction mechanism for the reaction of syngas on Rd(111) was identified[70]
Neural networks	A neural network was able to screen for active sites across a random, disordered nanoparticle surface. The most likely active sites for CO_2 conversion were identified for Au and Cu nanoparticle systems[71,72]

CNN, convolutional neural network; DNN, deep neural network; GBR, gradient boosting regression; KRR, kernel ridge regression; ML, machine learning.

battery's life[43]. A combined early-prediction and Bayesian optimization model has been used to rapidly identify the optimal charging protocol with the longest cycle life[44]. ML can be used to accelerate the optimization of lithium-ion batteries for longer lifetimes[53], but it remains to be seen whether these models can be generalized to different battery chemistries[54].

ML methods can also predict important properties of battery storage facilities. A neural network was used to predict the charge/discharge profiles in two types of stationary battery systems, lithium iron phosphate and vanadium redox flow batteries[55]. Battery power management techniques must also consider the uncertainty and variability that arise from both the environment and the application. An iterative *Q*-learning (reinforcement learning) method was also designed for battery management and control in smart residential environments[56]. Given the residential load and the real-time electricity rate, the method is effective at optimizing battery charging/discharging/idle cycles. Discriminative neural network-based models can also optimize battery usage in electric vehicles[57].

Although ML is able to predict the lifetime of batteries, the underlying degradation mechanisms are difficult to identify and correlate to the state of health and lifetime. To this end, incorporation of domain knowledge into a hybrid physics-based ML model can provide insight and reduce overfitting[53]. However, incorporating the physics of battery degradation processes into a hybrid model remains challenging; representation of electrode materials that encode both compositional and structural information is far from trivial. Validation of these models also requires the development of operando characterization techniques, such as liquid-phase transmission electron microscopy and ambient-pressure X-ray absorption spectroscopy (XAS), that reflect true operating conditions as closely as possible[54]. Ideally, these characterization techniques should be carried out in a high-throughput manner, using automated sample changers, for example, in order to generate large datasets for ML.

Electrocatalysts

Electrocatalysis enables the conversion of simple feedstocks (such as water, carbon dioxide and nitrogen) into valuable chemicals and/or fuels (such as hydrogen, hydrocarbons and ammonia), using renewable energy as an input[58]. The reverse reactions are also possible in a fuel cell, and hydrogen can be consumed to produce electricity[59]. Active and selective electrocatalysts must be developed to improve the efficiency of these reactions[60,61]. ML has been used to accelerate electrocatalyst development and device optimization.

Electrocatalyst materials discovery. The most common descriptor of catalytic activity is the adsorption energy of intermediates on a catalyst[61,62]. Although these adsorption energies can be calculated using density functional theory (DFT), catalysts possess multiple surface binding sites, each with different adsorption energies[63]. The number of possible sites increases dramatically if alloys are considered, and thus becomes intractable with conventional means[64].

DFT calculations are critical for the search of electrocatalytic materials[65] and efforts have been made to accelerate the calculations and to reduce their computational cost by using surrogate ML models[66–69]. Complex reaction mechanisms involving hundreds of possible species and intermediates can also be simplified using ML, with a surrogate model predicting the most important reaction steps and deducing the most likely reaction pathways[70]. ML can also be used to screen for active sites across a random, disordered nanoparticle surface[71,72]. DFT calculations are performed on only a few representative sites, which are then used to train a neural network to predict the adsorption energies of all active sites.

Catalyst development can benefit from high-throughput systems for catalyst synthesis and performance evaluation[73,74]. An automatic ML-driven framework was developed to screen a large intermetallic chemical space for CO_2 reduction and H_2 evolution[75]. The model predicted the adsorption energy of new intermetallic systems and DFT was automatically performed on the most promising candidates to verify the predictions. This process went on iteratively in a closed feedback loop. 131 intermetallic surfaces across 54 alloys were ultimately identified as promising candidates for CO_2 reduction. Experimental validation[76] with Cu–Al catalysts yielded an unprecedented Faradaic efficiency of 80% towards ethylene at a high current density of 400 mA cm^{-2} (FIG. 2c).

