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Artificial Intelligence for Green Energy: Case Studies in Materials Discovery, Perovskite Solar Cells, Hydrogen Production, and Grid Integration

Tanmay Saini
tanmay.manu1@gmail.com

ABSTRACT

With the growing global demand for energy, the use of renewable power, like wind and solar, has revealed that traditional energy management approaches are falling short. This has made artificial intelligence (AI) a key technology for advancing green energy. This review collates and analyses 38 sources to assess the use of AI throughout the green-energy supply chain, specifically on the following case studies: Materials and Catalyst Discovery, Perovskite Solar Cell Manufacturing and Recycling, Optimization of Hydrogen and Biofuel Production, and Management of Renewable Electricity Grids. In each case, the review examines the key issue, provides an accessible explanation of relevant AI techniques, and provides a summary of evidence and an assessment of the robustness of that evidence. From the beginning of the candidate identification process to process optimization, and finally to real-time forecasting and control, the analysis shows that AI plays an increasingly important role throughout the chain. There are also changing requirements for models: They must be tolerant of error, transparent, and have access to data. In all instances, the combined models, in which data-driven learning is combined with physical knowledge or optimization algorithms, outperformed the single-method models. Explainable AI helps to improve scientific understanding and accountability. The evidence base, however, suffers from inconsistent measures, limited size of the data sets, weak comparisons and lack of large-scale use. Self-driving laboratories, shared datasets and strong validation systems will be key for the future to ensure trust in AI in energy systems.

1. INTRODUCTION

Global energy consumption has gone up considerably over the past 150 years of economic growth and industrialization [1,2]. Energy resources are limited, too much supply results in loss of energy, and too few results in sustainability issues [1]. Improving individual devices, however, is not enough as energy is also lost between devices and across the system. Furthermore, contemporary energy systems are built on the use of a wide variety of energy sources and are required to manage energy supply and demand which is constantly varying.

The traditional energy management systems (EMS) were developed to keep track of and regulate electricity from a small number of reasonable, steady power generation facilities. The challenges for these systems lie with integrating electricity from multiple smaller electricity generation facilities and in integrating variable renewable electricity sources into older infrastructure. These setups require immediate decision making, and create a big challenge to the conventional EMS [2].

Since around 2014, the field of AI research and patents has experienced a surge of interest and activity, especially in the energy industry, thanks to the proliferation of computing power. Interestingly, about 17 patents for each research paper have been found in this area, showing a strong commercial interest. AI-based energy management is a combination of infrastructure, sensors, communication networks and information technology that is used to monitor, control and optimise energy production and consumption [1,2]. The main goals are to improve efficiency, reliability, integrate renewables, and cost savings [2].

Unlike traditional approaches, AI can analyze large datasets, recognize intricate relationships, and learn from data to make predictions and decisions. There have been several reviews of AI applications in the energy industry as a whole, with many listing the applications without providing detailed information about methodology or the reliability of the outcomes. This review is focussed on green energy, which is also known as renewable and low carbon energy and includes four detailed case studies. This review explores three key questions: What is AI's contribution to each component of the green-energy supply chain and how is this contribution realized; What is the quality and meaning of the supporting evidence; and What are the common pitfalls in all of the applications and what are the implications of these for future research?

1.1 Scope and Approach

These four case studies were selected as they span the entire green-energy value chain from discovery of materials to generation of devices, fuels and operation of the grid, and each has a comprehensive literature base. There are 38 sources cited that span a wide range of studies of the two fields as well as primary studies that present specific results, spanning the years 2018-2026. Relevant literature was retrieved from Google Scholar and Scopus. Nuclear energy is low carbon but is not included in this review, as its engineering, safety and regulatory environment is quite different from renewable energy. The results of some sections are based on a limited number of detailed studies [4-7] and this is indicated where appropriate and discussed in Section 7 and 8 where the limitations of these are discussed.

2. THE AI TOOLKIT FOR GREEN ENERGY SYSTEMS

The four case studies are similar in that they share common AI techniques, although they address quite distinct problems. This section will describe what these methods do, how they are trained and evaluated and explain them so that the evidence presented in subsequent sections can be interpreted.

