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Machine learning for a sustainable energy future

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Energy production is one of the key enablers for human activities such as food and clean water production, transportation, telecommunication, education, and healthcare; however, it is also the main cause of global warming. Hence, sustainable energy is critical for most United Nations (UN) Sustainable Development Goals (SDGs), and it is directly targeted in SDG7. In this review, we analyze the potential role of machine learning (ML), another enabler technology, in sustainable energy and SGDs. We review the use of ML in energy production and storage as well as in energy forecasting and planning activities and provide our perspective on the challenges and opportunities for the future role of ML. Although there are strong challenges for both sustainable energy supply (like conflict between the urgent energy needs and global warming) and ML applications (like high energy consumption in ML applications and risk of increasing inequalities among people and nations), ML may make significant contributions to sustainable energy efforts and therefore to the achievement of SDGs through monitoring and remote sensing to collect data, planning the worldwide efforts and improving the performance of new and more sustainable energy technologies.

1. Introduction

The UN Member States adopted "The 2030 Agenda for Sustainable Development" in 2015 to offer a shared vision for peace and prosperity for all member countries in the future. The 17 Sustainable Development Goals (SDGs) cover the basic human needs/rights from ending poverty and deprivation to improving health and education and reducing inequality in the entire planet, provide specific action plans through 169 targets for all countries in a global partnership while they also constitute the criteria to measure the progress.[1] Among 17 SDGs, "Affordable and Clean Energy" (SDG 7) and "Climate Action" (SDG 13) stand out as crucial goals in addressing both energy accessibility and climate change.

Global energy consumption has increased dramatically in response to industrialization, urbanization, and modernization; the world's gross electricity generation has increased from 9754 TW h in 1985 to 29 479 TW h in 2023 (multiplied by a factor of 3.02). However, the majority of world energy is still supplied by fossil fuels. As of 2023, renewable energy sources

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have a share of 30.2% in the mix of global electricity generation, and without hydropower, this corresponds to only 16.0%;[2] only 4% of transportation fuels are from renewable energy.[3,4] Fossil combustion also emits around 27 billion tons of CO_2 annually, causing global climate change, and emissions are expected to increase by 60% in 2030.[5] Global energy consumption is expected to increase by 50% by 2050, with renewables accounting for only 25% of the total.

Recent international efforts, such as the COP 28 summit, aim to accelerate the transition to clean energy, with a goal of tripling renewable energy capacity to 11 000 GW by 2030.[6] Even though the efforts to increase the share of cleaner energy technologies, like solar, wind, and biofuels in the energy mix, have increased significantly in recent years, there seems to be a long way to go to reach the desired stage. While solar and wind energy are gaining interest, they are unlikely to meet future energy demands alone.[7] Biomass should also be considered as a carbon-neutral alternative;[8] it especially plays a key role in developing nations, where it accounts for 38% of energy consumption,[9] primarily for cooking and heating.[10]

Renewable energy is critical for SDGs, particularly SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action).[11] While target 7.1 under SDG7 requires ensuring universal access to energy services, target 7.2 directly states the need for renewable energy (increase substantially the share of renewable energy in the global mix), which goes together with energy efficiency covered in target 7.3 (double the global rate of improvement in energy efficiency) for a sustainable energy future. Energy production rate, conversion technology used and resources utilized may also have impacts on various other SDGs as energy is one of the main enablers for various essential human activities like food and clean water production, transportation, telecommunication, education, and healthcare. Indeed, Nerini *et al.* stated in their perspective article that 113 targets (out of 169) require a change in the energy system.[12]

Although the SDGs and AI/ML seem to be unrelated at first glance, various works indicate the potential role of ML in reaching SDGs. To begin with, monitoring, data collection, and analysis of SDG-related activities at the global level, including implementation projects, will be much easier with AI/ML.[13] Second, AI/ML can be used for supply/demand forecasting for goods and energy and improving the effectiveness of planning and executing the efforts to provide these resources to the communities in need. Finally, ML has been used extensively in research and development, including in the fields related to SDGs, such as renewable energy technologies and storage systems.

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Our research groups have been collaborating on ML applications in the research of renewable energy technologies such as solar cells,[14–16] photocatalytic hydrogen production, CO_2 reduction,[17,18] algal biofuels[19,20] and oleaginous yeast,[21] lignocellulosic ethanol, biogas, and biochar production.[22–24] We also have a significant amount of ML works in supply/demand and capacity estimation of renewable energy as well as beyond Li-ion batteries for future energy storage needs,[25–28] which is also critical for achieving SDGs; there is a strong need for distributed energy storage coupled with solar and wind energy production in underdeveloped regions of the world, where the central energy supply may not be practical in the near future. In this feature article, we have reviewed the works published in the literature (including ours) and provided our perspective on the potential contribution of ML to the achievement of SDGs through renewable energy processes. To do that, first we have analyzed the relationships between SDGs, renewable energy, and ML. Then, we have reviewed ML applications in solar, wind, and bioenergy technologies from the SDGs' perspective, considering that they are the most commonly researched/investigated renewable energy technologies in recent years. Finally, we have reviewed ML applications in rechargeable batteries and discussed their relationship with SDGs.

2. Basic concepts and critical linkages

2.1. Machine learning basics

ML is the subfield of artificial intelligence that aims to learn from past data (or other similar events) using statistics and some algorithms (Fig. 1).[23] One can perform various functions (like clustering, classification, prediction, or association) by constructing a dataset and selecting appropriate algorithms for the purpose. For example, *k*-means clustering is one of the most common clustering algorithms, while algorithms such as *k*-means distribution, decision trees (DTs), artificial neural networks (ANNs), and support vector machines (SVMs) are used for classification. The prediction task can be considered as one of the most frequently performed ML tasks. It can be done using various algorithms such as ANNs, SVMs, random forest (RF), and gradient boosting.[29] In addition to the basic functions and algorithms summarized above, some more recent and effective tools like deep learning algorithms, transfer learning approach, physics-informed ML, and large language models have been developed in recent years.

A typical workflow for ML applications is presented in Fig. 2. In the dataset construction step, the data correlating descriptors (input variables) and desired performance variables (or outcome) can be collected from various sources. The pre-processing step

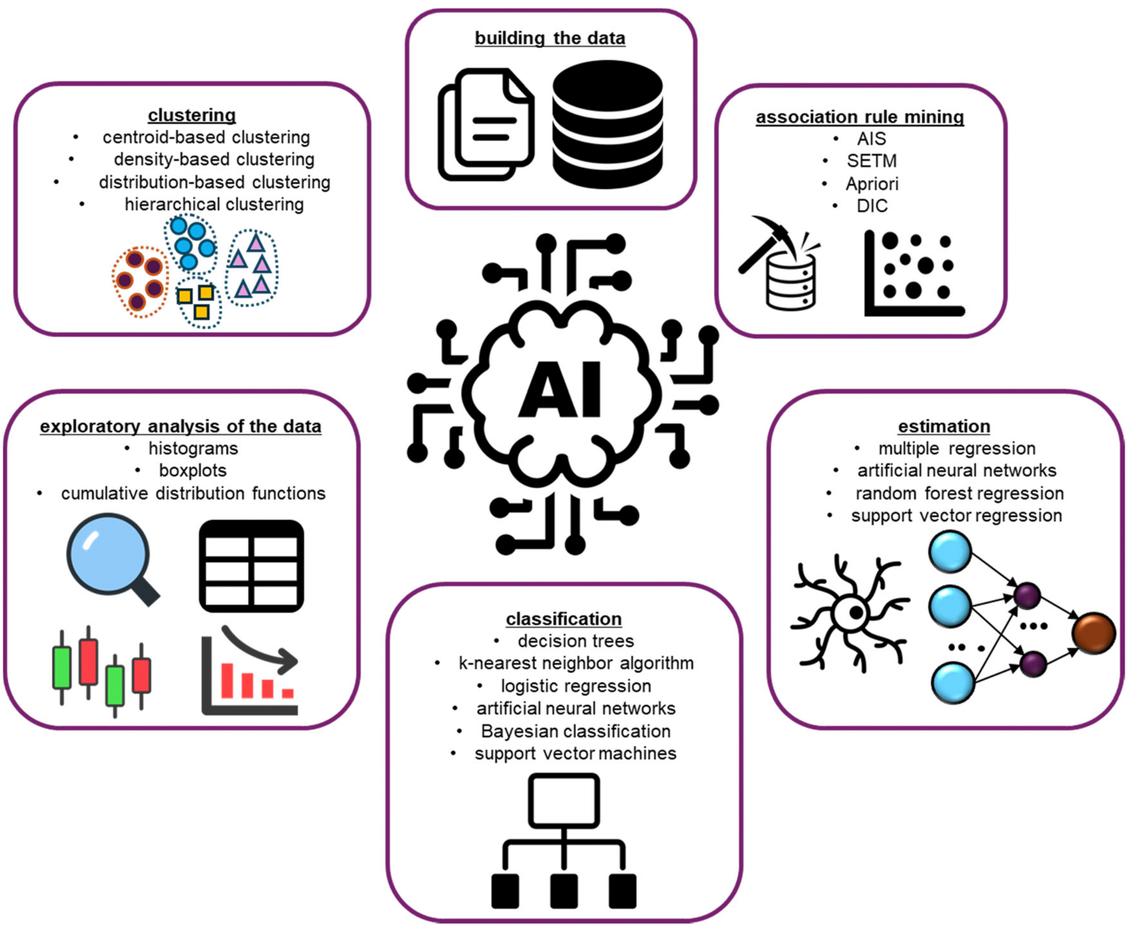

Fig. 1 ML tasks and their popular algorithms (reproduced with permission from Springer, Copyright© 2024).[23]

aims to prepare the data for analysis; the data are formatted in a machine-readable format, while the incomplete data points have to be completed or removed from the dataset. The potential descriptors should also be analyzed in terms of cross-correlations and redundancy, and their numbers should be reduced as much as possible (dimensionality reduction) as a smaller model for a given dataset is more robust.[30] For this, the insignificant descriptors can be eliminated (feature selection), and/or a new set of descriptors (like principal components) can be created to replace the original set (feature extraction).[31]

The model development step starts with the selection of appropriate algorithms, which is highly dependent on the objective of analysis and the structure of data. Then, the model is developed by dividing the dataset as training (to construct the model) and testing (verification of model performance on unseen data); often, k-fold cross-validation is implemented for model building (*i.e.*, to determine the optimal model hyper-parameters). Then, the model is tested using the testing data to determine its generalization ability.[29]

2.2. Machine learning for SDGs

The contribution of ML or artificial intelligence (AI) in general to SDGs can be analyzed at three levels. First, ML can contribute to the planning and execution of SDGs directly. As we will summarize below, there are strong correlations among various SDGs, and the actions needed to achieve most of the goals have to be planned and implemented by multi-organizational structures over multi-national geography. Hence, effective coordination of efforts is critical for success, requiring effective monitoring of activities, collecting relevant data, and making timely and effective decisions. The data needed are likely to be large and complex due to the diversity of issues and the size of populations and geography involved, and such complex data can only be collected using some automated systems and analyzed using effective tools like ML. For instance, remote sensing technologies can be used to monitor and collect data for climate, agriculture and fishing, clean water resources, pollution of rivers, and mass migrations of humans;[32] then the data collected can be analyzed using ML technologies to assess the current state and develop an effective action plan for related SDGs.

Indeed, a significant number of works have been published in SDG-related areas, such as the use of satellite images and ML or *meta*-analysis of mobile phones[33] to predict poverty, for remote sensing of agricultural activities,[34] and for monitoring inland water quality.[35] Various organizations like the UN Department of Economic and Social Affairs,[36] the Food and Agricultural Organization,[37] the European Space Agency Earth Observation for Sustainable Development,[38] and the Committee on Earth Observation Satellites[39] also provide data that can be used for the efforts to reach the targets of SDGs. For instance, Porciello *et al.*[40] argued that ML can be used to speed up evidence synthesis, which can be defined as the process of collecting/data information from different sources for decision-making in a specific area, to support SDGs and reporting a model for SDG2 (zero hunger).[41]

Second, ML may directly contribute to the efforts to reach some of the specific goals and targets. Vinuesa *et al.* have analyzed the relationship between AI and SDGs using a consensus-based expert elicitation process.[42] They considered a software technology as AI if it has at least one of the following capabilities: perception, decision-making, prediction, automated knowledge extraction and pattern recognition, interactive communication, and logical reasoning.[42] They found that AI can enable 134 targets across all SDGs while, interestingly, it can inversely affect 59 targets. AI may contribute to the building of smart and low-carbon cities through the range of interconnected technologies, including autonomous vehicles and smart appliances; however, large computing facilities required for AI/ML have significant energy consumption and carbon footprint.[43] Nevertheless, the potential contribution of AI to the well-being of humanity (including achieving SDGs) will still be well beyond its inverse effects, even though some extra care should be needed in practical applications.

ML may also be used for specific tasks involving SDG 7 (Affordable and Clean Energy) and SDG 13 (Climate Action), which are directly related to sustainable energy efforts. Forecasting renewable energy supply, optimizing the smart control/scheduling of energy systems, and accurately modeling emissions are just a few areas where ML can make significant contributions. As we will extensively discuss the ML applications in specific energy technologies in the following sections, we will restrict ourselves to a few cases that are specific to SDG 7 and SDG 13. For example, Marcillo-Delgado *et al.*[44] reported a case study that used compositional analyses of the electricity access problems for the most affected areas in the context of SDG7, while Matenga[45] used an ordinal k-means clustering algorithm to analyze the degree of closeness of an energy market to achieve SDG 7. Similarly, Li *et al.*[46] analyzed the

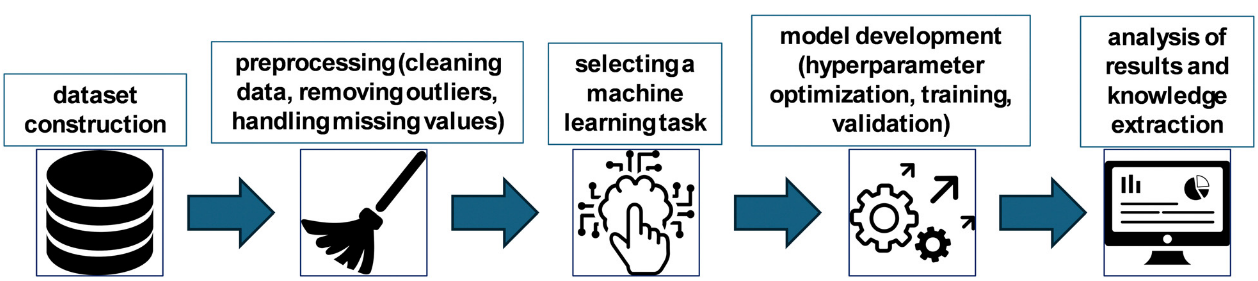

Fig. 2 A typical workflow for machine learning analysis.

energy deprivation for socially disadvantaged groups in India within the SDG7 framework using machine learning. There have also been published cases involving SDG13. For example, Lei *et al.*[47] reported an ML model for the prediction of air pollution in Macau, China, as an effort to meet SDGs, whereas Hwang *et al.*[48] used text mining analysis to determine climate change awareness and its relationship to SDG13 among various social groups.