Because of the large number of properties that electrocatalysts may possess

a Energy harvesting

Target property	Library creation	ML model	Prediction	Acceleration performance
Proper bandgap	212 hybrid perovskites	Gradient boosting regression	5,158 examined, 6 candidates	2 novel materials with ideal bandgap and stability

Accelerated discovery of lead-free perovskites for solar cells

b Energy storage

Target property	Library creation	ML model	Prediction	Acceleration performance
Lithium ion conduction	All materials from ICSD	Agglomerative hierarchical clustering	2,986 examined, 16 candidates	3 novel materials with unparalleled properties

Unsupervised discovery of solid-state lithium ion conductors

c Energy conversion

Target property	Library creation	ML model	Prediction	Acceleration performance
CO_2 reduction efficiency	12,229 surfaces of 244 Cu-intermetallics	Random forest regressor	4,000 examined with Cu-Al identified	2× Higher Faradaic efficiency (record)

Accelerated discovery of CO_2 electrocatalysts using active learning

d Energy management

Target	Data collection	ML model	Prediction	Performance
Optimized automatic generation control	Operation data of Hainan power grid	Relaxed deep learning model	Economic generation dispatch and control	80% cost reduction

Power grid optimization using relaxed deep learning

Fig. 2 | **Examples illustrating the use of ML techniques for a sustainable energy future. a** | Energy harvesting[23]. **b** | Energy storage[38]. **c** | Energy conversion[76]. **d** | Energy management[93]. ICSD, Inorganic Crystal Structure Database; ML, machine learning.

(such as shape, size and composition), it is difficult to do data mining on the literature[77]. Electrocatalyst structures are complex and difficult to characterize completely; as a result, many properties may not be fully characterized by research groups in their publications. To avoid situations in which potentially promising compositions perform poorly as a result of non-ideal synthesis or testing conditions, other factors (such as current density, particle size and pH value) that affect the electrocatalyst performance must be kept consistent. New approaches such as carbothermal shock synthesis[78,79] may be a promising avenue, owing to its propensity to generate uniformly sized and shaped alloy nanoparticles, regardless of composition.

XAS is a powerful technique, especially for in situ measurements, and has been widely employed to gain crucial insight into the nature of active sites and changes in the electrocatalyst over time[80]. Because the data analysis relies heavily on human experience and expertise, there has been interest in developing ML tools for interpreting XAS data[81]. Improved random forest models can predict the Bader charge (a good approximation of the total electronic charge of an atom) and nearest-neighbour distances, crucial factors that influence the catalytic properties of the material[82]. The extended X-ray absorption fine structure (EXAFS) region of XAS spectra is known to contain information on bonding environments and coordination numbers. Neural networks can be used to automatically interpret EXAFS data[83], permitting the identification of the structure of bimetallic nanoparticles using experimental XAS data, for example[84]. Raman and infrared spectroscopy are also important tools for the mechanistic understanding of electrocatalysis. Together with explainable artificial intelligence (AI), which can relate the results to underlying physics, these analyses could be used to discover descriptors hidden in spectra that could lead to new breakthroughs in electrocatalyst discovery and optimization.

Fuel cell and electrolyser device management. A fuel cell is an electrochemical device that can be used to convert the chemical energy of a fuel (such as hydrogen) into electrical energy. An electrolyser transforms electrical energy into chemical energy (such as in water splitting to generate hydrogen). ML has been used to optimize and manage their performance, predict degradation and device lifetime as well as detect and diagnose faults. Using a hybrid method consisting of an extreme learning machine, genetic algorithms and wavelet analysis, the degradation in proton-exchange membrane fuel cells has been predicted[85,86]. Electrochemical impedance measurements used as input for an artificial neural network have enabled fault detection and isolation in a high-temperature stack of proton-exchange membrane fuel cells[87,88].