2.1 Learning from Data Instead of Equations

In a conventional energy-system analysis, a system is modeled with physical equations, like those of heat flow or electrical load. They are valid for systems where the interactions are understood, but they are hard to construct, and may be slow to solve when the system contains many interacting components and manifestly fluctuating and erratic data [2]. The most popular application of AI in energy research is machine learning (ML), which differs by being trained, rather than programmed, by equations; many examples of energy input and output data are presented, and the model learns the relationship between the two from the data without any programmatic guidance [1,2]. As a result, ML is suitable for today's energy networks which generate a vast amount of information from smart meters, sensors and monitoring devices [2].

2.2 Three Learning Approaches

There are typically three types of ML methods [2]. For supervised learning, the model is trained on examples that are paired with the desired output, such as previous weather conditions and the electricity that a solar farm actually generated. After training it can generate the output for new inputs. Unsupervised learning is a type of machine learning that is used to discover hidden patterns or clusters within unlabeled data, such as identifying households that share similar consumption patterns. Reinforcement learning (RL): The model learns by trial and error by taking actions, getting a reward or penalty for those actions, and eventually learning a strategy to maximize the total reward. This makes RL a good option for sequential decisions, e.g., when to charge or discharge a battery [2]. Many applications use a mixture of these approaches, with the models being a mixture of multiple models, one for a particular application [2,6].

2.3 Training, Testing, and Data

All ML models are trained on a portion of the data set and tested on examples it has never seen before, to ensure that its predictions are correct [2]. The training data may be experimental and/or real measurement data, or data obtained from a computer simulation [2,7]. In materials research, one often has to deal with simulated data, such as that produced by the quantum-mechanical calculation density functional theory (DFT), which predicts a material's properties based on the arrangement of its atoms and electrons. Even though DFT is accurate, it has high computational cost; hence, ML models developed using DFT results are valuable since they can predict with much less time [7]. Deep learning (neural networks with many layers) and RL (reinforcement learning) are, in general, the top-performing methods, and their hybrids (deep RL) are effective methods for very large, dynamic power systems. [2]

A key risk in training is *overfitting*, in which a model memorizes the particular examples it was trained on rather than learning a general relationship. Such a model performs impressively on familiar examples but poorly on new ones. The risk is greatest when datasets are small, which, as later sections show, is common in laboratory-scale energy research.

2.4 What AI Is Used For

Across the green-energy literature, AI performs three main tasks. The first is *prediction*: forecasting renewable output from weather data and anticipating electricity demand [6], or predicting the properties of a candidate material before it is synthesized [7]. The second is *optimization*: finding the best settings for a system, such as balancing loads and scheduling energy flows in a grid [6], or identifying the operating conditions that maximize hydrogen or biodiesel yield [5,8]. The third is *autonomous operation*: continuously analyzing incoming data and making control decisions in real time, for example in building and industrial energy management [2].

2.5 How Performance Is Measured

Multiple studies report performances by multiple measures and the differences between them are important when comparing performances. Coefficient of determination (R^2): the amount of variation in the measured results explained by the model (value of 1 is a perfect fit, value of 0 has no explanatory power). The correlation coefficient (r) indicates how closely the predicted values correspond to the actual values (−1 to 1). The root−mean−square error (RMSE) provides a measure of the typical prediction error in the units of the quantity to be predicted, while the normalised mean squared error (NMSE) expresses the error in terms of the spread of the data. *Accuracy* is used for classification tasks and gives the percentage of cases a model assigns to the correct category. Because these measures are not interchangeable, results on one cannot be compared directly with those on another, a point returned to in Section 7.

2.6 Common Algorithms

Random forest: many decision trees with each trained on a random subset of data, whose predictions are averaged. *Gradient boosting:* decision trees built to correct the errors of the previous ones, built one after another; XGBoost and LightGBM are widely used. *Support vector machine (SVM):* can capture nonlinear relationships by finding boundaries or curves that fit the data with the widest possible margins. *Artificial neural network (ANN):* inspired by neurons, they are layers of interconnected nodes whose connection strengths are optimised during training. *Convolutional neural networks (CNNs):* specialise in grid-like data, such as images. *Recurrent neural networks (RNNs):* process sequences, such as time series. *Long short-term memory (LSTM) networks:* RNNs that retain information over longer sequences with *Bi-LSTM* reading sequences in both directions. *Bayesian optimisation:* search methods for when tests are expensive: builds statistical models of which settings are likely to work and chooses the next test accordingly. *Genetic algorithms (GA):* mimic natural selection by combining and mutating candidate solutions and keeping the best. *Particle swarm optimisation (PSO):* moves many candidate solutions through the search space with each being guided by its own best result and the group's best result.