Finally, ML is frequently used in the development of new technologies that will enable SDGs. As we will briefly discuss below, most of the new renewable energy technologies, especially solar cells and biofuels, both of which are critical for a sustainable future, have benefited ML for a long time. For example, ML has been used in numerous research steps, from material screening to performance tests and stability studies of perovskite solar cells,[16] which have been among the most popular research topics in recent years due to their great potential. Advances in computational power have facilitated the development of new materials *via* high throughput screening, computational chemistry, and physics-based modeling.[49] The creation of extensive experimental and computational databases, such as ICSD,[50] Materials Project,[51] and NOMAD,[52] has accelerated material property prediction and screening. These databases, together with DFT calculations, provide a foundation for material research focused on renewable energy systems. Physics-based models reduce the need for large datasets and enhance prediction accuracy by embedding fundamental physical principles, making them highly effective for material screening. For instance, Li *et al.*[53] developed a transfer learning approach to evaluate the stability of ABX3 inorganic perovskites as oxygen reduction electrocatalysts in solid oxide fuel cells. Their physics-informed model used structural and elemental parameters to predict formation energies, training on a dataset of 570 known compounds. It was then applied to forecast formation energies for 578 additional unknown compounds. In this way, 1148 data points were assembled to train a convolutional neural network for high-throughput screening. They found 98 stable perovskite structures, which were verified by DFT calculations. Jyothirmai *et al.*[54] investigated single-atom metal and nonmetal catalysts for pairing with g-C_3N_4 to enhance hydrogen generation efficiency, evaluating various ML algorithms for predicting the Gibbs free energy of hydrogen adsorption. In another study, Burns *et al.*[55] screened metal–organic frameworks (MOF) for CO_2 capture, and to support efficient screening, they developed ML models using standard adsorption metrics to predict MOF performance under specific purity and recovery requirements. Numerous reviews explore the applications of ML in material screening for sustainability purposes,[56] with a focus on specific clean energy domains like battery materials,[57] hydrogen generation photocatalysis,[58] and solar cell materials.[59]

ML may also have enormous impacts on other SDG-related technologies ranging from health and pharmaceuticals to new material design and manufacturing and environmental remediation. We can generalize this further by including the use of ML in monitoring, control, and optimization of chemical processes and plants as an indirect way of ML contribution to SDGs. Indeed, most of such efforts are to improve the efficiency of the processes to consume less energy and raw materials and to reduce emissions and waste; the energy and materials saved after these efforts can be redirected to contribute to the projects for SDGs while the reduced emissions may allow the use of fossil fuels over a longer period in less fortunate parts of the world if it is necessary. Table 1 provides the pros and cons of common ML algorithms in the field of renewable energy, with a more extensive list available elsewhere.[60]

2.3. Renewable energy for SDGs

The use of renewable energy technologies and improving energy efficiency are the basic ingredients of sustainable energy as both are among the targets of SDG 7; target 7.2 requires substantially increasing the share of renewable energy in the global energy mix, and target 7.3 aims to double the global rate of improvement in energy efficiency. The link between energy

Table 1 Most frequently employed ML techniques in the renewable energy field

Method	Advantages	Disadvantages	Tasks
Apriori algorithm	Simple and easy to implement	May require significant time and memory	Association rule mining
Centroid based clustering	Easy and quick to use, helpful for exploring and segmenting data	Needs a set number of clusters in advance and can be affected by starting conditions	Clustering
Hierarchical clustering	Effectively manages large datasets	Sensitive to outliers and computationally costly	Clustering
Logistic regression	Easy to interpret and effective with small datasets	Assumes linear relationships and is limited to classification tasks	Classification
Decision trees	Interpretable, both continuous and categorical data can be used	Can go to overfitting	Classification
Linear regression	Easy to apply, quick training	Can be used only for linear relationship	Estimation
Random forests	High accuracy, less likely for overfitting	Computationally more costly than decision trees and challenging to interpret	Estimation, classification
Support vector machines	Capable of handling high-dimensional data and non-linear relationships, with strong robustness to noise	Computationally costly and requires careful parameter tuning	Estimation, classification
Artificial neural networks	Can capture complex patterns, work with large datasets, and model non-linear relationships	Requires large data and can be challenging to interpret	Estimation, classification

and SDGs has been investigated by various investigators.[12,61,62] For example, the International Council for Science published a guide for the interactions among SDGs: the four SDGs, SDG 2 (zero hunger), SDG 3 (good health), SDG 7 (clean energy), and SDG 14 (life below water), were found to be in synergetic interactions with other SDGs. The council identified 316 target-level interactions (238 positive, 66 negative, and 12 neutral). Although no basic incompatibility among the SDGs was observed, some potential constraints and conditionalities were identified, indicating a need for coordination, management, and appropriate intervention to protect vulnerable groups, promote equity, and manage the demands for natural resources to balance economic and social development with environmental concerns. For example, the chapter of the report devoted to SDG7 stated that distributed renewable (solar and biogas) energy may make a significant contribution to the development of rural communities while the centralized infrastructure (even if they are also possible) may increase the cost of energy. It also stated in the report that the energy efficiency target may be considered a 'win–win' strategy as the amount of energy to be saved is equivalent to the amount of energy that does not need to be produced.

Nerini *et al.* also reported a work that analyzed interactions specifically between energy and SDGs, and mapped synergies and trade-offs using a consensus-based expert elicitation process in their perspective article.[12] They identified 113 targets, including target 13.2 (involving climate change) and target 3.9 (involving reducing deaths from pollution), that require changes in the energy system. They also found evidence showing synergetic interactions between 143 targets and SDG7, while there were also 43 trade-offs. As affordable, reliable, and sustainable energy is critical for most of the activities to ensure human well-being, which is the ultimate goal of SDGs, energy synergistically interacts with various SDGs and targets such as raising living standards through the provision of basic services, including healthcare, education, water, and sanitation (SDG2–4, 6–7, 9), improved household incomes (SDG8), and resilient rural and urban livelihoods (SDG1, 11). On the other hand, they stated that almost all trade-offs arise from the tension between the urgent action required for human well-being (ending poverty, providing clean water, food, and energy) and the careful planning for the efforts to integrate renewable energy production and energy efficiency.

Finally, we performed a keyword search using the keywords of sustainable development goal(s) in the "Energy fuels" category in the Web of Science (WOS) Database between the years 2014 and 2024 with the words resulting in 123 articles. Then, a keyword co-occurrence analysis (Fig. 3) was performed using VOSviewer (version 1.6.20) to observe the most frequently used keywords and the associations between each of them.[63] In the figure, larger nodes and labels indicate a higher frequency of keywords, whereas wider and closer connections between nodes suggest a closer relationship between two keywords or phrases.[64] The co-occurrence plot shows that SDGs are strongly associated with concepts like environment, climate change and CO_2 emissions as well as the energy transitions; the apparences of the biomass and bioenergy in plot the are especially important for the SDGs efforts in developing countries as the biomass is a domestic and generally abundant source while the biofuels are quite suitable to substitute fossil fuels in transportation without significant investment in vehicles and fuel distribution network.

3. Machine learning for energy supply/demand estimation

ML has been used for the effective planning and managing of regional and national energy systems for many years, including energy forecasting, capacity estimation for renewable energy (like solar or wind energy capacity of regions), optimization, fault detection, and stability in energy grids, managing battery systems, and energy trading.[61] Among all these functions, supply/demand forecasting is quite critical for SDGs; it is an indispensable task for the management of regional or national energy supply systems (distributed or central) to be effective. As a first step, the variables influencing energy consumption must be correctly identified to predict future consumption in a given country.[65] One of the key factors that influence the energy consumption of a country is its population as the energy consumption grows with increasing population. This trend can also be observed for the entire world, as shown in Fig. 4. The global population has increased from 4.84 billion in 1985 to 8.02 billion in 2023 (multiplied by a factor of 1.65) (Fig. 4a). During the same period, global gross electricity generation has increased even more from 9754 TW h in 1985 to 29 479 TW h in 2023 (multiplied by a factor of 3.02) (Fig. 4b).

Another important factor influencing energy consumption is the wealth of the people living in a country as measured by the gross domestic product per capita (GDP per capita), which may also be observed through improvements in the lifestyle of individuals like an increase in the number of electric equipment and computers owned, an increase in the number of vehicles used, and heating and cooling devices used to make the living spaces more comfortable.[67,68] Additionally, employment and inflation rates in a country are two other socio-economic factors that can affect energy consumption.[69] In the case of high unemployment and high inflation rates, consumers tend to reduce their expenses until they become economically better.[67] Finally, the variables related to climate, such as temperature, sunshine hours, humidity, precipitation, and wind speed, have all been shown to influence energy consumption by affecting heating and cooling needs.[70]

Today, the majority of world energy is still supplied by fossil fuels, as shown in Fig. 4b. As of 2023, renewable energy sources have a share of 30.2% in the mix of global electricity generation, and without hydropower, this corresponds to only 16.0%. In the case of underdeveloped countries, the total share of renewable energy is much lower, even though the population in these countries grows faster.[71] Unfortunately, fossil fuel sources are concentrated in a few countries in the world, resulting in foreign dependency in many countries.[67] Predicting how much energy these countries will use in the future is a very important

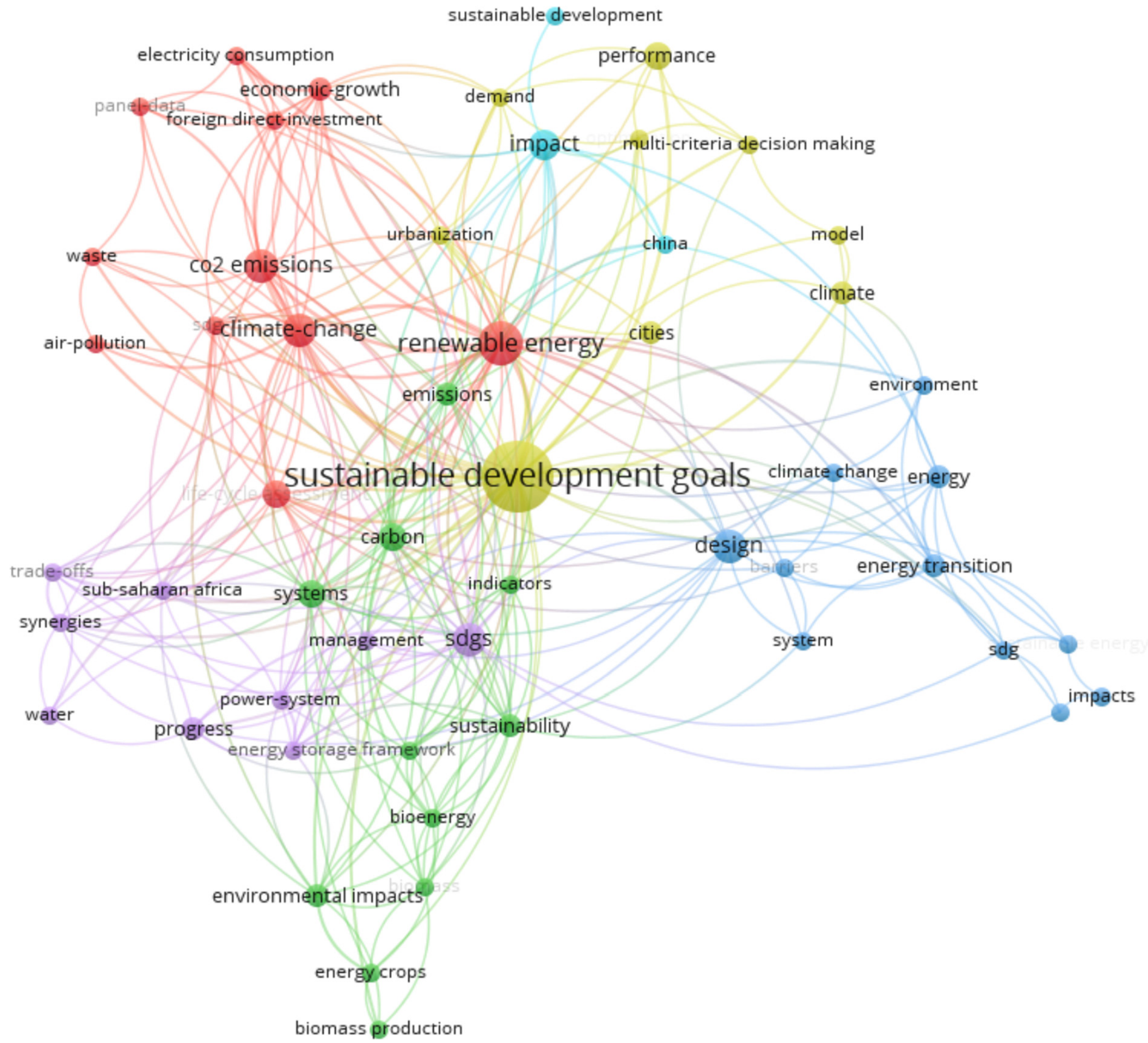

Fig. 3 Co-occurrence analysis for SDGs and energy/fuels between the years 2014 and 2024. Keywords that appear more than two times are displayed.

task in making new deals with exporting countries and creating long-lasting energy policies and smart strategies like developing renewable and sustainable energy programs.[44]

Energy consumption is usually forecasted in three time periods: short-term (a few hours to a few days), medium-term (a few weeks to a few months), and long-term (a few months to years),[72] and the number of publications on forecasting energy consumption over these horizons has increased significantly as reviewed recently.[73] Forecasting techniques are classified into two categories: conventional statistical methods (such as trend analysis, end-use analysis, and econometric approaches) and ML-based methods (such as fuzzy logic, ANNs, and SVMs), as explained elsewhere.[74] To forecast future energy consumption, the researchers apply a wide range of methodologies, such as multiple linear and nonlinear regression,[67,75] autoregressive integrated moving averages,[76–79] adaptive-network-based fuzzy inference systems,[80] multivariate adaptive regression splines,[76] and ML-based approaches like ANNs[80–88] and SVMs.[76,78,88]

The literature has expanded in recent years due to the emergence of deep learning techniques. For instance, Liu *et al.* developed a strategy to forecast energy consumption in buildings using deep reinforcement learning techniques.[89] In another example, a deep learning model was developed to estimate the generation of renewable energy and the demand for electricity in South Korea.[90] On the other hand, Lima *et al.* combined deep learning and portfolio theory to predict solar energy generation, and the strategy was compared to other significant methods in the literature, such as support vector regression and ANNs.[91]