ML approaches can also be employed to diagnose faults, such as fuel and air leakage issues, in solid oxide fuel cell stacks. Artificial neural networks can predict the performance of solid oxide fuel cells under different operating conditions[89]. In addition, ML has been applied to optimize the performance of solid oxide electrolysers, for CO_2/H_2O reduction[90], and chloralkali electrolysers[91].

In the future, the use of ML for fuel cells could be combined with multiscale modelling to improve their design, for example to minimize Ohmic losses and optimize catalyst loading. For practical applications, fuel cells may be subject to fluctuations in energy output requirements (for example, when used in vehicles). ML models could be used to determine the effects of such fluctuations on the long-term durability and performance of fuel cells, similar to what has been done for predicting the state of health and lifetime for batteries. Furthermore, it remains to be seen whether the ML techniques for fuel cells can be easily generalized to electrolysers and vice versa, using transfer learning for example, given that they are essentially reactions in reverse.

Smart power grids

A power grid is responsible for delivering electrical energy from producers (such as power plants and solar farms) to consumers (such as homes and offices). However, energy fluctuations from intermittent renewable energy generators can render the grid vulnerable[92]. ML algorithms can be used to optimize the automatic generation control of power grids, which controls the power output of multiple generators in an energy system. For example, when a relaxed deep learning model was used as a unified timescale controller for the automatic generation control unit, the total operational cost was reduced by up to 80% compared with traditional heuristic control strategies[93] (FIG. 2d). A smart generation control strategy based on multi-agent reinforcement learning was found to improve the control performance by around 10% compared with other ML algorithms[94].

Accurate demand and load prediction can support decision-making operations in energy systems for proper load scheduling and power allocation. Multiple ML methods have been proposed to precisely predict the demand load: for example, long short-term memory was used to successfully and accurately predict hourly building load[95]. Short-term load forecasting of diverse customers (such as retail businesses) using a deep neural network and cross-building energy demand forecasting using a deep belief network have also been demonstrated effectively[96,97].

Demand-side management consists of a set of mechanisms that shape consumer electricity consumption by dynamically adjusting the price of electricity. These include reducing (peak shaving), increasing (load growth) and rescheduling (load shifting) the energy demand, which allows for flexible balancing of renewable electricity generation and load[98]. A reinforcement-learning-based algorithm resulted in substantial cost reduction for both the service provider and customer[99]. A decentralized learning-based residential demand scheduling technique successfully shifted up to 35% of the energy demand to periods of high wind availability, substantially saving power costs compared with the unscheduled energy demand scenario[100]. Load forecasting using a multi-agent approach integrates load prediction with reinforcement learning algorithms to shift energy usage (for example, to different electrical devices in a household) for its optimization[101]. This approach reduced peak usage by more than 30% and increased off-peak usage by 50%, reducing the cost and energy losses associated with energy storage.

Opportunities for ML in renewable energy

ML provides the opportunity to enable substantial further advances in different areas of the energy materials field, which share similar materials-related challenges (FIG. 3). There are also grand challenges for ML application in smart grid and policy optimization.

Materials with novel geometries

A ML representation is effective when it captures the inherent properties of the system (such as its physical symmetries) and can be utilized in downstream ancillary tasks, such as transfer learning to new predictive tasks, building new knowledge using visualization or attribution and