3. CASE STUDY 1: MATERIALS AND CATALYST DISCOVERY

3.1 The Problem

Green-energy technologies depend on materials that convert, store, or separate energy and chemicals efficiently: light-absorbing materials in solar cells, catalysts for producing hydrogen, and porous materials that absorb carbon dioxide (CO_2). Traditionally, such materials are found through slow, repeated cycles of laboratory synthesis and testing, or by computationally expensive quantum calculations like DFT [7]. With an almost unlimited number of possible compositions, these methods can examine only a tiny fraction of the candidates.

3.2 How AI Is Applied

ML accelerates discovery by forecasting material properties directly, increasingly replacing first-principles calculations (methods based only on basic physics, of which DFT is one) while retaining similar accuracy [7]. A model trained on known materials can estimate the properties of thousands of untested candidates in the time a single DFT calculation would take. This enables *high-throughput virtual screening*, in which large libraries of candidates are evaluated computationally and only the most promising are synthesised [7,9]. Applications include predicting electronic arrangement and molecular properties, constructing *force fields* (models of the forces between atoms that allow their motion to be simulated), and speeding up quantum analyses using neural networks, Bayesian optimisation, and generative models [7]. Together, these form the basis of AI-assisted materials discovery for clean energy [9].

Catalysts, materials that speed up chemical reactions without being consumed, are a particular focus, especially for hydrogen production, CO_2 conversion, and clean-fuel synthesis [7]. One important tool is the *machine-learning potential*: a model that learns the energy and forces between atoms from quantum calculations, so that the behaviour of a catalyst surface can be simulated far faster than with DFT alone. To be read by a model, the 3D arrangement of atoms must first be converted into numbers; a common way of doing this is *Smooth Overlap of Atomic Positions* (SOAP), which encodes the neighbourhood of each atom in a form that does not change if the structure is rotated or shifted. SOAP-based ML potentials, together with Bayesian optimisation, genetic algorithms, and virtual screening, have supported electrocatalyst discovery, optimisation of catalyst composition, characterisation of catalytic surfaces, and prediction of reaction pathways [7]. AI has been applied to the sustainability-oriented design and assessment of green catalysts [10]; for example, calcium oxide (CaO) nanocatalysts for biodiesel production have been optimised using AI alongside reactor design [8]. Beyond catalysts, ML has accelerated the design of membranes for separation and clean-energy applications [11] and of *nanofluids* (liquids containing suspended nanoparticles) that improve heat transfer in renewable-energy systems [12].

3.3 From Screening to Inverse Design

Virtual screening still requires a list of candidates to be defined in advance. A newer approach, *inverse design*, reverses the process: researchers specify the properties they want, such as a particular ability to absorb sunlight, and a generative model proposes new structures likely to have them [7,13]. Many generative models work by compressing each known material into a short list of numbers, called its position in a *latent space*. This can be thought of as a map on which materials with similar properties sit

close together. Searching this map for regions predicted to have the target property, and then converting those positions back into chemical structures, permits the model to propose materials that were never in the first library [7,13]. Inverse design is therefore not limited to candidates that researchers have already thought of.

3.4 Application to Carbon Capture

The same tools are being applied to *carbon capture, utilisation, and storage* (CCUS), the set of technologies that trap CO_2 at emission sources and either store it or convert it into useful products. AI accelerates the discovery and optimization of *sorbents* (materials that adsorb CO_2 on their surface) and other functional nanomaterials [14]. In photocatalytic CO_2 conversion, which uses light-activated catalysts to turn CO_2 into fuels, AI combined alongside computational chemistry helps screen candidates and explain reaction pathways [15]. Separation membranes, which remain essential to carbon capture, benefit from the same ML design methods described above [11]. AI has been able to predict gas uptake in metal–organic frameworks (MOFs) – crystalline porous materials constructed from metal ions connected by organic molecules – with errors as low as 7.18% [7].