Another area in which ML can contribute is the integration of various renewable energy technologies to create an efficient grid. Although most of the energy of the world still comes from fossil fuels, the use of renewable energy systems has been increasing, continuously affecting the stability of grid operations due to the fluctuations in their energy output. Wind turbines operate only when there is wind, whereas solar panels generate electricity only when exposed to sunshine, and this variation is a fundamental challenge for integrating renewable energy into the grid system. ML can come into the picture at

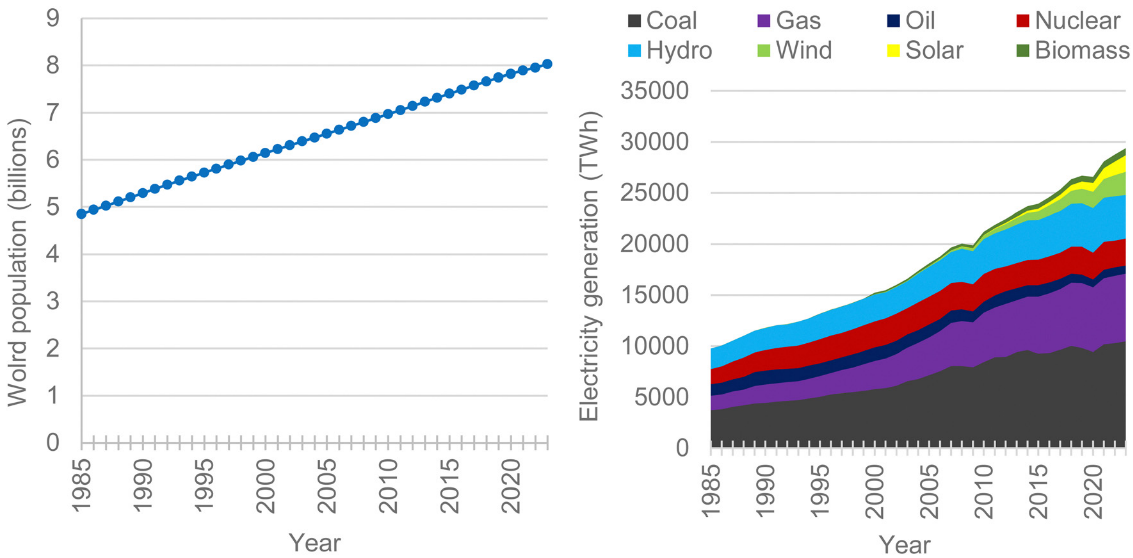

Fig. 4 Historical data for (a) the growth of world population[66] and (b) global electricity generation.[2]

this point to analyze the climatic patterns and predict electricity generation using renewable energy to balance demand and consumption.[92] Likewise, ML methodologies (such as nested learning) can be used to improve real-time power consumption monitoring and energy storage planning in order to maintain a balance between demand and supply.[93] Indeed, a recently published review paper examined various computational methods for reducing the impact of renewable energy sources on power system frequency.[94]

When a bibliometric analysis is done on the published articles, the recent trends in energy forecasting can be seen better. For this purpose, the "Energy fuels" category under the Web of Science Database was searched for the years between 2014 and 2024 with the words in the title: "energy forecast" or "energy prediction" or "energy estimation" or "electricity forecast" or "electricity prediction" or "electricity estimation", resulting in 2142 articles. The co-occurrence networks, which show the connections between keywords and their frequency of appearance together in publications, are given in Fig. 5a, where keywords that appear more than 25 times are displayed under different clusters. Additionally, in Fig. 5b, the keyword "machine learning" is centered, and its associations are exposed. It is shown that demand and consumption are the most frequent keywords associated with the target variables, whereas ANNs, deep learning, support vector regression, and classification are the most frequently used keywords associated with the methodological pathway for ML.

4. Solar energy

Solar energy, with its vast potential and growing technological advancements, may play a pivotal role in advancing SDGs. It can be used for water or space heating, electricity production, desalination of seawater, as well as water splitting and CO_2 reduction solar fuels.[95] Water heating is already quite common and can be easily spread on wider area while the technologies for water splitting and CO_2 reduction are not matured yet; the biggest contribution to SDGs will likely come from solar electricity and desalination.

4.1. Solar power generation

4.1.1. Solar power generation technologies. Solar electricity can be produced using concentrated solar power (CSP) plants or photovoltaic (PV) systems. In CSP plants, solar radiation is concentrated in a smaller area of absorbers to collect thermal energy to produce pressurized vapor and run a turbine for electricity production. There are various forms of thermal solar technologies that are usually distinct from the geometrical structures (such as parabolic troughs, solar towers, and solar dishes) used to concentrate solar.[96] The PV systems, on the other hand, directly convert solar radiation to electricity using some semiconducting materials. PV systems are also quite diverse, including single/multi-crystalline silicon, thin film, organic/polymeric, dye-sensitized, and perovskite solar cells.[97]

Although thermal technologies may also have a significant contribution to world electricity production, they may not be suitable to meet the targets of SDG7, especially in developing regions of the world, where small-scale distributed power generation will likely be more suitable, because they have to be built and operated on a large scale with high cost and administrative difficulties. In contrast, PV solar systems can be produced and installed for any size of application, like a water pump, an elementary school, a hospital, or an entire town. Single/multi-crystal silicon solar cells (first generation) are the dominant design in today's industry due to their efficiency and long-term durability. However, in recent decades, new solar cells have emerged, offering new materials and technologies to improve efficiency, reduce costs, and expand the possibilities of solar energy applications. Thin film solar cells (including the use of silicon as a thin film), dye-sensitized solar cells, organic solar cells, and perovskite solar cells, which

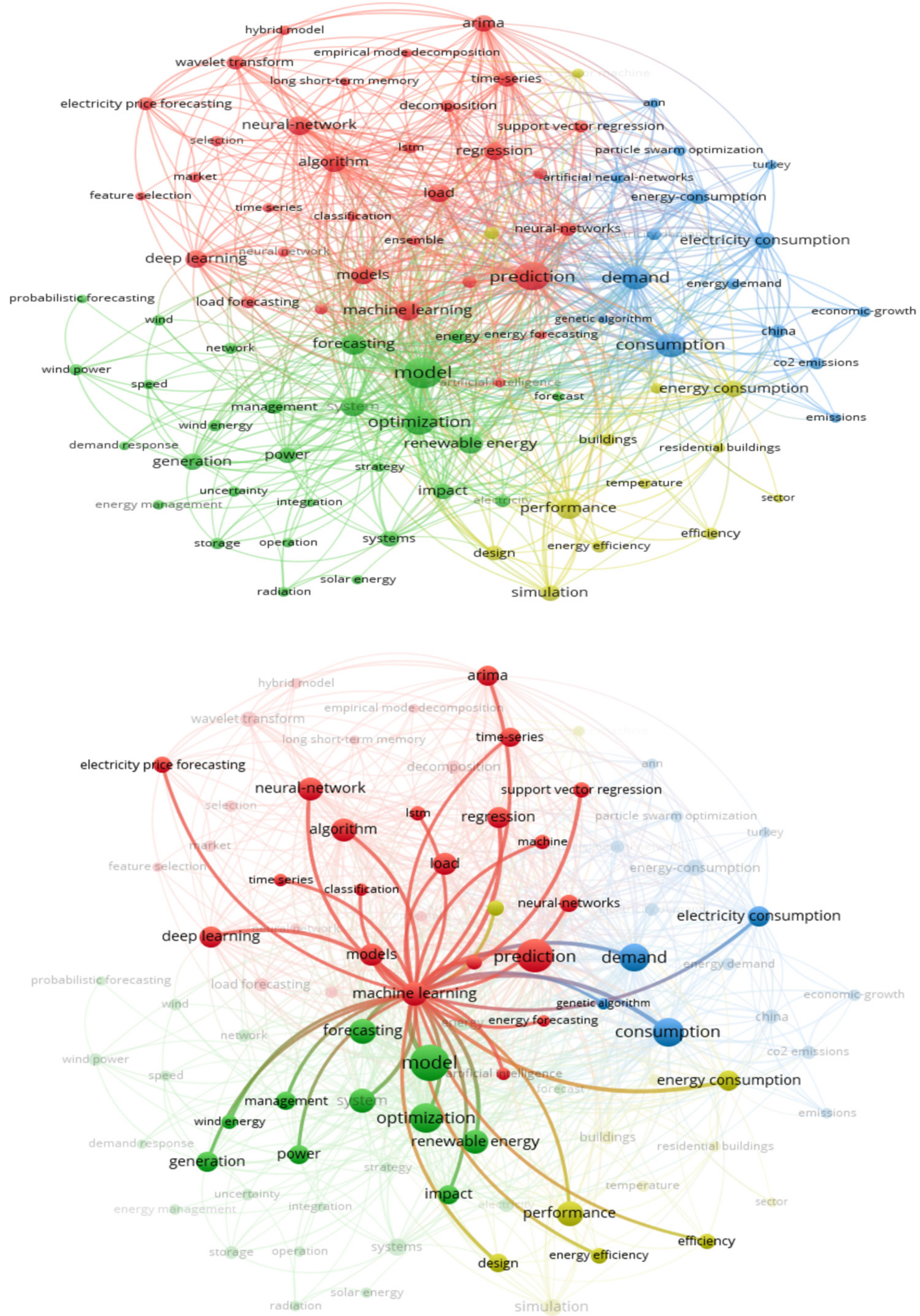

Fig. 5 Co-occurrence analysis for energy/fuels between the years 2014 and 2024: (a) co-occurrence analysis for energy forecasting and (b) co-occurrence analysis for ML use in forecasting.

use innovative materials to generate electricity more efficiently, are among the alternatives that have been investigated in recent years as reviewed by various investigators.[98,99]

The growth of solar energy use, especially for electricity production, is impressive. While the total electricity generation was only 1.2 GW in the year 2000, it reached 1418 GW in the year 2023, as shown in Fig. 6a. Moreover, the total annual electricity generation was found to be 1630 TW h (corresponding to a share of 5.5% in the total global electricity generation mix) in 2023, as indicated in Fig. 6b. Although the African continent receives a significant amount of solar irradiation, the share of solar power generation is much lower than that of the other regions.

4.1.2. ML applications in solar power generation. As solar energy technologies advance, ML may help in overcoming critical challenges related to efficiency, cost, and scalability. ML accelerates the development and deployment of solar energy

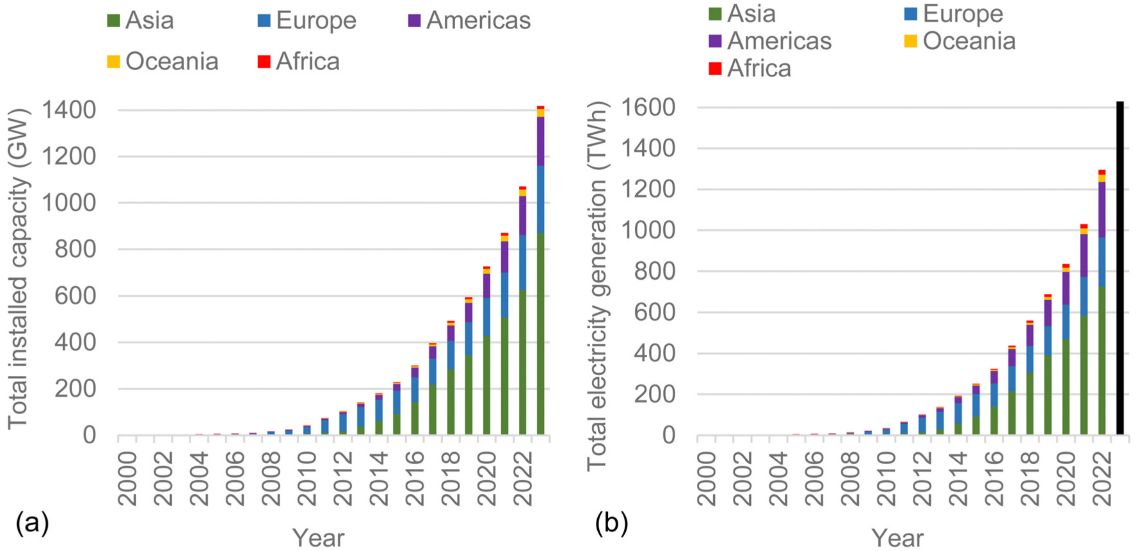

Fig. 6 Historical analysis of solar energy: (a) total installed capacity and (b) total electricity generation.[2,100]

solutions in a variety of ways, such as increasing efficiency, lowering costs, enabling large-scale implementation, and advancing complementary technologies like photocatalysis and desalination.[101] A bibliometric analysis over the past 10 years was conducted to understand the latest trends and emerging concepts in ML applications within solar energy research. The literature search was performed using the WOS, with the keywords ("solar") and ("energy" or "utilization" or "systems" or "to fuel" or "fuel") and ("machine learning" or "data driven"). A total of 2759 articles were identified and analyzed in the Bibliometrix package in R.[102] The co-occurrence analysis was performed using the Walktrap algorithm[103] for clustering, and an association was applied for normalization using the default settings of the Biblioshiny function.[102]

The word cloud of keywords reflects the most frequently occurring terms in the context of ML applications in solar energy (Fig. 7a). The size of each word corresponds to its frequency, with forecasting standing out as the most prominent keyword, indicating its significance in ML research related to solar energy. This is followed by PV, which highlights its central role in the application of ML for solar energy utilization. In addition to domain-specific keywords, several ML algorithms, such as ANNs, SVMs, RF, and deep learning, also emerge as common terms, emphasizing their popularity in this field. In addition to forecasting, optimization also appears as another task performed using ML. The co-occurrence diagram shown in Fig. 7b shows the relationships of major clusters with the frequent keywords. ANNs and deep learning are the most commonly used ML techniques in forecasting. For example, Soukeur *et al.*[104] used ANNs using 39-year historical data to successfully predict daily solar radiation in Oran and showed that it can be used to ensure optimal management of solar energy farms. Ledmaoui *et al.*,[105] on the other hand, compared the performance of ML algorithms for solar energy production and demonstrated that ANN resulted in the best predictive power.