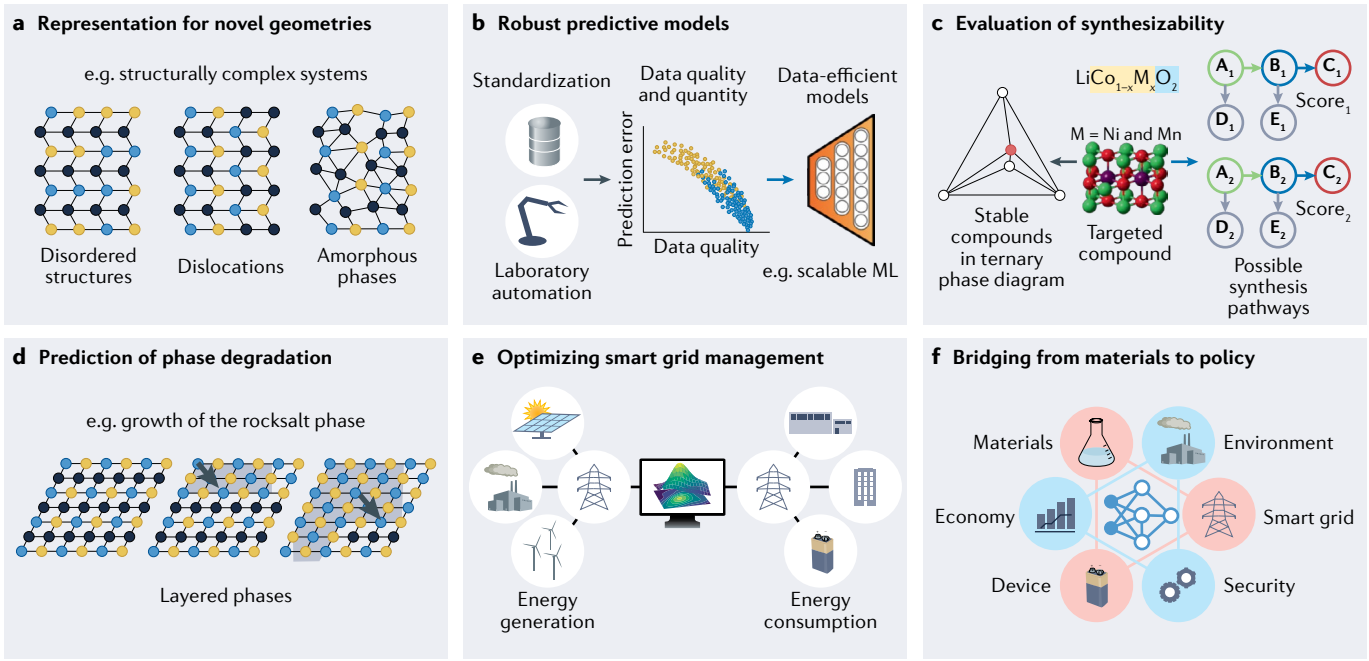

Fig. 3 | **Areas of opportunity for ML and renewable energy. a** | Energy materials present additional modelling challenges. Machine learning (ML) could help in the representation of structurally complex structures, which can include disordering, dislocations and amorphous phases. **b** | Flexible models that scale efficiently with varied dataset sizes are in demand, and ML could help to develop robust predictive models. The yellow dots stand for the addition of unreliable datasets that could harm the prediction accuracy of the ML model. **c** | Synthesis route prediction remains to be solved for the design of a novel material. In the ternary phase diagram, the dots stand for the stable compounds in that corresponding phase space and the red dot for the targeted compound. Two possible synthesis pathways are compared for a single compound. The score obtained would reflect the complexity, cost and so on of one synthesis pathway. **d** | ML-aided phase degradation prediction could boost the development of materials with enhanced cyclability. The shaded region represents the rocksalt phase, which grows inside the layered phase. The arrow marks the growth direction. **e** | The use of ML models could help in optimizing energy generation and energy consumption. Automating the decision-making processes associated with dynamic power supplies using ML will make the power distribution more efficient. **f** | Energy policy is the manner in which an entity (for example, a government) addresses its energy issues, including conversion, distribution and utilization, where ML could be used to optimize the corresponding economy.

generating similar data distributions with generative models[102].