3.5 Critical Assessment

The primary value of AI in materials discovery is its speed – it reduces the vast library of materials to a small list of potential candidates. Four caveats may temper the reported successes, however. One is that datasets of materials are often limited to well studied chemical families and a model trained on one family does not transfer well to other families [10,13]. Second, the accuracy of models built on the results of DFT and other simulated results is limited by the accuracy of the underlying data: a fast prediction is not necessarily a correct one [4]. Third, computational predictions should be validated experimentally, and validation at scale is difficult [10,13]. The limitation in practice is not on proposing candidates, but on testing candidates, which is why the closed-loop "self-driving laboratories" mentioned in Section 9 are viewed as the next step. Lastly, the evidence in this field is derived from review articles which provide a high-level summary of many studies [7,9] and the individual results such as 7.18% MOF error are encouraging, but should be interpreted as examples rather than typical performance.

4. CASE STUDY 2: PEROVSKITE SOLAR CELLS, FROM GREEN SOLVENTS TO RECYCLING

4.1 Background

The field of photovoltaic (solar) cells is one of the most intensively studied domains where AI is set to play a vital role in materials research. ML has identified promising compositions from large databases of candidate formulas in seconds and to optimise stability and *power conversion efficiency* (PCE), the percentage of incoming sunlight converted into electricity [7]. *Perovskite solar cells*, named after the crystal structure of their light-absorbing layer, have attracted particular interest. However, their fabrication relies on solvents that raise health and environmental issues, and their end-of-life recycling is not yet well established [4]. This case study follows a single line of research [4], supported by related work, through

three stages of a perovskite cell's life: choosing safer solvents, predicting cell performance, and recycling. This work sits within a wider movement to apply AI in *green chemistry*, the design of chemical products and processes that reduce hazardous substances, which includes deep learning for predicting whether compounds are biodegradable [16], AI-driven drug design coupled with green synthesis [17], and wider surveys of AI as an enabler of increasingly sustainable chemistry [18,19].

4.2 Selecting Greener Solvents

Problems in Green chemistry are good for ML because they are large data set problems, are complex reaction system problems, and are nonlinear relationship problems. One of the important problems in the manufacture of perovskites is whether the chemical precursors are soluble in a potential solvent. This can be estimated by Hansen solubility parameters, which are three numbers representing the strength of dispersion forces, polarity, and hydrogen bonding between a molecule. Random forest models were very accurate in predicting these relationships with an average correlation $r = 0.96$ for Hansen solubility prediction and green-solvent screening [4]. The models received descriptors, that is, numerical features describing a molecule's structure, shape, polarity and solubility [4].

Solvent selection was conducted in a two-step Bayesian process. The candidates were first narrowed down by evaluating the ability of each solvent to bind to the precursors and maintain the stability of the solution, followed by an efficiency model predicting which of the remaining solvents had the best potential for forming the perovskite films, based on crystal grain size, growth rate, and defect control [4]. The reasons behind the prediction results were indicated by the SHapley Additive exPlanations (SHAP) analysis. It concluded that the molecular weight, dispersion interaction, dipole moment, polarisability, and vapour pressure are the most important parameters, and it pointed to the use of triethyl phosphate (a solvent) and methylammonium chloride (an additive) as relevant parameters [4].

These numerical techniques were complemented by natural language processing (NLP) which translated published literature into machine-readable data. Despite limited data, an NLP model trained on roughly 30,000 perovskite-synthesis papers found 35 prospective solvents, while filtering out the endocrine disrupting chemicals with a 90% accuracy, using a context-aware model [4]. AI in conjunction with DFT further resolved at the atomic level the interactions between the solvents and the precursors, including the role of Lewis acid–base interactions (electron-pair sharing between molecules), hydrogen bonding and defect formation [4].

4.3 Predicting Device Performance

A gradient boosting model was used to predict the PCE of finished devices in the same study with an R^2 of 0.74 and an RMSE of 2.09 [4]. *Life cycle assessment* (LCA), a method for measuring a product's environmental impact from raw materials through to disposal, was integrated with AI to evaluate sustainability early in the design process. AI-integrated LCA clearly identified environmental hotspots, the stages contributing most to overall impact, and supported immediate decision-making [4]. Extending such lifecycle frameworks across the full sequence from innovation to use to recovery [13] links the manufacturing concerns of solar energy with the operational forecasting covered in Case Study 4 [6].