ML has been extensively implemented in specific solar power technologies in a variety of ways. As an example for CSP, the multiple deep learning models were used to predict the aggregated CSP energy production in Spain using a variety of inputs, including top-of-atmosphere irradiance, cloud cover forecasts, external temperature, and time-related variables such as the hour of the day and day of the year,[106] while a CSP plant

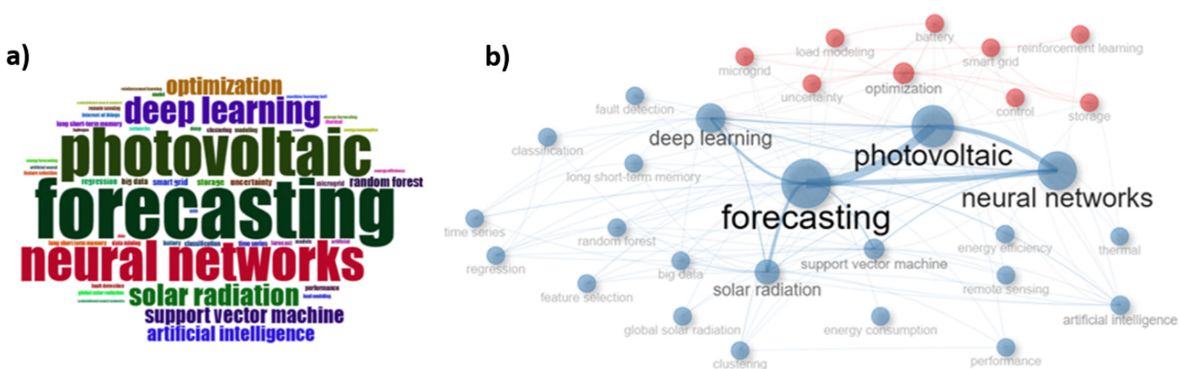

Fig. 7 Bibliometric analysis of ML in solar energy research: (a) word cloud and (b) co-occurrence network.

was simulated with ML to reduce the time compared to the traditional simulation model.[107] Pargmann *et al.*[108] introduced an ML-based differentiable ray tracing approach to accurately determine mirror imperfections and irradiance profiles; Narasiah *et al.*, on the other hand, developed an ML model for the discovery of a cost-efficient dry cooler design, which is essential for CSP plants.[109] As a last example, Pérez-Cutiño *et al.* utilized ML to detect broken receiver tubes using data from unmanned aerial vehicles and sensors from CSP plants.[110]

ML also has a crucial role in advancing PV technologies, including silicon-based solar cells; researchers have leveraged ML models to improve various aspects of silicon solar cell performance, including long-term performance predictions, efficiency optimizations, and manufacturing processes. For example, Lopez-Flores *et al.* worked on a model for PV production;[111] they used an artificial neural network model to predict PV plant metrics such as total profits, water consumption, waste, and emissions, including production timelines. Nguyen *et al.*, on the other hand, have predicted the annual energy output of building-integrated PV systems under realistic environmental conditions using ANN.[112] ML models may also analyze sensor data from solar panels to predict potential failures or efficiency drops before they occur; for example, Weiqing Li investigated the stiffness degradation in PV modules using ML and the finite element method.[113] Examples of other ML applications involving silicon-based PV panels can be found in various review articles published in the literature.[114,115]

The impact of ML on the new generation systems, like thin film technologies, dye-sensitized solar cells (DSSCs), organic/polymeric solar cells (OSCs), and halide perovskite solar cells (PSCs), is more direct and pronounced; for example, ML models can predict the optimal combination of materials, such as perovskites or organic materials, leading to improved light absorption and energy conversion rates. Indeed, the halide perovskite solar cells, which have drawn significant attention in recent years due to their high efficiency and expected low costs despite their inherent instability, may have the biggest share in the papers involving ML applications from material screening to performance prediction. For example, Zhang *et al.* focused on utilizing ML to accelerate the identification of small molecule passivation materials for PSCs, addressing a key challenge in improving their efficiency using DFT-generated data,[116] and they identified key molecular traits that enhance passivation performance. They then discovered three new molecules, which were experimentally validated, showing a notable increase in performance. Our group, on the other hand, analyzed experimental data collected from the literature to determine the conditions for high power conversion efficiency,[117] stability,[118] hysteresis, and reproducibility of PSCs.[14] Additionally, we investigated 2D/3D perovskite structures using eXtreme gradient boosting (XGBoost), random forest regression, and ANNs.[15] There are also various reviews published on ML applications in perovskite solar cells,[119–121] including one of ours.[16] Given the rapid rise in popularity and research on perovskite materials, there has been a growing need for systematic data management to make the vast amount of research data more accessible and usable. In response, Jacobsson *et al.* developed the Perovskite Database Project (PDP), which extracts and organizes meaningful device data from peer-reviewed studies on metal-halide perovskite solar cells.[122] The database includes information on over 42 400 PV devices, with up to 100 parameters per device.

4.2. Solar fuel production

4.2.1. Solar fuel production technologies. Solar energy is also being used to generate (green) hydrogen, a clean fuel that has immense potential in sectors such as transportation, industry, and energy storage. One notable approach is the PV water electrolysis method, which has shown considerable promise for green hydrogen production. Although hydrogen production through water electrolysis has been known for over 200 years, the efficient use of electrolyzers still requires significant scientific work.[123] Hydrogen produced this way has a share in global hydrogen production of only 4% due to economic and technical difficulties.[124] There are several methodologies related to electrolysis, including alkaline water electrolysis, anion exchange membrane (AEM) water electrolysis, proton exchange membrane (PEM) water electrolysis, and solid oxide water electrolysis. However, identifying complex rules or pathways that result in high performance may require optimizing variables such as support and surface elements, membrane type, electrolyte type, cathode and anode gas diffusion layers, flow rate, and temperature.[123,125,126]

Solar energy can also be used directly to produce hydrogen through photocatalytic (or photoelectrochemical) systems, in which solar irradiation is used to generate photoelectron–hole pairs to be used to split water to hydrogen or reduce CO_2 in the presence of water to generate a variety of solar fuels (such as hydrogen, CO, methane and methanol); the second process has the additional benefit of reducing CO_2 emission. Although this technology has not matured yet, it has been investigated significantly due to its potential to contribute to the efforts toward sustainable energy in the future. There may be some variation in the process described above with the use of different reaction systems like type I, type 2, and *z*-scheme heterojunctions or when performing the process in a photoelectrochemical cell. However, the major challenges remain the same: finding semiconductor(s) that effectively work under visible light and cocatalyst(s) that will separate electron–hole pairs effectively before their recombination. Various semiconductors have been tested for photocatalytic water splitting and CO_2 reduction so far: metal oxides (like TiO_2, ZrO_2, CeO_2, and ZnO_2), perovskites (like $NaTaO_3$ and $SrTiO_3$),[127] nitrides (especially g-C_3N_4), sulfides (like CdS, ZnS, and CuS),[128] MOFs[129] and halide perovskites.[130] Similarly, various cocatalysts such as noble metals (like Pt, Au, Pd, Ag, Rh), metal/metal oxides (Cu-based, Ni-based, Cd-based materials), and alloys (like Au/Cu and Pt/Cu) have been used together with the semiconductors.[131] The details of the processes can be found in numerous publications, including some review articles.[132]

4.2.2. ML applications in solar fuels. In solar fuel production, ML is used for material discovery and development, performance prediction, and optimization of operational conditions. As discussed in a recent study,[133] advanced modeling techniques and ML-based methodologies can be used to discover the ideal combination of variables that leads to high performance.

For instance, Zhao *et al.* successfully applied dynamic hierarchical modeling and control to high-temperature PEM electrolyzer cell systems.[134] Furthermore, Mohamed *et al.* used five different ML techniques to forecast hydrogen generation rate and density.[135] Yin *et al.*, on the other hand, concentrated their study on the uses of ML approaches in membrane design and discovery.[136] As a last example, Kim *et al.* focused on developing optimal ML techniques for understanding the operational features of PEM electrolyzers.[137]

As far as the photocatalytic and photoelectrochemical systems are concerned, material screening is a popular area for ML applications due to the large number of materials with potential semiconductor properties and the continuous development of new synthesis methods. For instance, Zhou *et al.* introduced a novel ML-driven methodology for the rapid screening of metal oxide photocatalysts for water splitting.[138] Similar to the perovskite database project mentioned above, Isazawa and Cole created a Photocatalysis Dataset for water-splitting applications.[139] They developed a dataset of 15 755 records extracted from 47 357 papers, focusing on water-splitting activity with photocatalysts. Similar studies were also performed for CO_2 reduction. For instance, Khwaja and Harada used first-principles screening and ML for high throughput screening of synthesizable, light-absorbing, and water-stable MOFs for the photoreduction of CO_2.[140] Performance prediction, such as estimating product rates (in photocatalysis) or power conversion efficiencies (in photoelectrochemical systems), represents another key application of ML in solar hydrogen production. Liu *et al.* developed a regression fusion model to predict the hydrogen production rate for TiO_2 photocatalytic water splitting using ML.[141] Our group also used ML for performance prediction of water splitting in photocatalytic[142] and photoelectrochemical[143] systems, as well as CO_2 reduction over metal oxide semiconductors[18] and MOFs.[17] We also reviewed ML applications in catalysis and photocatalysis,[29] while we concentrated only on the perovskite semiconductors in another review.[16]

4.3. Solar desalination for clean water production

4.3.1. Solar desalination basics. Solar thermal desalination uses solar energy to heat water and produce steam, which is then condensed into freshwater. It is energy-efficient and can be applied on a small scale for rural communities or on a large scale for cities. Desalination processes can be grouped as electrochemical, thermal, and membrane-based processes. Electrochemical methods, such as electrodialysis (ED), use ion-selective membranes and an electric field to separate ions from seawater, while thermal systems such as humidification–dehumidification systems (HDH), multi-effect distillation (MED), multi-stage flash (MSF), solar still (SS), and solar chimney (SC) utilize evaporation–condensation cycles to produce freshwater from saltwater. On the other hand, the membrane-based processes, comprising reverse osmosis (RO) and membrane distillation (MD), employ semipermeable membranes that separate water from salt and other impurities.[144] These technologies can also be grouped in terms of the way they use solar energy; some systems, such as HDH, SS, and SC, use solar energy directly, while others, like solar-powered ED, MSF, and RO, utilize solar electricity.[145]

Solar desalination may be one of the critical technologies to achieve SDGs, especially SDG6 (ensure availability and sustainable management of water and sanitation for all); it may effectively address the global water crisis, which has been elevated in recent years due to factors like population growth, pollution of water sources and poor farming. This is particularly crucial in water-scarce regions like Africa and the Middle East, where access to fresh water is limited, but solar energy is abundant. Although significant progress has been made in recent years, and the combined capacity of present desalination plants worldwide has reached 95 million m^3 d^{-1},[144] these technologies have to develop further and spread to wider geographies to solve the clean water requirement of the future.

4.3.2. Machine learning in solar desalination. ML may help to enhance desalination by improving efficiency and energy consumption through modeling and optimizing the processes; applications are quite diverse. For example, Salem *et al.* used a multilayer perceptron to predict the efficiency of water desalination.[146] Priya *et al.* used ML for a two-dimensional material search for water desalination systems.[147] Plasencia *et al.*, on the other hand, utilized SVMs and DTs for the analysis of reverse osmosis desalination.[148] At the same time, Acevedo *et al.* employed the ANNs to predict the permeate output in a gap membrane distillation (PGMD) module from the operational parameters.[149] Karunakaran *et al.* used various ML algorithms to model and optimize the forward osmosis (FO) process.[150] In another example, Kandeal *et al.* predicted the performance of a double slope solar still (DSSS) using ML algorithms under the climatic conditions of Egypt.[151] Similarly, Wang *et al.* investigated the hourly performance of tubular solar stills.[152] While these ML models used data generated by the investigators themselves, An *et al.* analyzed the productivity of a humidification–dehumidification system using data collected from various sources in the literature.[153]

5. Wind energy

5.1. Wind power generation

Wind energy, as a renewable energy source, has some advantages, like continuous generation of electricity during the day and nighttime, less CO_2 emissions, and high efficiency. It is important for achieving SDGs because the wind is free and widely available around the world. On the other hand, it has some disadvantages like environmental impact, limited life expectancy, and variable power output.[154] Meteorological and environmental factors have a significant impact on the instability and uncertainty of wind power, which causes challenges to its integration into electricity generation.

The utilization of wind energy has grown significantly over the years, with the global installed wind power capacity increasing from 17.0 GW in 2000 to the impressive milestone of 1 TW in 2023, as displayed in Fig. 8a;[100,155] as indicated in Fig. 8b, the electricity generated by wind turbines reached 2304 TW h (about a share of 7.8% in the total global electricity generation mix) in the same year.[2] It is observed that wind-based electricity generation in Asia has grown the most in the past 23 years,

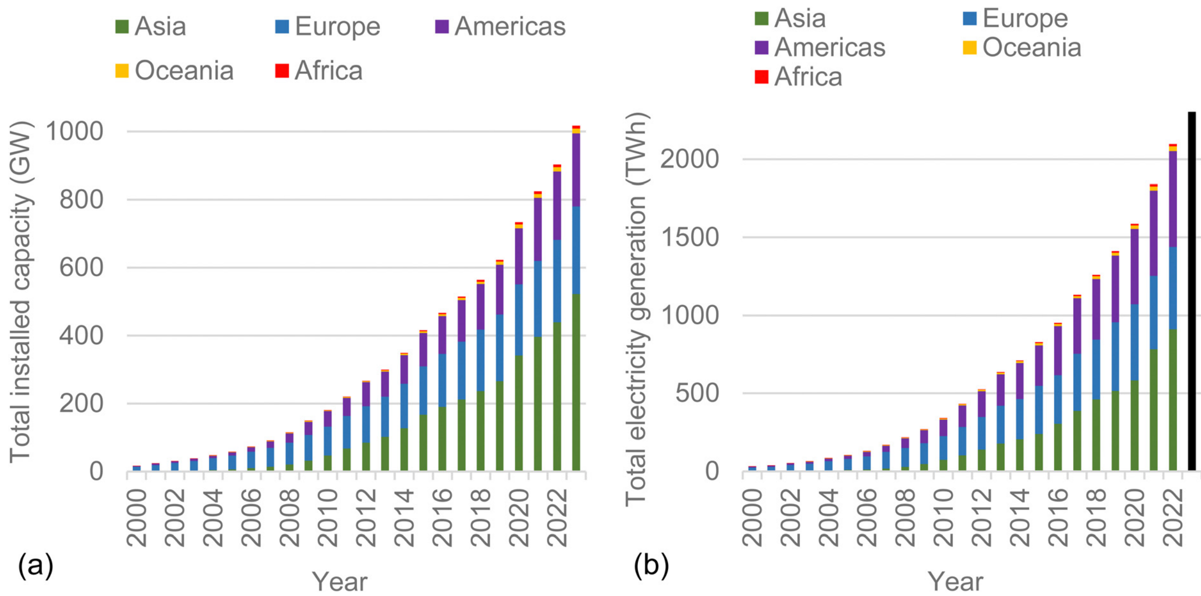

Fig. 8 Historical analysis of wind power: (a) total installed capacity and (b) total electricity generation.[2,100]

reaching a capacity of 522.4 MW, followed by Europe (258.0 MW) and the Americas (214.3 MW) in 2023. Africa is the last among other regions, which makes the implementation of sustainable development goals, including wind energy, even more important for this region.