For materials, the inputs are molecules or crystal structures whose physical properties are modelled by the Schrödinger equation. Designing a general representation of materials that reflects these properties is an ongoing research problem. For molecular systems, several representations have been used successfully, including fingerprints[103], SMILES[104], self-referencing embedded strings (SELFIES)[105] and graphs[106–108]. Representing crystalline materials has the added complexity of needing to incorporate periodicity in the representation. Methods like the smooth overlap of atomic positions[109], Voronoi tessellation[110,111], diffraction images[112], multi-perspective fingerprints[113] and graph-based algorithms[27,114] have been suggested, but typically lack the capability for structure reconstruction.

Complex structural systems found in energy materials present additional modelling challenges (FIG. 3a): a large number of atoms (such as in reticular frameworks or polymers), specific symmetries (such as in molecules with a particular space group and for reticular frameworks belonging to a certain topology), atomic disordering, partial occupancy, or amorphous phases (leading to an enormous combinatorial space), defects and dislocations (such as interfaces and grain boundaries) and low-dimensionality materials (as in nanoparticles). Reduction approximations alleviate the first issue (using, for example, RFcode for reticular framework representation)[8], but the remaining several problems warrant intensive future research efforts.

Self-supervised learning, which seeks to lever large amounts of synthetic labels and tasks to continue learning without experimental labels[115], multi-task learning[116], in which multiple material properties can be modelled jointly to exploit correlation structure between properties, and meta-learning[117], which looks at strategies that allow models to perform better in new datasets or in out-of-distribution data, all offer avenues to build better representations. On the modelling front, new advances in attention mechanisms[118,119], graph neural networks[120] and equivariant neural networks[121] expand our range of tools with which to model interactions and expected symmetries.

Robust predictive models

Predictive models are the first step when building a pipeline that seeks materials with desired properties. A key component for building these models is training data; more data will often translate into better-performing models, which in turn will translate into better accuracy in the prediction of new materials. Deep learning models tend to scale more favourably with dataset size than traditional ML approaches (such as random forests). Dataset quality is also essential. However, experiments are usually conducted under diverse conditions with large variation in untracked variables (FIG. 3b). Additionally, public datasets are more likely to suffer from publication bias, because negative results are less likely to be published even though they are just as important as positive results when training statistical models[122].

Glossary

Active learning
Machine learning techniques that can query a user interactively to modify its current strategy (that is, label an input).

Artificial intelligence
(AI). Theory and development of computer systems that exhibit intelligence.

Automatic generation control
A system for adjusting the power output of multiple generators at different power plants, in response to changes in the load.

Closed-loop approach
A technology development pipeline that incorporates automation to go from idea to realization of technology. 'Closed' refers to the concept that the system improves with experience and iterations.

Data augmentation
Process of increasing the amount of data through adding slightly modified copies or newly created synthetic data from existing data.

Deep belief network
A generative graphical model, or alternatively a class of deep neural network, composed of multiple layers of latent variables, with connections between the layers but not between units within each layer.

Deep learning
(DL). Machine learning subfield that is based on neural networks with representation learning.

Generalization
The ability to adapt to new, unseen data, drawn from the same distribution as the one used to create the model.

Generative learning
Machine learning techniques that learn to model the data distribution of a dataset and sample new data points.

Interpretability
Degree to which a human can understand a model's decision. Interpretability can be used to build trust and credibility.

Inverse design
A design method where new materials and compounds are 'reverse-engineered' simply by inputting a set of desired properties and characteristics and then using an optimization algorithm to generate a predicted solution.

Long short-term memory
A special kind of recurrent neural networks that are capable of selectively remembering patterns for a long duration of time.

Machine learning
(ML). Field within artificial intelligence that deals with learning algorithms, which improve automatically through experience (data).

Multi-agent system
A computerized system composed of multiple interacting intelligent agents.

Multi-kernel-ridge regression
The combination of ridge regression (a method of estimating the coefficients of multiple-regression models in scenarios where the independent variables are highly correlated) with multiple kernel techniques.