4.4 Recycling at End of Life

The same study applied AI to end-of-life processing. A neural network predicted suitable recycling methods for hazardous components with approximately 70% accuracy [4]. A random forest model identified 10 suitable de-encapsulation reagents having an RMSE of 0.167 [4] and a support vector machine identified 23 reagents with a reactivity score of 0.819 [4].

4.5 Critical Assessment

This is the most apparent case from the literature reviewed that involved using AI throughout the entire lifespan of a product, and there are three implications to be drawn from this case. First, accuracy declines as the target moves further from the molecular properties: solubility is mainly determined by the molecular structure, and has $r = 0.96$, while the efficiency of the device is determined by several processing steps and is $R^2 = 0.74$, so about a quarter of the variation in efficiency is not explained. Second, the accuracy of the prediction at 70% for the recycling method implies that approximately three in ten predictions were incorrect, so such models should be used to narrow down the choices for the human expert to consider rather than for definitive predictions. Third, the SHAP results are not only statistically significant, but also scientifically significant: the factors identified, such as dipole moment and vapour pressure, are chemically meaningful, which adds more confidence to the fact that the model is capturing real chemistry and not just a coincidence. The primary concern is the limited number of studies that have been conducted, with all of this evidence from a single study [4] and a larger number of independent studies with different perovskite compositions and laboratories would be required to confirm and generalise the results.

5. CASE STUDY 3: OPTIMISING HYDROGEN AND BIOFUEL PRODUCTION

5.1 Background

One of the cleanest, most versatile energy carriers, hydrogen could also fulfil the demand for the future in energy and industrial sectors, but its mass-scale implementation is hindered by the energy efficiency of hydrogen production, storage, and transport, alongside the energy cost. Usual production methods have been assigned a colour code to indicate the method and carbon intensity [5]. One of the more prevalent methods is steam methane reforming, which involves reacting water vapour with the natural gas over a catalyst at 700–1000 °C and at high pressure, but requires a lot of energy and produces CO_2. Partial oxidation provides about 30% of the world's hydrogen, while autothermal reforming integrates the two methods such that the heat from the partial oxidation reaction is balanced by the heat utilized for the reforming reaction. Chemical looping technology is a solid based oxygen carrier process technology that allows for the generation of high purity hydrogen along with a concentrated CO2 stream that is easier to capture. Electrolysis (electrolysis of water to hydrogen and oxygen with electricity) results in no direct carbon emissions if powered by renewable sources, but is only about 5% of the production. Biological methods such as dark fermentation (conversion of organic matter by bacteria in the absence of light) have drawbacks such as low conversion efficiency [5].

5.2 How AI Is Applied

In these routes AI is predominantly used as an optimisation tool, with a strong quantitative evidence base [5]. ANNs have been optimized for biomass pyrolysis (i.e., heating of organic matter without oxygen), dark fermentation, and steam methane reforming for the prediction of gas composition and thermal efficiency and identification of the optimal operating conditions [5]. Support vector machines (SVM) demonstrated a higher prediction accuracy of hydrogen yield than neural networks (NN) in comparative studies, and the use of AI in combination with genetic algorithms (GA) and particle swarm optimisation (PSO) allowed the best SVM results to be obtained, with an output 2.1 times higher than in the unoptimised case [5].

Several studies have compared the performance of AI with response surface methodology (RSM), which is a traditional statistical method that fits a simple curved surface to the experimental data. A support vector machine (SVM) was trained with a Bayesian algorithm with adjusted R^2 values greater than 0.99, and with a lower error than the RSM, while an SVM and an artificial bee colony optimiser (another nature-inspired search method) were used to obtain an R^2 of 0.9464 and a correlation of 0.9751 between the predicted and the observed hydrogen output [5]. The R^2 for the electrolysis ranged from 0.989–0.997 for comparisons of an RNN, LASSO (a variant of standard regression that discards unimportant variables), XGBoost, linear regression, and LightGBM, some linear models reaching 0.999 [5].