A bibliometric analysis was also conducted to determine the general trends in the scientific community for wind power capacity estimation within the "Energy fuels" category under the Web of Science Database with the words in the title: "wind energy estimation/prediction/forecast" or "wind power estimation/prediction/forecast" for the years between 2014 and 2024, resulting in 988 articles. Accordingly, the keyword co-occurrence analysis is shown in Fig. 9, where it is displayed that "speed" is the most frequently used keyword surrounded by "wind power forecasting", "wind power prediction", "artificial neural networks" and "optimization".

5.2. ML applications in wind power generation

Predicting wind speed and direction is crucial for estimating wind power to establish renewable energy strategies and organize and coordinate grid operations.[156] Wind speed/power prediction can be classified into four categories based on its time horizon: very short-term (from a few seconds to 30 minutes ahead), short-term (from 30 minutes to 48 hours ahead), medium-term (from 48 hours to one week ahead), and long term (from 1 week to years ahead).[157] Various tools based on statistics and ML have been used and discussed by different researchers to predict wind speed or power for these time horizons.[158] Forecasting methods such as auto-regressive moving average (ARMA), auto-regressive integrated moving average (ARIMA),[159] and discrete-time Markov chain models[160] are quite effective in predicting short- or very short-term wind speeds. Additionally, as a part of ML techniques, ANNs[161,162] have become widespread for wind power prediction, as well as kernel ridge regression,[163] SVMs,[163,164] and deep learning-based methodologies.[165,166]

ML can also be used to predict wind speeds in target locations based on data from neighboring regions where wind speeds have been measured for many years. For instance, Velo *et al.* used ML to predict the wind speed of a target location using the wind speed and direction data from nearby stations in Galicia, Spain.[167] Similarly, Fadare used ML methods with geographical variables as descriptors to predict wind speeds in some target locations in Nigeria.[168] Likewise, in one of our previous studies, we modeled mean monthly wind speed as a function of several geographical variables, atmospheric variables, and the month of the year to predict wind speed for some target locations in the Aegean region of Turkey.[169]

A wind turbine has several mechanical parts and electrical equipment that sometimes work under extreme environmental conditions. Moreover, wind farms are typically located in remote areas where a wind turbine failure is difficult for a person to prevent immediately. As a result, some detection sensors are used to collect data from wind farms, and using these data, it is possible to monitor wind turbine conditions[170] and predict failure in wind turbines using ML approaches[171] so that the operator can stop the turbine operation to avoid potential damage.[172] On the other hand, false alarms generate unnecessary downtime, which results in productivity losses and higher maintenance expenses. As a result, detecting false alarms is also one of the most important components in making wind energy competitive with other energy sources.[173,174]

Physics-informed ML, which is a novel approach that combines physical rules and ML algorithms to generate models that are both data-driven and physically consistent, has been popularized recently for condition detection or anomaly detection.[175] For instance, Schröder *et al.* used the transfer learning approach to detect abnormal behavior in wind turbine sensor data using a

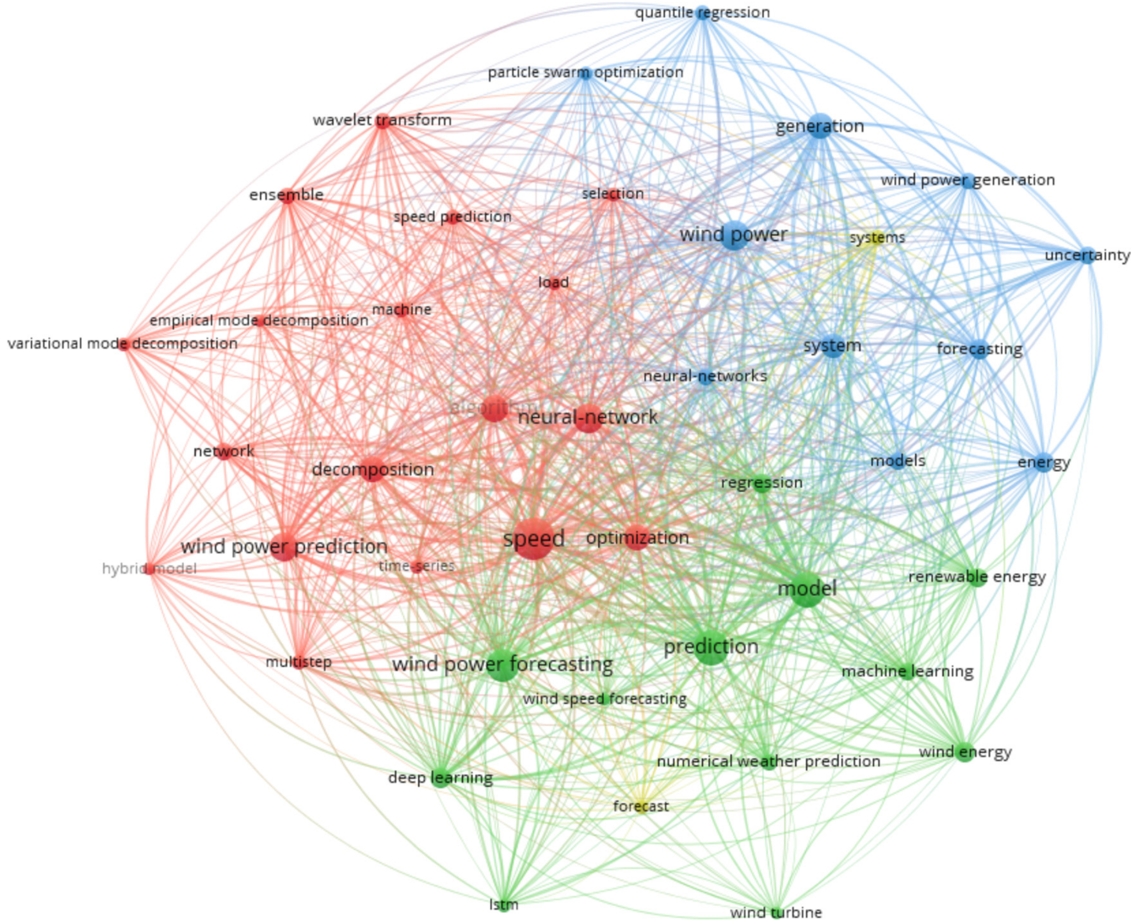

Fig. 9 Co-occurrence analysis for wind power capacity estimation. Keywords that appear more than 25 times are displayed.

physics-constrained artificial neural network.[176] Similarly, de N Santos *et al.* used a similar approach for health monitoring of wind turbine fatigue using physics-guided learning of neural networks.[177] Perez-Sanjines *et al.* applied physics-informed deep learning for fault detection of wind turbine gearboxes.[178] Physics-informed ML can also be used for different purposes in the field of wind energy. For example, Baisthakur and Fitzgerald estimated the aerodynamic forces on wind turbine blades using physics-informed neural networks.[179] On the other hand, Wang *et al.* used LiDAR (light detection and ranging) data as the data source and combined the principles of fluid dynamics to build a physics-informed neural network for observing wind turbine wake dynamics.[180] Cobelli *et al.* used a similar methodology to model wind fields in wind farms, specifically for reconstructing the inflow velocity field of a single wind turbine.[181]

6. Biofuels

Biofuels, derived from organic biomass, offer a sustainable alternative to fossil fuels and align with SDGs (particularly SDG 7 and SDG 13).[182] They play a crucial role in decarbonizing the transportation sector and advancing the net-zero emission goal. However, the long-term sustainability of biofuels requires addressing social, environmental, and economic factors, including land use, feedstock sources, and food security. Balancing these challenges is essential to maximize the positive impact of biofuels on both SDGs and the global goal of net-zero emissions. Given the socio-demographic, political, and technological changes in developing nations, achieving the SDGs presents a significant challenge.[11] Biofuels, particularly those derived from organic waste, can support integrated biorefineries and energy production while also contributing to waste management and the circular economy.[183]

To determine the general trends in the scientific community and to see the relationship between biofuels and sustainable development goals, a bibliometric analysis was also conducted in the WOS database with the words in all fields: ''biofuel/biomass/bioenergy'' and ''sustainable development goals/sdg'' for the years between 2014 and 2024, resulting in 847 articles. Fig. 10 shows the keyword co-occurrence analysis, where the ''sustainable development goals'' is in the center, surrounded by various bioenergy sources and types as well as production methods like ''biodiesel'', ''biochar'', ''microalgae'', ''pyrolysis'', and ''anaerobic digestion'' together with the words related to the environment like ''CO_2 emission'', ''climate change'', *etc.*

6.1. Biofuel technologies

6.1.1. Biomass sources. Biomass is used in both non-energy (*e.g.*, biomaterials, chemicals) and energy applications,

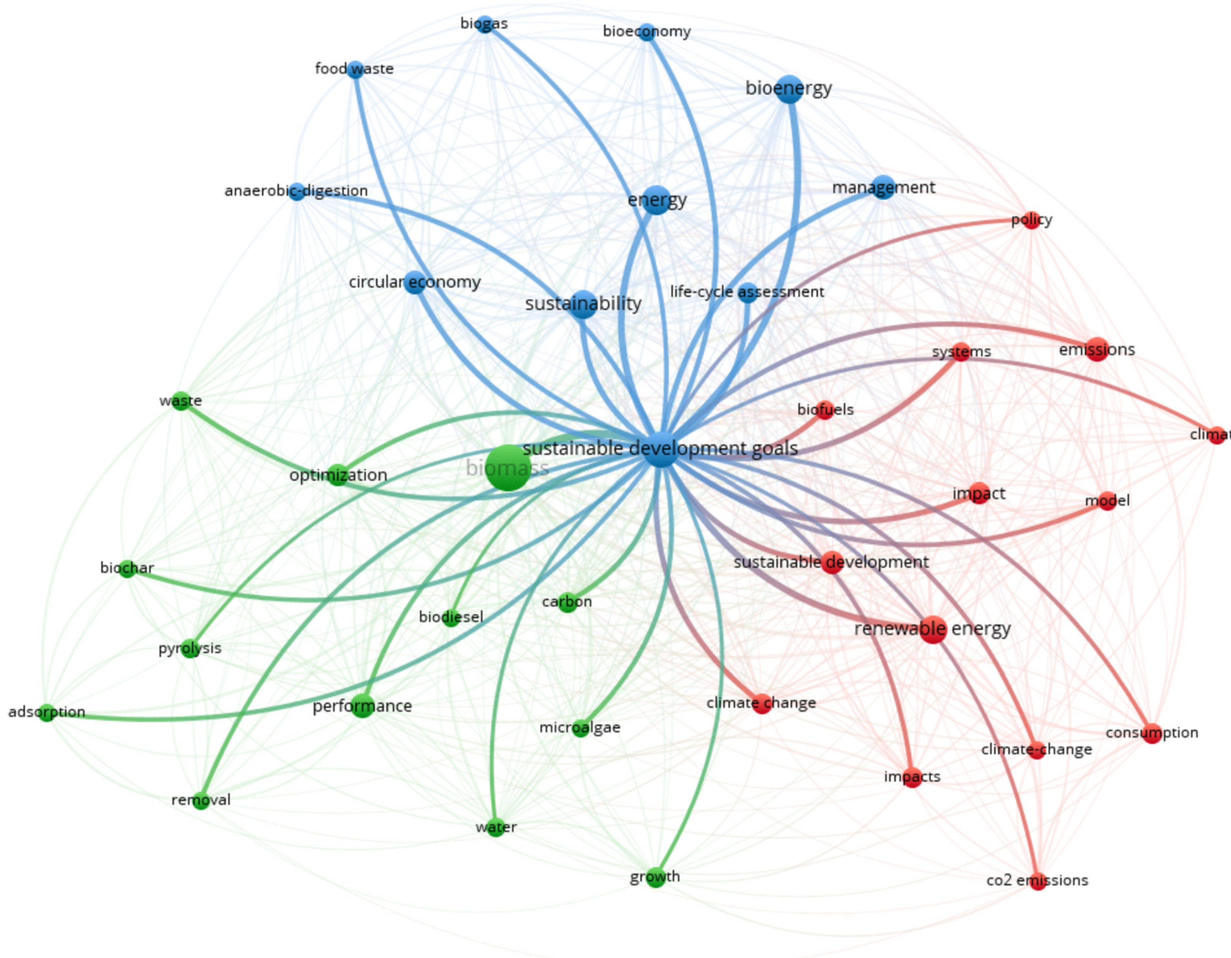

Fig. 10 Co-occurrence analysis for SDGs and biofuels from 2014 to 2024. Keywords that appear more than 25 times are displayed.

including traditional and sustainable fuel production, by using various conversion techniques to produce biofuel.[184] In developing regions, biomass remains a key energy source for households and industries, while its potential in the global energy transition is also growing.[185] Biofuels derived from biomass, such as bio-hydrogen, biogas, and biodiesel, offer a promising pathway for sustainable energy.[186] However, competition with food crops for arable land remains a challenge. First-generation biofuels use edible biomass such as seeds, grains, and sugars, while second-generation biofuels utilize lignocellulosic feedstocks and waste materials. Third-generation biofuels, which employ high-lipid microorganisms like microalgae, provide additional benefits such as carbon sequestration and water treatment while requiring less land and offering high productivity.[184] Currently, the technology for third-generation biofuels has not yet reached maturity. High-yield strains of bacteria and microalgae have been identified, and the technology for transesterification has improved significantly. Though these biofuels have shown promise, commercial scalability remains limited due to the lack of supply chain standardization.[186]

As a major representative of second-generation biofuel feedstock, lignocellulosic feedstocks, such as agricultural residues, forestry waste, and energy crops, offer several advantages.[187] These biomass sources are abundant, renewable, and low-cost, providing a consistent supply for biofuel production.[187] Utilizing waste biomass supports rural economies by creating new markets for agricultural waste and aligns with circular economy principles by repurposing materials, increasing resource efficiency, and reducing environmental impact. As a major representative of third-generation biofuel feedstock, microalgae is a promising renewable resource for bioenergy production due to its high oil content and various biomolecules, including lipids, proteins, and carbohydrates; it is produced *via* photosynthesis, using carbon dioxide and nutrients like nitrogen, potassium, and phosphorus.[188] It offers advantages such as requiring minimal arable land and having high biomass productivity; it can be grown in various environments, including open raceway ponds. Its high lipid content, ranging from 20% to 50%, makes it suitable for biofuel production, particularly for transportation fuels.