Multiphysics models
Models that involve the analysis of multiple, simultaneous physical phenomena, which can include heat transfer, fluid flow, deformation, electromagnetics, acoustics and mass transport.

Multiscale modelling
The field of solving problems that have important features at multiple scales of time and/or space.

Neural networks
A neural network is composed of parameterized and optimizable transformations.

Recurrent neural networks
A class of artificial neural networks where connections between nodes form a directed or undirected graph along a temporal sequence.

Regularization
Process of incorporating additional information into the model to constrain its solution space.

Reinforcement learning
Machine learning techniques that make a sequence of decisions to maximize a reward.

Representations
Features used in a representation learning model, which transforms inputs into new features for a task.

Retrosynthesis
Technique for solving problems in the planning of chemical synthesis.

Robotic workflows
A robotic equipment automated chemical synthesis plan.

Screening strategy
Design process composed of several stages where materials are iteratively filtered and ranked to arrive to a few top candidates.

Supervised learning
Machine learning techniques that involve the usage of labelled data.

Transfer learning
Machine learning techniques that adapt a learned representation or strategy from one dataset to another.

Uncertainty quantification
Process of evaluating the statistical confidence of model.

Unsupervised learning
Machine learning techniques that learn patterns from unlabelled data.

Addressing these issues require transparency and standardization of the experimental data reported in the literature. Text and natural language processing strategies could then be employed to extract data from the literature[77]. Data should be reported with the belief that it will eventually be consolidated in a database, such as the MatD3 database[123]. Autonomous laboratory techniques will help to address this issue[19,124]. Structured property databases such as the Materials Project[122] and the Harvard Clean Energy Project[125] can also provide a large amount of data. Additionally, different energy fields — energy storage, harvesting and conversion — should converge upon a standard and uniform way to report data. This standard should be continuously updated; as researchers continue to learn about the systems they are studying, conditions that were previously thought to be unimportant will become relevant.

New modelling approaches that work in low-data regimes, such as data-efficient models, dataset-building strategies (active sampling)[126] and data-augmentation techniques, are also important[127]. Uncertainty quantification, data efficiency, interpretability and regularization are important considerations that improve the robustness of ML models. These considerations relate to the notion of generalizability: predictions should generalize to a new class of materials that is out of the distribution of the original dataset. Researchers can attempt to model how far away new data points are from the training set[128] or the variability in predicted labels with uncertainty quantification[129]. Neural networks are a flexible model class, and often models can be underspecified[130]. Incorporating regularization, inductive biases or priors can boost the credibility of a model. Another way to create trustable models could be to enhance the interpretability of ML algorithms by deriving feature relevance and scoring their importance[131]. This strategy could help to identify potential chemically meaningful features and form a starting point for understanding latent factors that dominate material properties. These techniques can also identify the presence of model bias and overfitting, as well as improving generalization and performance[132–134].

Stable and synthesizable new materials

The formation energy of a compound is used to estimate its stability and synthesizability[135,136]. Although negative values usually correspond to stable or synthesizable compounds, slightly positive formation energies below a limit lead to metastable phases with unclear synthesizability[137,138]. This is more apparent when investigating unexplored chemical spaces with undetermined equilibrium ground states; yet often the metastable

phases exhibit superior properties, as seen in photovoltaics[136,139] and ion conductors[140], for example. It is thus of interest to develop a method to evaluate the synthesizability of metastable phases (FIG. 3c). Instead of estimating the probability that a particular phase can be synthesized, one can instead evaluate its synthetic complexity using ML. In organic chemistry, synthesis complexity is evaluated according to the accessibility of the phases' synthesis route[141] or precedent reaction knowledge[142]. Similar methodologies can be applied to the inorganic field with the ongoing design of automated synthesis-planning algorithms for inorganic materials[143,144].