Beyond production, AI supports the hydrogen supply chain, for example by optimising the location of refuelling stations and by combining scenario planning, optimisation, visualisation, and data management in decision-support tools [5]. For hydrogen storage in porous materials, ML models, including graph neural networks (which represent each material as a web of connected atoms) and ANNs, predicted uptake with accuracies of up to 97%. SHAP analysis identified temperature, pressure, the *isosteric heat of adsorption* (how strongly hydrogen binds to the material's surface), and the *BET surface area* (the total internal area available for adsorption) as the controlling factors [5]. The results are consistent with dedicated reviews of AI for hydrogen and battery technologies [20], smart-grid integration [21], renewable hydrogen systems [22], and renewable production routes [23], and with a review of nanomaterials for hydrogen and CCUS [14].

5.3 A Related Route: Biofuels

Biofuel research shows a similar pattern. AI and ML have moved process design beyond adjusting one factor at a time and classical statistical optimisation, towards data-driven prediction of yields and fuel properties [24]. One study combined principal component analysis (PCA) with an ANN to link the chemical composition of biodiesel to its fuel properties, identifying which components most influence its quality [25]. Broader reviews describe AI applications in characterising feedstocks (the raw biological materials used), modelling conversion processes, and assessing whole bioenergy systems [26]. Because biodiesel production depends on catalysis, the AI-optimised CaO nanocatalysts discussed in Section 3.2 link this case study to materials discovery [8,10]. As in hydrogen production, the dominant methods are ANNs and SVMs, often combined with genetic algorithms or particle swarm optimisation [5,24].

5.4 Critical Assessment

The literature on hydrogen presents some of the best performance numbers reported in this review, but these should be interpreted with caution. Simple linear regression, with R^2 of 0.999 for electrolysis, suggests a very linear relationship between the inputs and the output, so there is little additional benefit from more complex AI models over this range of study. Very high R^2 values may instead reflect small datasets from laboratory experiments, where the risk of overfitting (Section 2.3) is greatest, and results obtained under such controlled conditions may not hold in industrial plants. The choice of baseline matters as well: a 2.1-fold improvement over unoptimised conditions shows that tuning is worthwhile, but not that AI outperforms established engineering methods. The comparisons with RSM are more informative because they test AI against a recognised conventional method. Finally, most hydrogen applications use AI to tune the operating conditions of existing processes instead of discovering new ones, so they complement, and do not replace, the materials-discovery work in Case Study 1.

6. CASE STUDY 4: FORECASTING AND GRID INTEGRATION OF RENEWABLES

6.1 The Problem

The main obstacle to embedding renewable energy into electricity networks at scale is that wind and solar generation are intermittent and variable, which has motivated the use of AI for forecasting, energy management, and control [6]. The challenge is especially acute in *microgrids*, small local electricity networks that can operate either connected to or separately from the main grid, and in *hybrid renewable energy systems*, which combine several sources such as solar, wind, and storage [6].

6.2 How AI Is Applied

In microgrids and mixed systems, AI predicts demand and solar and wind output; manages energy flows, *demand response* (shifting consumers' usage to match available supply), and the control of combined sources within economic and operating limits; and improves long-term planning, grid reliability, and real-time scheduling [6]. In a study combining wind, wave, and solar generation, PSO coupled with an ANN achieved the fastest convergence (3,367.5 seconds) and an NMSE of 1.10%, outperforming the other hybrid optimisation–ANN algorithms tested [6].

Comparative study shows that each method family has particular strengths and weaknesses (Table 1). The most consistent finding is that hybrid architectures, such as ANNs paired with genetic algorithms, PSO, or dynamic programming, and fuzzy-logic controllers tuned by GA or PSO, outperform single methods during convergence, robustness, and forecast precision [6]. *Fuzzy logic* is a rule-based approach that handles uncertainty using degrees of truth (for example, "fairly sunny") rather than strict yes/no categories.

Table 1. Strengths and weaknesses of AI method families for microgrid and renewable-energy management, summarised from Talaat et al. [6].