Interest in co-producing commodity and perennial bioenergy crops is growing due to their agricultural and environmental benefits. One key factor is the use of marginal lands (areas with suboptimal conditions for commodity crops or high susceptibility to environmental degradation) for bioenergy crop cultivation. Targeting these lands with advanced, high-yielding bioenergy crops can promote sustainable biofuel production while enhancing ecosystem services. This approach also addresses concerns about indirect land use change, which is a significant issue in large-scale biomass production.[189] Marginal lands, as defined by the FAO and others, are those with limited agricultural potential, requiring additional inputs but offering negligible returns. These lands include fallow or idle plots, abandoned farmlands, barren lands with hostile conditions (*e.g.*, high salinity, aridity), grasslands, shrublands, and contaminated sites. Utilizing these areas for bioenergy crops like microalgae or lignocellulosic biomass reduces competition with food resources and conserves freshwater supplies.[190]

6.1.2. Biofuels. The development of biofuels, primarily ethanol and biodiesel, has gained significant attention as a means to combat climate change and meet emission reduction targets, and their technological maturity level has reached a certain limit.[191] Also, as global demand for diesel and biodiesel rises, the by-products of biodiesel production, such as crude glycerol, offer valuable opportunities for producing hydrogen, ethanol, and other biochemicals.[192,193] There are other biofuels that may be produced with different forms and properties, and used for different purposes. For example, biochar, produced through slow pyrolysis of biomass, has gained attention for its potential applications like carbon sequestration, soil amendment, and wastewater treatment in addition to its traditional role as fuel.[11] Similarly, pellets, another solid biofuel with high heating value and low moisture content, are valued for their low storage costs and high combustion efficiency.[194] Biohydrogen, a promising carbon-neutral energy carrier, is produced biologically through methods such as microbial electrolysis, dark fermentation, and biophotolysis.[195] The yield and quality of biofuels strongly depend on several factors, including feedstock type, reaction conditions, and the use of catalysts.[184]

6.2. Machine learning for biofuels

The use of ML for biofuels, with the perspective of achieving SDGs, can be evaluated using the following four critical research areas: (i) optimum use of lands, (ii) developing low-investment solid biofuels, (iii) improving the performance of mature biofuels like biodiesel and bioethanol, and (iv) the development of new biofuel technologies. The first area (optimum land use) involves the identification of potential land for biomass cultivation, particularly focusing on sustainable sources like lignocellulosic feedstock and microalgae. As an example, Ching *et al.* developed early prediction models for *Spirulina platensis* biomass yield, achieving good results with ridge regression.[186] Similarly, Igou *et al.* applied deep learning to predict open raceway pond microalgal productivity using sensor data.[196] Chen *et al.*, on the other hand, assessed marginal lands for microalgae cultivation, using GBM to predict biomass production potential. Their study identified over 7.37 million km^2 of suitable land for biofuel cultivation, with marginal land areas concentrated in equatorial regions.[190]

As the second area, the solid biofuels, such as bio-briquettes and pellets, which offer an affordable energy solution with low investment costs, especially for developing regions of the world, were investigated. For example, Bamisaye *et al.* used adaptive neuro-fuzzy inference system (ANFIS) models to predict the calorific value and fixed carbon content of bio-briquettes made from waste biomass,[197] whereas Mancini *et al.* predicted pellet quality using various ML models. Naive Bayes achieved the best results for classifying pellet samples based on ash content, with recall values as high as 0.92 for low-ash samples.[194] Shafizadeh characterized hydrochar from lignocellulosic biomass, sewage sludge, and other waste materials using DTR models, finding that ash and carbon content, along with operating temperature, are key factors in hydrochar production.[198]

The third area involves the issues related to the more effective use of mature biofuel technologies (biodiesel and bioethanol). For example, Wong *et al.* used an extreme learning machine to predict engine performance when running on ethanol.[199] Kale *et al.* investigated the optimization of homogeneous charge compression ignited engines using biofuel blends; SVMs were employed to model fuel parameters, showing that energy content and cooling potential are the most influential for predicting engine characteristics.[200] Luna *et al.*, on the other hand, predicted cold filter plugging points and kinematic viscosity in biodiesel blends using ridge regression and AutoML, achieving predictive accuracy close to experimental error.[201] Aghbashlo *et al.* developed models to optimize the exergetic performance of diesel engines using biofuel-diesel blends.[202]

Finally, the ML research focuses on optimizing key process parameters for better prediction and control of yields in new technologies. For example, Khandelwal *et al.* applied ML models like XGB and CatBoost to predict gas yields from supercritical water gasification of lignocellulosic biomass,[6] while Djandja *et al.* developed models to predict bio-oil yields in solvothermal liquefaction, identifying biomass conversion as a crucial intermediate step.[3] In another example, Yang *et al.*, on the other hand, explored microwave pyrolysis with various ML models, where GBR and RF showed promising results. Our group also investigated the use of algal biofuels, oleaginous yeast, and lignocellulosic materials.[19–21,203]

7. Batteries for energy storage

Developing high-capacity and low-cost batteries is also critical for achieving SDG 7 and its targets mainly because electrochemical energy storage systems are highly efficient, directly converting chemical energy into electrical energy in a single step. Moreover, these systems can be designed specifically according to the need at the required location and capacity and would be suitable for indoor or outdoor operations; such flexibility would be especially vital in developing regions of the world, where the central power generation and distribution network is not sufficient. Another evident impact of the development of high-performance, affordable rechargeable batteries would be on SDG 13: Climate Action. Yet, there are less apparent relationships between rechargeable batteries and the other SDGs. For instance, Hannan *et al.* conducted a comprehensive study on the connection between battery energy storage systems and the SDGs and proposed that batteries positively affect the success of 60 targets (35.5%).[204]

Recent research trends in the development of rechargeable batteries are critically linked to several SDGs. For instance, the use of earth-abundant and geography-independent active materials, the improvement in the battery manufacturing and recycling methods that are more environmentally friendly and cost-effective, the development of battery systems suitable for secondary use, and the design of hybrid renewable energy storage systems combining different energy generation and storage systems will have a crucial influence on the success of not only SDG7 and SDG13 but also SDG 3 (good health and well-being), SDG 6 (clean water and sanitation), SDG 8 (decent work and economic growth), SDG 9 (industry, innovation, and infrastructure), SDG 11 (sustainable cities and communities), SDG 12 (responsible consumption and production), SDG 14 (life below water), SDG 15 (life on land), and SDG 16 (peace, justice, and strong institutions). ML plays a key role in all of these research approaches.

To determine the general trends in the scientific community and to see the relationship between batteries and SDGs, a bibliometric analysis was conducted under the WOS Database with the words in all fields: ''battery'' and ''sustainable development goals/sdg'' for the years between 2014 and 2024, resulting in 203 articles. Fig. 11 shows the keyword co-occurrence analysis, where the ''sustainable development goals'' is in the center, surrounded by various keywords such as ''lithium-ion batteries'', ''energy storage'', ''life cycle assessment'', ''circular economy'', *etc.*

7.1. Li-ion batteries

Currently, the Li-ion technology, with its specific energy of up to 170–250 W h kg^{-1} and cycle life of up to 3000 cycles, dominates the market for mobile and stationary energy storage solutions. In addition, Li-ion batteries have high voltages (3.05–4.2 V), high specific power (200–1000 W kg^{-1}), and low self-discharge rates (less than 10% per month), making these batteries highly attractive. In parallel, researchers continue to work on developing Li-ion batteries with better performances for the completely electrified future.[205] The current research areas typically focus on the main components of the batteries: the positive and the negative electrodes where reversible electrochemical reactions take place, electrolytes for ionic transport, and separators for the electrical isolation of the electrodes.

The anodes of Li-ion batteries can be inspected under three categories: insertion, conversion, and alloying materials. Graphite, with a theoretical capacity of 372 mA h g^{-1}, belongs to the insertion-type anode family and became very popular due to its high electrochemical stability and cost-effective easy production. TiO_2-based anodes are other intercalation-type anodes showing high cycle life and fast kinetics;[206] other intercalation-type anodes, including transition-metal oxides, nitrides, and phosphides, are not as common despite having high capacity and capacity retention due to their low voltages.[207] Finally, alloying-type anodes were developed to reduce the side effects of pure lithium metal compared to alloyed metals. Silicon anodes are also a hot topic in the Li-ion battery literature as they are environmentally friendly and abundant in nature with capacities higher than 4200 mA h g^{-1}. However, the silicon anodes have significant volume expansion problems and thus are not commercialized yet.[208]

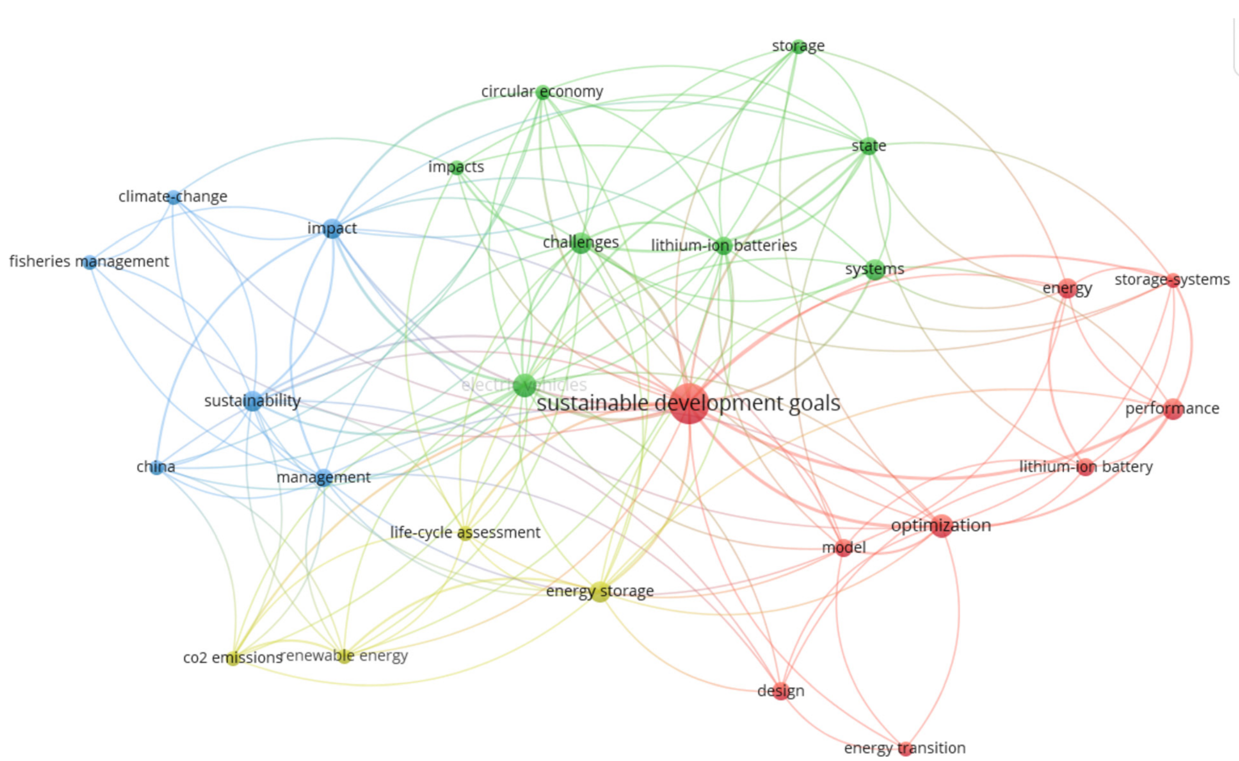

Fig. 11 Co-occurrence analysis for SDGs and batteries from 2014 to 2024. Keywords that appear more than 25 times are displayed.

The material choice is also critical for the positive electrodes to improve cell potential, thus increasing the specific power and power densities, surpassing the cycle life, and diminishing the cell cost. However, there is no perfect cathode material for every application of Li-ion batteries yet. Layered transition metal oxides, spinels, olivines, and phosphate-based materials are the main materials at the focus. One of the biggest advantages of layered transition metal oxides is the easy transport of Li ions in their layered structures in the 2-dimensional space. The lithium metal oxides, $LiMO_2$, are formed using various metal/metals, mainly cobalt, manganese, and nickel, with different ratios. The first commercialized cathode material, $LiCoO_2$, belongs to this family. Although the oxides $LiNiO_2$ and $LiMnO_2$ are also options, the mixed oxides show optimum solutions for the shortcomings of single oxides for Li-ion batteries. $LiNi_xCo_{1-2x}Mn_xO_2$ is currently one of the most preferred cathode chemistries[209] where Ni increases the voltage and capacity, while Mn and Co are responsible for improving the cycle life and rate capability of the batteries.[210] Another popular cathode chemistry belongs to the phosphate family: lithium–iron–phosphate, $LiFePO_4$. Although NMC has the largest market share, the LFP cathodes also gained popularity due to their longer cycle life and safer nature. In addition, they do not contain rare metals such as cobalt.[211]

Though not an active material, electrolytes of Li-ion batteries also play a crucial role in the realization of the full potential of the electrodes in terms of electrochemical reactions, stability, cycle life, and safety aspects.[212] Hence, electrolyte development is also widely investigated in the literature. The liquid electrolytes of Li-ion batteries contain various kinds of solvents and several additives. Typically, the non-aqueous solvents, namely ethylene carbonate (EC), propylene carbonate (PC), ethyl methyl carbonate (EMC), and diethyl carbonate (DEC), are used with tetrafluoroborate ($LiBF_4$), hexafluorophosphate ($LiPF_6$) and perchlorate ($LiClO_4$) lithium salts.[213] Several thousand additives from diverse chemistries have been utilized in Li-ion batteries.[212] Meanwhile, solid-state electrolytes (SSE) have also been widely investigated in the literature as they are believed to be the future of Li-ion batteries, and that is why we classified these batteries as beyond Li-ion batteries (discussed next).[214]

7.2. Beyond Li-ion batteries

Although not commercialized yet, new chemistries, so-called beyond Li-ion batteries, are also widely investigated to find alternatives with less ecological fingerprints and without supply chain problems. In this regard, both charge carrier anodes (Na, K, Zn, and Mg), new cathodes (S and O_2), and SSEs were studied. In our recent review article, we analyzed the literature trends and performed a bibliometric analysis with the help of text mining to see the trends beyond Li-ion batteries.[215] The results showed that Li–S and Na-ion batteries have been the most popular battery chemistries for almost 15 years. This is followed by Zn-based batteries (Zn–air and Zn-ion), Li–air, and finally K-ion batteries. These batteries are still in the development stage since they all have various problems. Although the cell requirements, hence the answers to the questions shown in Fig. 12, may change depending on the application, none of the new chemistries has replaced the Li-ion batteries yet and reached the desired performances in terms of energy density, power capability, and cycle life set by the customers for a completely sustainable future.

Members of metal-ion batteries, both mono- and multivalent batteries, work similarly as all of them have the rocking chair mechanisms where a single ion transfers between the two electrodes.[216] The most popular univalent chemistries are sodium- and potassium-ion batteries, and the biggest advantages of these metals are their low cost and natural abundance.