Synthesis and evaluation of a new material alone does not ensure that material will make it to market; material stability is a crucial property that takes a long time to evaluate. Degradation is a generally complex process that occurs through the loss of active matter or growth of inactive phases (such as the rocksalt phases formed in layered Li-ion battery electrodes[145] (FIG. 3d) or the Pt particle agglomeration in fuel cells[146]) and/or propagation of defects (such as cracks in cycled battery electrode[147]). Microscopies such as electron microscopy[148] and simulations such as continuum mechanics modelling[149] are often used to investigate growth and propagation dynamics (that is, phase boundary and defect surface movements versus time). However, these techniques are usually expensive and do not allow rapid degradation prediction. Deep learning techniques such as convolutional neural networks and recurrent neural networks may be able to predict the phase boundary and/or defect pattern evolution under certain conditions after proper training[150]. Similar models can then be built to understand multiple degradation phenomena and aid the design of materials with improved cycle life.

Optimized smart power grids

A promising prospect of ML in smart grids is automating the decision-making processes that are associated with dynamic power supplies to distribute power most efficiently (FIG. 3e). Practical deployment of ML technologies into physical systems remains difficult because of data scarcity and the risk-averse mindset of policymakers. The collection of and access to large amounts of diverse data is challenging owing to high cost, long delays and concerns over compliance and security[151]. For instance, to capture the variation of renewable resources owing to peak or off-peak and seasonal attributes, long-term data collections are implemented for periods of 24 hours to several years[152]. Furthermore, although ML algorithms are ideally supposed to account for all uncertainties and unpredictable situations in energy systems, the risk-adverse mindset in the energy management industry means that implementation still relies on human decision-making[153].

An ML-based framework that involves a digital twin of the physical system can address these problems[154,155]. The digital twin represents the digitalized cyber models of the physical system and can be constructed from physical laws and/or ML models trained using data sampled from the physical system. This approach aims to accurately simulate the dynamics of the physical system, enabling relatively fast generation of large amounts of high-quality synthetic data at low cost. Notably, because ML model training and validation is performed on the digital twin, there is no risk to the actual physical system. Based on the prediction results, suitable actions can be suggested and then implemented in the physical system to ensure stability and/or improve system operation.

Policy optimization

Finally, research is generally focused on one narrow aspect of a larger problem; we argue that energy research needs a more integrated approach[156] (FIG. 3f). Energy policy is the manner in which an entity, such as the government, addresses its energy issues, including conversion, distribution and utilization. ML has been used in the fields of energy economics finance for performance diagnostics (such as for oil wells), energy generation (such as wind power) and consumption (such as power load) forecasts and system lifespan (such as battery cell life) and failure (such as grid outage) prediction[157]. They have also been used for energy policy analysis and evaluation (for example, for estimating energy savings). A natural extension of ML models is to use them for policy optimization[158,159], a concept that has not yet seen widespread use. We posit that the best energy policies — including the deployment of the newly discovered materials — can be improved and augmented with ML and should be discussed in research reporting accelerated energy technology platforms.

Conclusions

To summarize, ML has the potential to enable breakthroughs in the development and deployment of sustainable energy techniques. There have been remarkable achievements in many areas of energy technology, from materials design and device management to system deployment. ML is particularly well suited to discovering new materials, and researchers in the field are expecting ML to bring up new materials that may revolutionize the energy industry. The field is still nascent, but there is conclusive evidence that ML is at least able to expose the same trends that human researchers have noticed over decades of research. The ML field itself is still seeing rapid development, with new methodologies being reported daily. It will take time to develop and adopt these methodologies to solve specific problems in materials science. We believe that for ML to truly accelerate the deployment of sustainable energy, it should be deployed as a tool, similar to a synthesis procedure, characterization equipment or control apparatus. Researchers using ML to accelerate energy technology discovery should judge the success of the method primarily on the advances it enables. To this end, we have proposed the XPIs and some areas in which we hope to see ML deployed.

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