Genetic algorithms	Handle multiple objectives at once; simple to implement	Long computation times; may converge prematurely on a sub-optimal solution
Deep learning (CNN, LSTM, Bi-LSTM)	Excellent at fault diagnosis, maintenance prediction, and solar-irradiance forecasting from noisy, complex data	Decisions lack transparency; require large training datasets
Particle swarm optimisation	Suits nonlinear problems; converges quickly	Can become stuck in a locally, rather than globally, optimal solution
Fuzzy logic	Handles uncertainty well	Depends on rules set by experts; cannot learn on its own
Hybrid models	Best convergence, robustness, and accuracy overall	Greater design complexity

6.3 Supporting Evidence

The results are supported by work on distributed-energy planning and coordination in smart grids [27], reviews of AI for managing variable renewable energy [28], microgrid power forecasting with an environmental perspective [29], bibliometric study of AI in renewable energy [3], AI in renewable-powered desalination [30], and reviews of predictive maintenance and optimisation [31,32]. At national scale, an explainable AI framework has modelled India's hydro, nuclear, and renewable electricity generation [33]. Making forecasting and dispatch decisions auditable through explainable AI (XAI) is an emerging theme across this literature [34].

6.4 Critical Assessment

Grid applications encounter a trade-off not seen as sharply in the other case studies. Deep learning models, the most accurate option for complex forecasting, are also the least transparent and the hungriest for data [6], yet grid operators are accountable for blackouts and must be able to justify their decisions, which is why XAI is attracting attention [34]. Combined models deliver the best accuracy but at the cost of complexity and computation time: even the fastest of these in the multi-source study took 3,367.5 seconds, nearly an hour, to converge [6]. This is fine for day ahead planning, but not suitable for second by second control, so the appropriate approach at the right time is needed. Unlike the previous case studies, the grid AI is directly deployed on critical infrastructure and failures have "real" impacts, making cybersecurity, reliability and interoperability with existing systems key issues. [27]

7. DISCUSSION

7.1 The Role of AI Changes Along the Chain

In materials discovery, AI searches and generates: Candidates are proposed which are subsequently tested in experiments, and thus errors in individual projections will not lead to the failure of the entire project since they can be detected before building anything. Midstream, involving solar manufacturing and fuel production, AI fine-tunes settings of established processes, mistakes costing material and labor but never endanger lives. AI makes or informs instant decisions downstream in a grid where mistakes have immediate repercussions [6,27]. Consequently, the demand that is placed on the models gets more and more stringent as they are passed down the chain: the tolerance for errors is reduced, and the demand for transparency, reliability, and speed is increased. This suggests that a method should not be judged by a single standard across applications; a materials-screening model with 70% accuracy can be valuable, whereas a grid controller performing at that level would be unacceptable.

7.2 Data Availability Shapes Performance

Performance is highest where data are plentiful and well structured, such as solubility parameters for a wide range of known solvents [4] or long time series of weather and electricity demand [6], and lower where outcomes depend on numerous poorly recorded factors, such as device efficiency or recycling outcomes [4]. The perovskite case shows how this limitation can be partly overcome: NLP converted roughly 30,000 papers into structured records [4], suggesting that published literature is itself an under-used source of training material.

7.3 Hybrid and Physics-Informed Models Perform Best

In all four case studies, the strongest results come from combining methods rather than relying on one. Hybrid optimisation–ANN models outperformed single methods for grid management [6]; coupling AI with genetic algorithms and PSO improved hydrogen yields [5]; and combining DFT with ML provided both rapidity and atomic-level understanding in materials and solvent design [4,7]. Each approach fills the void of the other: physics-based calculations provide reliable knowledge in regions where data is limited, while ML provides speed and flexibility in regions where physics is slow or too complex.

7.4 Explainability Serves Two Purposes

Explainable AI is serving different functions at both ends of the spectrum. In materials/potential research, SHAP serves as a discovery tool—such as characterizing dipole moment and vapour pressure as parameters that drive solvent performance [4] or identifying binding strength and surface area as parameters that determine hydrogen storage [5]—can provide scientific insight that can inform future experiments. For grid operation, explainability is used to support accountability, so that operators and regulators can track the automated decisions made [34]. Explanations that match with scientific models boost confidence that a model has learned real relationships in both.

7.5 Limitations of the Evidence

The comparison reveals poor evidence bases. First, the results cannot be directly compared across or within the four cases because the different studies employ different metrics (R^2, r, RMSE, NMSE and accuracy). Secondly, the benefit of AI can be overstated as the improvements are sometimes compared to suboptimal conditions instead of the best conventional approach. Third, many of the highest reported numbers are obtained from data sets too small to prevent over-fitting and not real world. Fourth, a majority of the documents are reviews rather than primary documents, and there are few reports of full-scale industrial or “grid” deployment. Future results would be much more easily compared from a more easily interpreted shared set of reference datasets and standard reporting practices, such as size, split into test and reference sets, and comparison to a traditional baseline.