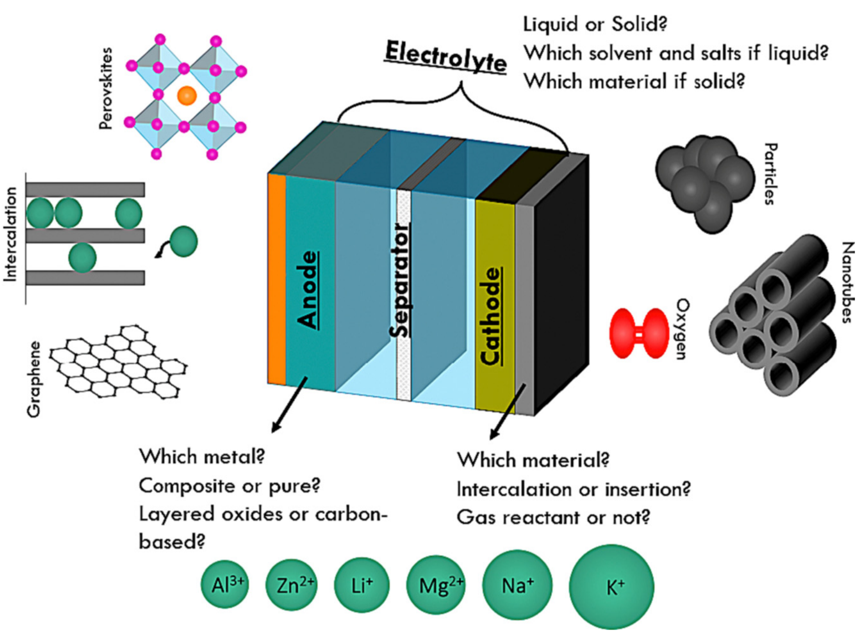

Fig. 12 The basic variables involved in the battery cells (reproduced with permission from Wiley, Copyright© 2022).[215]

However, due to the change in the ion size of Na^+ (~1.02 Å) and K^+ (~1.38 Å) compared to Li^+ (~0.76 Å), special materials should be designed specifically with large internal spaces for these new chemistries.[216] In addition, multivalent metals, due to the multi-ion transfer, have much higher theoretical capacities. Zn-ion batteries are among the most popular battery chemistries, but they also face Zn metal stability problems and limited available positive electrode materials.[217] In this respect, as seen from the keyword analysis of the beyond Li-ion literature, given in Fig. 13, electrode designs are the top priority for metal-ion batteries. On the other hand, conversion chemistries, such as Li–S, Zn– and Li–air batteries, have attracted attention recently due to their high specific energy. The polysulfide shuttle mechanism, the insulating nature of sulfur, and volume expansions during cycling are the main obstacles of metal-sulfur batteries. The metal-air battery problems are also associated with positive electrodes, where oxygen redox reactions are problematic.[218] Hence, the cathode and electrolyte design are found to be at the heart of research areas.

Furthermore, keyword analysis showed that graphene and carbon are the most frequently found materials, especially in the form of nanotubes and nanosheets, indicating that most of these batteries show a potential direction in new material selection and adaptation. On the other hand, aqueous electrolytes and metal oxides are found to be promising, given that only successful results are published in academia. Meanwhile, the high repetition of electrocatalyst and reduction keywords shows the problems faced due to the electrochemical reactions for metal–air batteries. Similarly, composite and polysulfide keywords show the polysulfide shuttle mechanism effect, which

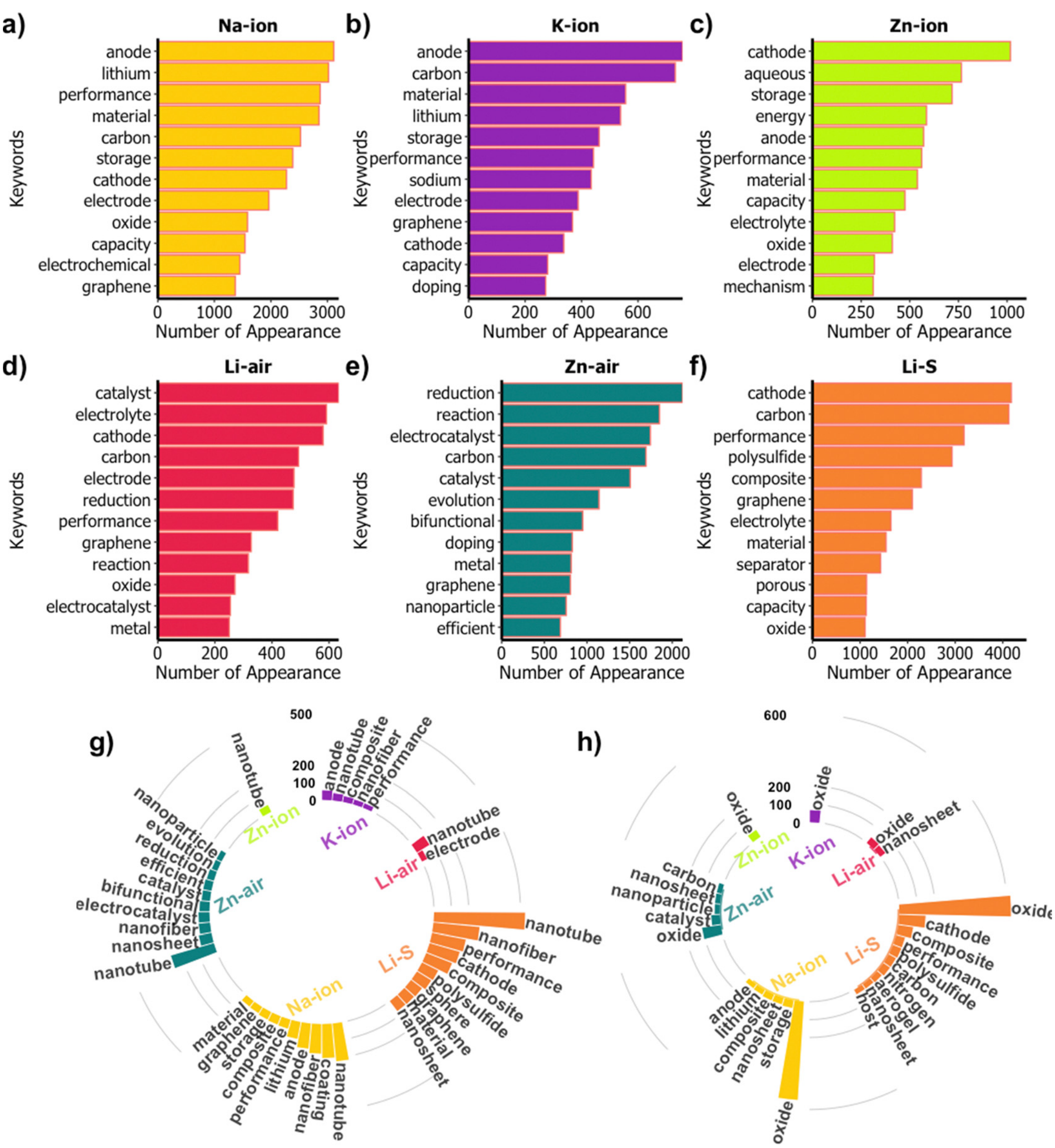

Fig. 13 The single-word keyword analysis for beyond Li-ion batteries (a)–(f) and the word associations with carbon (g) and graphene (h) (reproduced with permission from Wiley, Copyright© 2022).[215]

is the main problem of the sulfur cathodes in Li–S batteries. The text mining analysis also shows the significance of data and data tools in quickly gaining insights into the subject. With better tools such as ML, the exploration of batteries and battery materials can be accelerated.

7.3. ML applications in battery systems

ML is used in the battery field for material screening and property and performance predictions. With ML, structure–property–performance linkage can be found easily, which shortens the path to discovering novel materials. In order to do that, datasets obtained by in-house experiments, computational calculations, or the collection of literature findings are utilized. Our experience with these strategies has been successful in applications beyond Li-ion batteries.[25,26,28] In parallel to our studies, ML applications have also been widely used in the recent years in battery literature.[215]

The application of ML in Li-ion batteries is mainly focused on state-of-charge (SoC) and state-of-health (SoH) predictions with real-time data monitoring in real devices; given the maturity of the battery chemistry, no beyond Li-ion chemistry is at that stage yet.[219] Typically, the voltage, current, and temperature data of the cells have been used as the inputs to predict the SoC and SoH outputs.[220,221] On the other hand, ML techniques have also been used to advance Li-ion battery materials and manufacturing processes. In these works, the data are generally obtained from density functional theory (DFT) calculations in addition to some experimental studies where various parameters are predicted. For electrodes, the voltages of various materials and discharge capacities were predicted.[222,223] Similarly, the predictions of redox potentials of electrolyte additives,[224] as well as refractive indexes and viscosities of ionic liquids,[223] were also performed. In addition, aqueous electrolyte optimization was deployed using ML.[225] In another interesting work, image analysis was performed using DTs to detect the surface defects of separators used in Li-ion batteries.[226]

ML has also been used for various purposes beyond Li-ion batteries. In our group, ML applications in Li–S, Li–air, and Na-ion batteries were performed successfully.[25–27] For instance, Kilic *et al.* reported promising materials and material types to attain high-capacity Li–S batteries using the association rule mining technique.[26] In the following work, the analysis was narrowed down to the batteries using ionic liquid electrolytes to find the ionic liquid types to be used in the electrolytes of Li–S batteries, leading to an increase in specific energy.[27] Recently, the ionic liquid electrolytes were further investigated by a database that included ionic liquid properties obtained from computational calculations to identify the suitable anion–cation families. There are also various works by the other groups related to material development for uni- and multivalent metal-ion batteries and metal-air batteries.[227,228] In a valuable work performed by Joshi *et al.*, a web page was developed to give an interphase that can easily calculate the voltages of various materials as the electrodes for Na- and K-ion batteries with a dataset containing 3977 data points with 80 features obtained from the Materials Project.[229]

SSEs are important for all battery chemistries, including Li-ion chemistry, since liquid electrolytes increase safety concerns. In addition, with SSEs, high-power and high specific energy batteries are possible. Hence, SSEs have been widely investigated in both battery literature and the industry to replace the liquid electrolytes of Li-ion batteries.[230] With the growth of big data and increased computational power, the fast screening of promising SSE materials has become one of the favorite tools as it is cheaper and takes less time compared to the traditional trial-and-error procedure. In addition, ML is also used to elaborate on the structure–activity relationships in SSEs. The DFT method is defined as an ideal method to calculate microscopic atomic-scale features, whereas high throughput screening is found to be useful in increasing the material space for the investigation of SSEs. Furthermore, the combination of ML with DFT eliminates the downsides of DFT with statistical learning algorithms.[231] For example, the adoption of ML and DFT provided 130 promising materials based on ionic conductivity for SSE applications, and maximum packing efficiency and volume per atom are some of the most important features.[232] Similar works focused on the ionic conductivity of the solid membranes include predictions of polymers,[233] ternary crystals,[234] and ceramics, as well as classification of LLZO materials.[235] The mechanical property predictions[236] were also conducted for Li-ion transfer. Hence, the findings of these studies can be used for any batteries that use lithium-ion as the charge career. There are also works related to Na-ion conducting membranes.[237] In addition, clustering analyses were performed for Raman maps of polymer materials using *k*-means algorithms.[238]

To sum up, ML is widely used in the development of both Li-ion and beyond Li-ion batteries and probably will be used to a greater extent in the future. However, it should be noted that although ML is a very helpful tool, it also has some limitations. Although we greatly improved in creating large databases, these still need to be improved. Databases with relevant features and corresponding performance values are very much desired. However, creating these databases using computational tools such as electrochemical modeling is more straightforward since experimenting with these many batteries is time- and resource-consuming. Still, experiments can be performed to validate the results found by ML algorithms. Also, the ML models should be carefully selected to create generalizable models that correctly direct the research to promising materials with the available data to create a more sustainable future.

8. Future perspective

8.1. Challenges and opportunities for SDGs in general

As stated in the 2022 progress report by the UN, the defining principle behind SDGs is ‘‘leave no one behind’’.[239] Are we in that position now, after 60% of the time was spent and just six years away from the deadline? According to the same report, we are far from the desired state despite some progress. The report issued in 2023 also shows similar results from a different perspective.[240] If we look at SDG 7 in more detail, the 2023 report states that, although more people have access to electricity in 2021 compared to 2015, the gap is still too large to close for the developing regions. For example, in Sub-Saharan Africa, only 50% of people have access to electricity compared to 39% in 2015, which may be considered significant progress; however, the bottom line is half of the people do not have electricity yet. According to the 2023 report, the international flow of finance to developing countries for renewables was also declining.

Acting together as an entire planet and reaching SDGs, requiring that more efforts should be spent by the developed countries for the benefit of developing countries, was probably always challenging (possibly such efforts were not even tried before). Unfortunately, new challenges were added after 2015, making the situation worse. The first big setback came with the COVID-19 pandemic; the shortage of goods and services, including vaccines, affected those who already have difficulties in meeting those needs. The COVID-19 pandemic also seems to weaken the solidarity among the countries as each one entered into a survival mode. Then, the Russia–Ukraine war began (or escalated to the current state) in February 2022, worsening the worldwide food and energy supplies, both of which are critical for SDGs, as both countries are among the major wheat exporters while Russia is also a major energy supplier (especially natural gas for Europe). The political problems around the world, including those in the energy-rich Middle East, indicate that, unfortunately, the conditions may not improve to favor SDGs in the near future.

On the other hand, there are also opportunities to realize SDGs; the biggest one is the 2030 Agenda for Sustainable Development itself. Even if the specific targets of SDGs may not be reached by 2030, the efforts will likely continue to increase the awareness of the need for a more sustainable world, publicize the demands in this direction, and obtain the contribution of people, organizations, and governments through ever-growing means of worldwide communications.

As a result of the continuously increasing frequency of recorded temperature, drought, flooding, and other climatic events, global warming has become visible to even the most skeptical eyes in recent years. Although it is far from being called an opportunity, it may increase the awareness of the need for sustainability, including SDGs; for instance, the need for renewable energy could not be more apparent as energy is one of the main causes of global warming while it is also indispensable for many human activities.[241]

8.2. Challenges and opportunities for solar energy

Solar energy technologies like photovoltaics, concentrated solar power, solar desalination, and photocatalysis each present unique challenges and opportunities for advancing sustainable development. The initial investment in solar infrastructure is relatively high, which can hinder widespread adoption, particularly in developing regions.[221] In addition to the cost, solar power generation is highly dependent on weather conditions, creating a challenge for a consistent energy supply; the fluctuations make the integration harder. Most solar technologies require large land areas or the mining of rare minerals, which generates some social and environmental impact.[242] Despite its downsides, however, solar energy seems to be indispensable for a sustainable future, especially in less developed regions of the world.

CSP, despite being more capital-intensive and geographically constrained, offers advantages in large-scale energy production and storage, providing stable, utility-scale power solutions.[243] PV systems, on the other hand, are more versatile and scalable (from small-scale residential setups to large commercial solar farms), providing flexibility in application depending on the energy needs and availability of resources. They also support the development of decentralized energy systems, which can increase energy security, reduce transmission losses, and make energy production more resilient to disruptions. The current challenges related to efficiency limitations, concerns over material availability, and waste management may be overcome with new innovations in materials (like perovskites) and cell manufacturing.[244]

As far as solar fuel production is concerned, green hydrogen production using electrolyzes powered by solar electricity will likely be significant in the near future as the growth of current market share indicates;[245] developments in both electrolyzer and solar technologies will contribute to the much wider adaptation of solar electrolyzers. The photocatalytic and photoelectrochemical processes, on the other hand, are still far from making significant contributions to solar fuel production, even though they also seem to hold transformative potential for the long-term future.

Solar desalination, while promising for water-scarce regions, also has challenges related to high energy requirements and the slow pace of water purification compared to conventional desalination technologies. Additionally, the upfront costs of installing solar desalination plants can be prohibitive. However, harnessing solar energy to desalinate seawater offers a renewable, low-emission solution for producing fresh water, which is crucial for maintaining water security in rural regions. The integration of solar desalination plants with renewable energy sources or solar energy sources such as CSP or PV can decrease energy requirements and create economic benefits.[246] By overcoming these challenges through technological innovation, cost reduction, and supportive policies, these solar technologies hold immense potential to advance global sustainability goals, particularly in regions where energy and water access are critical issues, such as Africa.

8.3. Challenges and opportunities for wind energy

There are numerous opportunities for the expansion of wind energy installations, like boosting regional economies by creating job opportunities in manufacturing, construction, repair, and operation, as well as improving the national energy mix by introducing a clean, renewable energy source.[247] On the other hand, there are several challenges as well. For instance, to harness wind energy efficiently, the wind pattern of the target location is very important. Environmental and geographical elements cause significant local changes in wind speed and direction;[248] hence, a good site must be selected having a stable and high wind speed throughout the year. In addition to high average wind speed, a wind farm must be built in a location sufficiently far from the noise-sensitive human population, with a site that does not affect the lives of wildlife or block the air traffic route.[249] As a result of these issues, optimal wind sites are frequently in remote locations, sometimes on the top of a distant hill, creating installation challenges such as the transportation of large-scale equipment and other construction materials. Moreover, those remote locations can be out of the range of the national grid system. Hence, the national grid network must be upgraded to connect wind-rich areas with population centers that require electricity.

Although the wind potential of Africa is estimated to be around 10 600 TW h (with an average wind speed of 5.1 m s^{-1} at an altitude of 10 m), wind energy remains underexploited despite the growing energy demand.[250] This is because of policy-related issues (most African countries lack policies promoting wind energy) and several technical issues like the integration of a fluctuating wind energy generation with the outdated national energy grids, as well as economic issues like the operational expenses, the cost of wind energy equipment, and the cost services given to the industry.[251] To overcome these issues, strong policy frameworks are required in African countries, such as providing tax reduction or long-term credit opportunities for investors, as well as encouraging local producers to manufacture expensive equipment to localize value chains.

8.4. Challenges and opportunities for biofuels

A key challenge with first-generation biofuels is their competition with food crops for arable land. This challenge has diminished with the use of second-generation biofuels, which use waste materials, and third-generation biofuels, which rely on high-lipid microorganisms like microalgae. However, despite their advantages, like carbon sequestration and minimal land use, more technological advancements are needed to reach the commercialization of these biofuels.

Various biofuels are produced with various conversion methods using a large variety of biomass sources. The application of ML to those fields is vastly explored. From a general point of view, it can be said that ML models are more successful in thermochemical conversion.[252] This success is largely due to the relative ease of combining data from diverse experimental studies, creating robust datasets suitable for ML model training. In contrast, biological conversion methods present challenges due to the heterogeneity of input variables across different experiments. Integrating datasets from multiple studies often requires extensive preprocessing and meticulous data curation, leading most research to rely on single-study data for model development, which limits the generalizability of these models.[203]

Variability between different biomass sources also creates challenges for the generalization of ML models. Early ML models mainly focused on single biomass types; however, with the growing interest in coprocessing and co-cultivating multiple biomass feedstocks (and even incorporating other materials like plastics), research has shifted towards developing ML models that can accommodate mixed biomass sources.[20] Advanced ML techniques, along with the incorporation of variables related to biomass characteristics, have facilitated this transition, yielding promising results. For instance, variability in feedstock composition of different lignocellulosic biomass is mitigated through variables like proximate and elemental analyses, which are consistently pivotal in model development;[23] on the other hand, however, achieving a generalizable model remains a significant challenge, particularly in biodiesel production from sources like microalgae and other oleaginous microorganisms, where feedstock variability continues to hinder model reliability.

The economics of biofuels plays a critical role in achieving SDGs; hence, identifying promising biomass feedstock and processes that can maximize the production of desired/needed biofuels while minimizing costs and meeting quality specifications is a critical task. However, both feedstock and biofuel needs, as well as financial resources for investment, are different for different regions of the world due to the differences in climate conditions and living standards. This will impose an additional challenge in generalizing the experience gained in biofuels, including ML applications, to the entire planet. On the other hand, ML may also offer valuable assistance in identifying the optimal biomass-to-biofuel conversion routes and optimizing them for specific areas. This complex challenge requires a multi-disciplinary/multi-organizational approach in which ML can help navigate the vast solution space efficiently using the data, experience, and expertise in various disciplines and organizations.

8.5. Challenges and opportunities for batteries

If we center particularly on the advancement of rechargeable batteries, several critical concerns must be focused on to succeed in the SDGs. The first concern is related to raw material extraction and processing. Li-ion chemistries typically contain raw materials such as lithium, cobalt, manganese, nickel, copper, aluminum, and fluorine. Yet, there are several issues with the extraction and processing of these raw materials. For instance, the recovery of Li metal from mineral deposits is highly energy intensive as it involves high temperatures, high carbon emissions, and the evolution of acidic liquid effluents. Similarly, the recovery of Li metal from brines may lead to the sharing of limited water sources. Co, Ni, Mn, Cu, and Al mining is similarly energy-intensive, all producing water pollution. In addition to the environmental impacts, Co mining is associated with human rights issues. On top of these, currently, these materials travel up to 50 000 miles from the mine to the final consumer. Sustainability needs to be prioritized to localize the supply chain. For instance, the use of earth-abundant active materials in developing next-generation batteries should be highlighted. Recent approaches in the Li-ion battery literature focus on developing Ni-rich cathodes to decrease the amount of Co within the compound or advance LFP cathodes that do not contain nickel or cobalt. Moreover, research beyond Li-ion battery chemistries has accelerated the development of metal-ion batteries, in which Li is substituted by a more abundant element such as Na, Mg, Al, or Zn, the replacement of metal oxide cathodes with sulfur or oxygen ones, the search for solid-state electrolytes that are less volatile and less toxic to the environment, and the investigation of anode-less batteries.[253]

The second challenge concerns battery manufacturing: even disregarding raw material mining and refining, 30–55 kW h of energy is required to create a 1 kW h Li-ion battery.[253] Subsequently, battery manufacturing should be revised to promote sustainability. The most urgent issue in the short term would be the development of the dry electrode coating process. Currently, NMP solvent is used to prepare the electrode slurry. But NMP is highly toxic, and the evaporation and following recovery of NMP is one of the most significant energy users in a plant. Subsequently, switching to a dry coating process could significantly reduce carbon footprint and cost and lower energy consumption. Furthermore, optimized charging protocols with shorter and more energy-efficient formation cycles can lead to significant advancements in the manufacturing process.

Battery recycling is another important issue to be considered. The life cycle assessment (LCA) of batteries is commonly used to investigate the environmental effect of the product from cradle to gate, cradle to grave, and grave to cradle. LCA of Li-ion batteries shows that recycling active materials typically consumes less energy and produces less greenhouse gases and SOx emissions than mining and refining these materials. Battery recycling is also critical to prevent the depletion of the limited minerals. There are various recycling methods, and these processes should also be considered based on sustainability. One should also keep in mind that the environmental and economic impact of battery recycling also depends on transportation costs and governmental policies.[254]

The secondary use of batteries should also be considered. As discussed above, battery recycling is critical for sustainability. But conventional battery recycling methods are still energy-intensive, costly, and emission-heavy. Moreover, with the significantly increasing demand in the EV market, the number of retired batteries will soon be considerably high, and recycling may not be possible for all. Consequently, repurposing and reusing the retired EV batteries will be required to achieve the SDGs. Second-life batteries can be used in stationary energy storage, EV charging infrastructure, grid stabilization, and off-grid storage for rural areas or disaster relief.[255] Some critical aspects for increasing the secondary use of batteries would be focusing on materials and battery design for longevity, developing market mechanisms and policy setups that support the battery repurpose and reuse, and designing battery management systems to manage these retired batteries effectively and safely in their second life.[256]

Last but not least, the importance of hybrid renewable energy storage systems should be emphasized, specifically for providing reliable, sustainable, and clean energy for rural areas and developing countries. These hybrid systems may combine PV power, wind power, hydrogen storage, rechargeable batteries, and supercapacitors. Subsequently, the design of such systems not only has environmental and economic advantages but also can increase access to energy in remote communities and reduce the necessity of diesel generators for backup in the case of a power outage or grid failure.[257]

8.6. Challenges and opportunities for ML

Data availability and quality are generally the biggest challenges for ML, which employs algorithms relying on statistical learning in any field. The dataset should contain sufficient information (*i.e.*, input–output relationships) for the model to be built or analysis to be performed and large enough for reliable inference and generalization. These challenges will exist, and they will probably be bigger in ML applications in SDGs; especially the data collected from different sources (like different countries or regions, different types of organizations, and different disciplines and expertise) will have significant levels of noise, incompatibility, mismatches, and even conflicts. On the other hand, the availability of remote monitoring and sensing technologies and the presence of numerous data sources (including national and local governments, offices of various UN organizations, and international institutions) constitute a big opportunity for the use of ML in macrolevel applications (such as the analysis and modeling of atmospheric, agricultural, economic or demographic data) for policy development and execution. This could be improved further with closer collaboration among multinational organizations, governments, industry associations and non-government organizations.

The data availability for individual technologies, on the other hand, has been increasing continuously in recent years with a different set of solutions. One of the most common strategies to improve data availability is the creation of an ever-growing number of databases containing experimental and computational databases.[16,20] Some examples of experimental databases are Pauling File Database,[258] Inorganic Crystal Structure Database (ICSD),[259] Cambridge Structural Database,[260] Crystal Open Database,[261] CRYSTMET,[262] ZINC database,[263] and PubChem[264] while The Material Project,[265] Automatic FLOW for Materials Discovery Library (AFLOWLIB),[266] The Computational Materials Repository,[267] Open Quantum Materials Data (OQMD),[268] AiiDA,[269] and JAVIS- DFT[270] are examples for the computational (mostly based on density functional theory) databases. Currently, most of the databases contain material properties, and they are used for material screening or estimating the other properties; in recent years, however, discipline-specific (like perovskite solar cells[122] or catalysis[271]) databases have been developed in increasing numbers although they are not as sophisticated as material databases due to the difficulty in making generalizations in complex structures with complex functions. Other opportunities that will contribute to the improvement of data availability are the ever-growing trend in open-access publications and the availability of repositories for the storage of research data and computer codes.

Implementation of transfer learning, which involves information transfer from a model to analyze a different (but similar) problem with a smaller number of data points, may also be used to ease the data availability problem. Some of the ML implementations, such as the analysis of demographic, agricultural, and climate data, as well as energy forecasting, optimization of national grid networks, or analysis of energy trading, are quite similar in different countries; hence, the models developed in the countries with high data availability can be used for similar analysis involving other countries through transfer learning algorithms when sufficient amount of data is not available. The same is also true for the analysis of research and development data in specific energy technologies, while data augmentation techniques allowing the use of experimental and computational data as well as low- and high-accuracy data can also be employed to ease the problem arising from the insufficiency of available data.[272]

Another important challenge is the lack of technological infrastructure and budget to build in less developed geographies for which the SDGs were set in the first place. The monitoring and data collection, which also require infrastructure, have to be local, even though ML analysis could be done remotely (even that would not be the best option anyway). To overcome this, collaborations should be made between local authorities/experts and their counterparts in other countries or international organizations.

Finally, the concerns for the high energy consumption and greenhouse emissions of data storage and large ML models, which are likely to be required in SDG-related activities, have to be resolved. Although it is not easy to forecast the potential energy consumption and emissions for AI-related issues in the future, the current numbers can provide some ideas to understand the scale of the problem. According to the International Energy Agency,[273] the data centers use about 1–1.3% of global electricity consumption (excluding energy used for cryptocurrency mining) while they account for 1% of energy related GHG emission. These numbers are quite significant, and they are very likely to increase more in the future with the increasing sizes of databases and ML/AI models. On the other hand, one should also consider the amount of energy saved and GHG emission avoided with the use of AI; for example, Tomlinson *et al.*[274] reported that AI-generated one-page text or an image consumes less energy than those generated by humans. Even though the high energy consumption and GHG emissions associated with ML/AI are inevitable, they are probably justifiable; however, there seems to be a need for further clarification in people's minds.

9. Concluding remarks

Sustainable energy is one of the major enablers for SDGs, as it is directly related to some goals (especially SDG 7 and SDG 13) while indirectly affecting others as numerous works identified positive and negative interactions between energy and the targets of SDGs. Similarly, ML or AI, in general, may directly or indirectly contribute to the efforts toward SDGs, starting from monitoring, collecting, and analysis of worldwide SGD-related data, assisting the planning for SDGs through forecasting energy supply/demand and capacity of resources at local and global levels, and supporting research and development in the fields related to SDGs including solar, wind, and biofuel technologies. Although there are significant challenges to reach the targets of SDGs on time (in 2030), the efforts are likely to continue beyond 2030 with increasing awareness and technological progress.

To maximize the benefit of ML in achieving SDGs and parallel efforts beyond 2030, the data availability should be improved first. Although this issue in scientific research has to proceed with its own dynamics, the accessibility of national, regional, and international levels of SDG-related data (involving climate, demography, economy, health, education, and so on) can be improved with special efforts by international organizations taking part in SDGs. The effective coordination of activities involving the use of ML in SDGs seems to be another area that requires special attention; the people and organizations that should take part in such efforts will likely be from various unrelated disciplines, interest groups, and economic, social, and cultural background with different agendas and goals. Harmonizing such diverse groups will be a challenging task by itself and have a critical impact on the effective use of ML in SDGs.

Data availability

No primary research results, software, or code have been included, and no new data were generated or analyzed as part of this review.

Conflicts of interest

There are no conflicts to declare.

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