8. OBSTACLES AND CONSTRAINTS

The characteristics of its usefulness in energy systems define its limitations, technical, economic and regulatory [27]. In fact, AI performance relies on a significant amount of quality data, but data is often incomplete, noisy, and limited in quality [27]. Deep learning models are particularly data and time intensive, and produce "black box" decisions, which is the driving force behind XAI [6,34]. The inclusion of AI in critical infrastructure, cybersecurity, and reliability and interoperability (the ability of new systems to integrate with existing systems) is an additional constraint [27]. The dataset bias (10,13), the poor transferability of models between families of chemicals, and the inability to validate predictions on a large scale in the lab are the specific limitations in materials and catalyst research. Computational models built from first principles remain numerically expensive and the resulting models are as accurate as the data on which they are based [4].

From an economic standpoint, implementing AI requires considerable upfront investment, which may involve upgrading outdated systems and equipment, and the potential return on investment is unpredictable [27]. Regulatory and ethical issues encompass transparency in AI decisions, equity in energy and resource allocation, and accountability for misaligned energy and resource decisions [27].

This review has some constraints. It is a narrative and not a systematic review, which means that not all sources may be relevant to the scope. A few sections are based on a relatively limited number of detailed investigations [4– 7] and the conclusions are as firm as the work on which they are based. The choice of the four case studies gives depth and sacrifice coverage; other important applications like wind turbine maintenance and battery management are not detailed.

9. FUTURE DIRECTIONS

The literature suggests a greater level of integration of AI in self-improving closed-loop systems. The most noticeable example is the self-driving lab, where generative models suggest candidate materials, AI filters the candidates, plans the synthesis, robotic platforms do the synthesis and testing, and the outcomes are used to refine the next set of candidates [7]. This would address the experimental-validation

bottleneck in Case Study 1. One of the key components, automated synthesis planning, was maturing, with retrosynthesis models working from the target molecule to the prediction of the correct reaction achieving 78% correct answers and 98% among their top ten answers in a test set [7]. Laboratory to industry scale up of validated models, as done in green catalysts and eco friendly materials [10,13] are the direction of work. Improved uncertainty assessment (reporting the confidence that a model has in each prediction) is a near-term priority, as is better transfer between chemical and materials families, and a design goal that considers the full product lifecycle [13,33].

The next step in all four case studies involves developing predictive systems, adding uncertainty to decision making, further developing XAI to allow for consequential decisions to be audited, and creating the validation frameworks that are required for regulatory acceptance [34]. Comparing as in Section 7 reveals three additional priorities: shared reference datasets and standard reporting to allow for fair comparisons of results; field-scale demonstrations to ensure that results under real operating conditions, and not only in the laboratory; and governance and human monitoring, as the progress of AI in energy is not only a matter of improved algorithms, but also of how they are managed and regulated [27].

10. CONCLUSION

In this review, four case studies from the materials discovery-to-grid operation spectrum of AI in green energy were explored. Despite the diversity of the applications, they have a toolkit of supervised, unsupervised and reinforcement learning; a single workflow where experimental or simulated data are leveraged to build models that predict and optimise faster than the standard; and common data quality, interpretability, cost and trust challenges.

The comparison brings three main conclusions: First, the purpose of AI and, consequently, the criteria for evaluating it, vary throughout the chain, from creating candidates upstream to real-time control downstream. Second, a combination of data-driven learning with physical knowledge or optimisation algorithms consistently outperformed single methods in the studies reviewed. Third, the data is encouraging, but the metrics are not consistent, the data sets are often small and the baseline standards are weak, and headline figures should be viewed as a potential, not a proven, level of performance.

These developments have been found in studies at the national economy level, beyond the laboratory. In developed and developing countries, AI and green technological innovation are tied to better energy efficiency [35]; AI has been connected to high-quality energy development and the transition to clean energy [36, 37]; and patent analyses reveal that AI is a catalyst for innovation in renewable energy [38]. Whether AI ultimately contributes to a safe, efficient, low-carbon energy system will depend less on further gains in accuracy than on resolving the questions of validation, transparency, and governance identified in this review.

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